On behalf of the organizing committee and the New York local section of the ACS, we are pleased to welcome you to the 40th Middle Atlantic Regional Meeting, MARM 2008.

The theme of this meeting is Chemistry and Health, reflecting the importance and impact of the health sciences in the region. This theme is visited throughout the program in several exciting special topics sessions and symposia series, and all fundamental areas of chemistry are strongly represented. Our Program Co-Chairs, Jack Norton and John Sowa, have assembled a program of over 600 abstracts across nearly 60 symposia and poster sessions that feature top national and international speakers. Ronald Breslow and Roald Hoffmann, our keynote speakers, make their addresses after the afternoon program on Sunday and Monday, respectively. Barbecue dinners follow each night and are held nearby the evening poster sessions. We hope you will meet friends and colleagues, old and new, during these events!

There is an extensive program for students, which begins on Saturday with the 56th NY-ACS Undergraduate Research Symposium. Workshops in leadership and career related topics follow throughout the meeting, and student research is incorporated into all technical poster sessions for a unique opportunity to network with potential mentors and employers. There are activities for chemical educators of all backgrounds, including the NSF-sponsored POGIL workshop, plus sessions on innovative curriculum materials and instructional strategies. Two of the highly popular ACS Leadership Development workshops are also offered, along with two workshops for chemical entrepreneurs from the ACS Division of Small Chemical Businesses.

We are especially pleased to host the spring meeting of the United States section of the Royal Society of Chemistry on Saturday night and extend our greetings to all of its members and guests. We hope you will visit the MARM 2008 Expo on Sunday and Monday for exhibits by local and national scientific companies. All are invited to attend the other social events at MARM, such as the Directors Breakfast and the Women Chemists Committee Luncheon, and you are especially encouraged to stay for dinner on Tuesday night for the annual Awards Banquet in recognition of several very worthy individuals and groups. Finally, while you are here in Bayside, we hope you will take some time to experience the incredible culture and diversity of New York City by exploring Queens and the rest of the boroughs of the city.

We are grateful to the many sponsors and advertisers listed on the following pages for their generous support of MARM 2008, and also to Queensborough Community College of CUNY, which has offered their campus and facilities for a truly outstanding event. This meeting would have been impossible without the tremendous effort of the organizing committee and all of the volunteers that have given their time and energy since the beginning. We thank you all and look forward to an exciting and successful MARM!

Sincerely yours,

Paris Svoronos  
General Co-Chair  

David M. Sarno  
General Co-Chair
May 17, 2008

Dear MARM 2008 Participants,

On behalf of the more than 160,000 members of the American Chemical Society, I am pleased to extend greetings to the attendees of the 40th Middle Atlantic Regional Meeting (MARM) at Queensborough Community College of the City University of New York, Bayside, New York.

The organizers have chosen the theme “Chemistry and Health” because of the importance and impact of the health sciences in the Middle Atlantic region. This and many other topics are explored in over 60 technical sessions that will be of interest to academic and industrial chemists, students, and entrepreneurs. These include symposia such as Analysis of Biomolecules, Antimicrobials, Biocatalysis and Biomimetic Catalysis, Chemistry and the Arts, Forensic Chemistry, HIV/AIDS, Ionic Liquids, Metal Complexes in Chemotherapy and Diagnostics, and Protein Misfolding. Please take this opportunity to interact with your colleagues and to discuss developments taking place in your field.

I do hope you also take the time to fully explore the interesting array of education programs, workshops and short courses, career enrichment and professional development activities, awards, vendor expo, and networking and social events. MARM is also host to the 56th NY-ACS Undergraduate Research Symposium, and the Spring Meeting of the United States Section of the Royal Society of Chemistry.

I am grateful to the many volunteers, especially the members of the New York local section and the other 15 participating MARM sections of the American Chemical Society – representing over 30,000 members! – for their hard work and dedication to create an intellectually stimulating, as well as personally enjoyable experience here in Bayside. Together we will achieve the Vision of our Society: "Improving people's lives through the transforming power of chemistry."

Sincerely,

Bruce E. Bursten, Ph.D.
President

ACS Vision: Improving people’s lives through the transforming power of chemistry
May 2008

Dear MARM 2008 Participants,

On behalf of Queensborough Community College, a college of The City University of New York, I am delighted to offer my warm greetings to all those who are participating in the American Chemical Society’s 40th Middle Atlantic Regional Meeting – MARM 2008.

I am especially proud that Queensborough Community College is hosting the first MARM ever to be held at a community college. Our faculty members have been aggressively pursuing and securing grant awards in the sciences, resulting in new programs in laser and engineering technology. Their efforts have also created a new student research lab on campus. And, most importantly, our students have been energized by their interactions with our science faculty and are successfully conducting research and choosing careers in the sciences.

The scholarship support that our students have received from the American Chemical Society has made a tremendous difference. Thank you for partnering with us to create a committed and enthusiastic pool of future scientists for our region and our country.

I am very pleased to welcome two special guest lecturers and renowned chemists to our campus for the event – keynote speaker Ronald Breslow, Chemistry Professor at Columbia University and past ACS President, and Roald Hoffmann, Professor at Cornell University, poet, playwright and Nobel Prize winner in chemistry. The theme of this year’s meeting, Chemistry and Health, is a timely and important topic that highlights the impact of the health sciences in the New York Metropolitan area.

I welcome all attendees, and hope you all have an enjoyable and enlightening time.

Sincerely,

Eduardo J. Martí, Ph.D.
President
The Chancellor

May 2008

Dear President Marti:

I am delighted to extend a warm welcome to all of the students, faculty, and science professionals attending the American Chemical Society’s 40th Middle Atlantic Regional Meeting—MARM 2008—at Queensborough Community College.

I am particularly proud that Queensborough is the first community college, and first CUNY college, to host this regional meeting of the American Chemical Society. Through its Decade of Science initiative, CUNY is renewing the University’s commitment to creating a healthy pipeline to science, technology, engineering, and mathematics fields by advancing science at the highest levels, training students to teach in these areas, and encouraging young people, particularly women and minorities, to study in these disciplines.

Queensborough is actively participating in CUNY’s Decade of Science, achieving growing recognition for its faculty grant awards in the sciences, which are funding new labs and programs in laser and engineering technology. Queensborough’s science faculty are dedicated to the success of their students, as evidenced by the multiple American Chemical Society scholarships awarded to Queensborough students and by the students’ success in CUNY and ACS science competitions.

On behalf of The City University of New York, I thank you for your hard work and leadership in bringing the American Chemical Society’s Middle Atlantic Regional Meeting to CUNY and to New York City, and I wish all of the participants a successful meeting.

Sincerely,

Matthew Goldstein

535 East 80th Street, New York, New York 10075
May 17, 2008

Dear Friends:

It is a great pleasure to welcome all those attending the American Chemical Society’s 40th Middle Atlantic Regional Meeting.

This meeting provides a wonderful opportunity for attendees to share knowledge and professional expertise, to network, and to collaboratively take stock of innovations in the chemical sciences. This meeting is the first MARM to be hosted in New York City—and we are proud to welcome this gathering of professionals, students, and educators dedicated to promoting the health sciences in the New York City metropolitan area.

On behalf of our City, I am pleased to recognize those associated with the American Chemical Society for hosting this event and contributing so much to the health and well-being of our City. I also applaud Queensborough College — a vital part of our City’s community college system — for once again demonstrating their dedication to promoting the highest standards of academic and professional excellence by hosting this conference. I welcome all attendees to New York, and encourage everyone to venture out and take advantage of the many attractions and diverse neighborhoods that make this City one of the world’s greatest places to live, to work, and to visit. Please accept my best wishes for an enjoyable event and continued success.

Sincerely,

Michael R. Bloomberg
Mayor
May 17, 2008

Dear Friends:

It is a pleasure to extend my warmest greetings to all those gathered to celebrate the American Chemical Society’s 40th Annual Middle Atlantic Regional Meeting at Queensborough Community College of the City University of New York.

I am especially pleased to welcome the American Chemical Society to its first-ever regional meeting in a New York City community college.

As the world’s largest scientific society with more than 160,000 members, ACS provides essential and exceptional educational, science and career programs in chemistry. Additionally, ACS offers educational opportunities to underrepresented minority undergraduates and to economically disadvantaged high school students through its ACS Scholars and Project SEED programs, respectively.

I commend ACS for the invaluable role it has played for over a century in educating the public and policymakers in issues ranging from public health to environmental protection.

Please accept my wishes for a most enjoyable Middle Atlantic Regional Meeting 2008!

Sincerely,

Gary L. Ackerman
Member of Congress
May 17, 2008

Dr. Eduardo J. Marti
President
Queensborough Community College
222-05 56th Avenue
Bayside, NY 11364-1497

Dear Dr. Marti:

It is a great pleasure on this special occasion to welcome all of you to the American Chemical Society's 40th Middle Atlantic Regional Meeting - MARM 2008 - here at Queensborough Community College.

I congratulate Queensborough for being the first community college to host a Middle Atlantic Regional Meeting of the American Chemical Society. With all of Queensborough’s recent achievements in the sciences, it is only fitting that it be the first CUNY College to host a regional meeting of the American Chemical Society. I congratulate Queensborough on hosting this prestigious meeting and maintaining its continued standard of excellence in the field of sciences. Your work is truly inspiring.

I would also like to thank the American Chemical Society for its generous financial contributions to Queensborough Community College, coming in the form of academic scholarships, grant awards in the sciences, new labs, and expanded programs. I salute the Society for its generosity to this campus and for its unwavering support and investment.

Please know that you can continue to count on my strong support.

Sincerely,

Charles B. Rangel
Chairman
Committee on Ways and Means
May 17, 2008

Dr. Eduardo J. Marti
President
Queensborough Community College
222-05 56th Avenue
Bayside, NY 11364-1497

Dear President Marti:

It is my very great pleasure to extend greetings to you and all of the many participants in the American Chemical Society's 40th Middle Atlantic Regional Meeting (MARM 2008) at Queensborough Community College. In light of the fact that this is the first MARM ever to be held in New York City, the first MARM to be held on a CUNY campus, and the first MARM at a community college, this is truly an historic event for Queensborough Community College and everyone involved.

As the world's largest scientific society, with more than 160,000 members, the American Chemical Society has clearly made extraordinary contributions to the world of scientific research and advancement. I am certain that MARM 2008, being held from May 17th through the 21st, will provide extraordinary opportunities for all participants to network, share knowledge, and engage in vital dialogue with some of our country's most respected scientific minds.

As MARM 2008 commences, I would like to acknowledge Columbia University Professor Ronald Breslow, the keynote speaker, and Roald Hoffman, a Nobel Laureate and Cornell University professor. Your participation in MARM 2008 will undoubtedly make MARM 2008 an outstanding success, and it is a pleasure to welcome you to Queensborough Community College.

Please accept my very best wishes for a highly productive and exciting meeting, and for continued success in the years to come.

Sincerely,

Malcolm A. Smith
Senate Democratic Leader
May 17, 2008

Dr. Eduardo J. Marti
President
Queensborough Community College

Dear President Marti,

I would like to take this opportunity to welcome all the attendees of the American Chemical Society’s 40th Middle Atlantic Regional Meeting.

This is the first time in the history of the American Chemical Society that the MARM has been held in New York City. It is also the first time the meeting has been convened at a community college.

As a former electrical engineer, it is a true honor to have over 1,000 scientists, chemists, professors and educators from throughout the Mid-Atlantic region bring their annual meeting to Queens.

I would like to thank you for your hard work, dedication and leadership in putting together this meeting for the American Chemical Society Mid-Atlantic Region. Your staff and faculty have once again shown their unwavering commitment to bringing new programs and educators from throughout the country to QCC.

I would also like to recognize Dr. Paris D. Svoronos, Chair of the Department of Chemistry and MARM 2008 General Chair. Additionally, I would like to extend a welcome to keynote speaker Columbia University Professor Ronald Breslow and Noble Laureate and Cornell University Professor Roald Hoffman.

Once again, it is my distinct pleasure to extend my warmest welcome to all the attendees of the MARM during your visit here in Queens.

Cordially,

[Signature]

Senator Frank Padavan
May 17, 2008

Dr. Eduardo J. Marti
President
Queensborough Community College
222-05 56th Avenue
Bayside, NY 11364

Dear President Marti:

Please extend my best wishes and warm regards to the members of the New York Section of the American Chemical Society and all those in attendance at the 40th Annual Middle Atlantic Regional Meeting (MARM), May 17-21, 2008.

Your shared dedication to clinical innovation, public health education and the ongoing support for chemistry students and professionals deserves the recognition and appreciation of the City of New York.

Special congratulations to your keynote speaker, Columbia University Professor Ronald Breslow, and featured speaker Cornell University Professor Roald Hoffman.

Best wishes for a successful event.

Sincerely,

Tony Avella
Council Member
District 19 - Northeast Queens

TA:es
May 17, 2008

Dr. Eduardo J. Marti, President
Queensborough Community College
222-05 56th Avenue
Bayside, New York 11364

Dear Dr. Marti:

I am writing to congratulate Queensborough Community College for being the first community college to host the American Chemical Society’s 40th Middle Atlantic Regional Meeting–MARM 2008.

I am truly proud that representing New York City is “Queen’s Own” Queensborough Community College.

With all of Queensborough’s recent achievements in the sciences, it is appropriate that Queensborough also be the first CUNY College to host this regional meeting of the ACS. Befitting of The City University of New York’s proclaimed “Decade of Science,” (2005-2015), Queensborough has received student scholarships awarded from the American Chemical Society and faculty recognition for their growing grant awards in the sciences and new labs and expanded programs.

I welcome the American Chemical Society and its regional members to New York City and to the borough of Queens. Again, I offer Queensborough Community College my congratulations and best wishes on hosting this wonderful event.

Sincerely,

AUDREY I. PHEFFER
Member of Assembly

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ACS Board of Directors

**Bruce E. Bursten, President**  
*University of Tennessee*  
Dr. Bursten is Dean of the University of Tennessee's College of Arts and Sciences and a distinguished professor of chemistry. He received his bachelor's degree from the University of Chicago and Ph.D. from the University of Wisconsin, Madison. He has been an ACS member since 1974.

**Catherine T. Hunt, Immediate Past President**  
*Rohm and Haas*  
Dr. Hunt is leader of technology partnerships at Rohm and Haas, Spring House, PA. She received her A.B. from Smith College and her Ph.D. from University of California, Davis. She has been an ACS member since 1977.

**Dr. Thomas H. Lane President Elect**  
*Dow Corning*  
Thomas H. Lane is director of global science and technology outreach at Dow Corning, Midland, Michigan. He received his B.S. in Chemistry from Purdue University, his M.S. in Chemistry from Central Michigan University, and his Ph.D. from Open University, Milton Keynes, England. He has been an ACS member since 1973.

**Madeleine Jacobs, Executive Director & CEO**  
*American Chemical Society*  
Previously serving as the Editor-in-Chief of Chemical and Engineering News (C&EN), 2004 marks Ms. Jacobs first year as Executive Director of the American Chemical Society. She worked for C&EN from 1969 until 1972 and returned again in 1993. She is a much-honored science journalist, an internationally sought after public speaker, and brings an extensive familiarity and understanding of Society programs, products, and services.

**Anne T. O'Brien, Director, District I**  
Dr. O'Brien retired as Manager of Research Information Sciences at Wyeth-Ayerst Research, a Division of American Home Products in Pearl River, NY in 2002. She received her B.S. in chemistry from Marymount College and her Ph.D. in organic chemistry from Fordham University. She has been an ACS member since 1959.

**Madeleine M. Joullie, Director, District III**  
Dr. Joullie is a professor of chemistry at the University of Pennsylvania, Philadelphia. She received her B.S. in chemistry from Simmons College and her Ph.D. in Chemistry from the University of Pennsylvania. She has been an ACS member since 1947.
# MARM 2008 Organizing Committee

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**We thank our corporate sponsors!**

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<td><a href="http://www.metronyawis.org/">www.metronyawis.org/</a></td>
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<td><a href="http://www.molecularandmicroanalysis.com">www.molecularandmicroanalysis.com</a></td>
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<td>Metrowomen Chemists Topical Group of the New York and North Jersey ACS Sections</td>
<td><a href="http://www.newyorkacs.org/comm_women.html">www.newyorkacs.org/comm_women.html</a></td>
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We thank our symposia sponsors and event sponsors!

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<td><strong>STREM CHEMICALS, INC.</strong></td>
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<td><strong>ACS Women Chemists Committee</strong></td>
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Exhibitors at MARM 2008

Make sure to visit the MARM 2008 Expo, where you will find refreshments during our coffee breaks, a great place to meet with colleagues, and representatives from the following companies. The Expo will take place on Sunday, May 18 and Monday, May 19 on the First Floor and Lower Level of the Medical Arts Building.

ACS Division of Small Chemical Businesses (SCHB)
http://membership.acs.org/S/SCHB/
The mission of the Division is to aid in the formation, development and growth of small chemical businesses. To this end, the Division offers programming at National and Regional ACS meetings, as well as exhibiting. The booth at National meetings is shared – an opportunity for small firms to test this market at nominal costs.

American Institute of Pharmaceutical Technology
www.aiptnet.com
AIPIT is a Career College in the field of Pharmaceutical Technology and Clinical Research over 17 years. Programs such as Quality control, Quality assurance, Regulatory affairs, Validation engineering, Method and Process Development (R & D), and Manufacturing Technology. College provides industrial skills/education/ hands on training for the pharmaceutical/biotech/allied chemical industries.

Analiza
www.analiza.com
Analiza is a contract research organization providing low cost, fast, highly accurate assays for key physicochemical and ADME properties for early drug discovery. Our LogD and solubility assays are miniaturized versions of the gold standard shake-flask methods.

Biotage
www.biotage.com
Biotage is a global life science technologies company specializing in microwave synthesizers, resin-bound scavengers, reagents and catalysts, flash chromatography systems and cartridges, evaporation systems and sample preparation products. Our clients include major pharmaceutical companies, contract research organizations, government research centers, and leading academic institutes.

CEM
www.cem.com
The worldwide leader in advanced microwave laboratory instrumentation, CEM provides visionary technology for today’s microwave chemistry applications, including chemical synthesis, analytical chemistry, process control, acid digestion, biosciences, and organic extraction.

Chemglass, Inc.
www.chemglass.com
Over 60 years, our tradition of excellence in manufacturing has made our products an integral part of the chemistry performed in laboratories throughout the world. Chemglass utilizes raw materials purchased from primary glass manufacturers and reworks these materials to fabricate standard catalog items and components as well as custom glassware.
Exhibitors at MARM 2008

Dell, Inc. Healthcare and Life Sciences  
www.dell.com/lifesciences
Dell, Inc. Healthcare and Life Sciences division is focused on simplifying IT across the enterprise and lifecycle – helping customers accelerate discovery, ensure secure data management, leverage mobility and virtualization, and expedite commercialization of breakthrough enterprises.

EDU-CHEM Innovations  
www.edu-chem.com
EDU-CHEM Innovations is a small Company with GREAT capabilities to help you teach Technology more effectively, economically and enjoyably! Offering a comprehensive assortment of Analytical Chromatography, Spectroscopy and Electrochemistry to meet the Teaching Lab needs of any College or University... from Gen Chem through Graduate Research... with complete Academic Support!

Energy Beam Sciences, Inc.  
www.ebsciences.com
Energy Beam Sciences is a world leader in the manufacture and distribution of products in the field of Electron Microscopy. We manufacture consumables such as filaments, apertures and specimen mounts. We are also the exclusive US distributors for SEM specimen preparation products from the Polaron Range and Emitech; Detector and Camera Systems from KE Developments; and Alicona MeX Software.

HiScope System Company  
www.hiscope.com
HiScope is the Distributor and Service Company of 3-D View Microscope Products including Hitachi Portable SEM and Hirox Digital Video-Microscope Products.

Hoffmann & Baron, LLP  
www.hoffmannbaron.com
The attorney’s of Hoffmann & Baron, LLP possess expertise in the acquisition, protection, and strategic planning for all forms of intellectual property which include patents, trademarks, copyrights, unfair competition, trade secrets, licensing, technology-related agreements, and due diligence. The firm serves clients in all major scientific fields including biochemistry, chemical processes and systems, organic and inorganic chemistry, and nanotechnology, among others.

MeasureNet Technology Ltd  
www.measurenet-tech.com
MeasureNet Technology specializes in Laboratory Information Management Systems (“LIMS”) for Teaching Labs: Gen Chem, Analytical, Instrumental & more. Using rugged, long-lived Workstations instead of “disposable” PCs; Students focus on the Experiment & Data, not individual Software. Simple Probes, advanced Spectrophotometers and complex Chromatographs can all be connected to MeasureNet!
Exhibitors at MARM 2008

**MicroLab, Inc.**  
[www.microlabinfo.com](http://www.microlabinfo.com)  
MicroLab’s products are innovative high quality instruments and software for college and university chemistry laboratories. Our FS-522 integrates a unique FASTspec™ 360-940 nm spectrophotometer – Fluorescence, Absorbance, Scatter, and Transmission – with sensors for pressure, temperature, pH, conductance, REDOX, and more, providing a cost-effective, high performance laboratory tool.

**TA Instruments**  
[www.tainstruments.com](http://www.tainstruments.com)  
More worldwide customers choose TA Instruments as their preferred thermal analysis, rheology and microcalorimetry supplier. With direct offices around the world, TA Instruments is uniquely qualified to meet customer needs for high technology thermal analysis, rheology and microcalorimetry products, excellent training and customer support.

**Shimadzu Scientific Instruments**  
[www.ssi.shimadzu.com](http://www.ssi.shimadzu.com)  
Since 1975, Shimadzu USA (“SSI”) has been providing an extensive range of products, software and unrivaled customer service, meeting the needs of the analytical laboratory industry. Today Shimadzu continues that tradition as a global leader in the development of solutions for the world’s technology hurdles. We are crafting tools for the next inspiration.

**Shodex**  
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“Capture the Essence” with Shodex polymer-based HPLC columns. We emphasize rapid analysis of proteins using solid-sphere particles in conventional HPLC and UHPLC pressures. For small molecule analysis, our unique polymer-based restricted-access material column can retain polar and non-polar compounds. Other small molecule SEC columns are introduced.

**Tosoh Bioscience**  
[www.separations.us.tosohbioscience.com](http://www.separations.us.tosohbioscience.com)  
Tosoh manufactures and supplies HPLC Columns, media, and instrumentation. Featured at this show is our new GPC system, the EcoSEC.

**Varian**  
[www.varianinc.com](http://www.varianinc.com)  
*Inspiring Excellence™* is at the Heart of Our Business. We’re a diversified, global technology leader helping customers innovate with confidence, enhance their competitiveness, and boost their efficiency. Our businesses—Scientific Instruments and Vacuum Technologies—bring together our high quality, innovative and user-friendly products with industry-leading service and support to create genuinely inspired solutions.

**Vernier**  
[www.vernier.com](http://www.vernier.com)  
Stop by the Vernier Software & Technology booth to see our exciting LabQuest interface. LabQuest can be used either as a computer interface, or a stand-alone device with a vivid color screen, and built-in data acquisition and analysis. Learn about our low-cost solutions for spectroscopy, our auto-ID sensors as well as our Advanced Chemistry with Vernier lab book.
GENERAL MEETING INFORMATION for MARM 2008

Registration
On-site registration will begin at 7:00 a.m. Saturday, May 17, 2008. Payment can be made by cash, credit card or check. Registration will take place in the Medical Arts Building. The registration schedule is as follows:

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<tr>
<th>Day</th>
<th>May</th>
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<td>Saturday</td>
<td>17, 2008</td>
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<td>Wednesday</td>
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Refreshments
Either the Science Building Cafeteria or the Oakland Dining Hall will be open for breakfast and lunch during MARM (beginning with lunch on Sunday). A complimentary continental breakfast will be served in the Medical Arts Building on Sunday morning before the start of the technical program. Light refreshments will be served during the scheduled morning and afternoon breaks, and also prior to the plenary lectures on Sunday and Monday. There are also several restaurants within convenient distance of the campus.

Technical Sessions
Most technical sessions will be held in the Medical Arts Building. A small number will be held in the Library Building and the Science Building.

Programming for Students and Educators
MARM 2008 offers a variety of programs for students, including the NY-ACS Undergraduate Research Symposium, Student Affiliates activities, careers workshops and panel discussions, and a short course on analytical chemists in industry.

Programs for educators begin on Saturday with a free POGIL workshop and Student Affiliates activities. They continue on Sunday with laboratory probe ware workshops, the NY-ACS Nichols Teacher Forum, and a full-day Chemical Education symposium.

Mixers
On Sunday and Monday evenings, a casual barbeque dinner will be served outside the Student Union Building. These follow the plenary addresses and are held during the PM poster sessions. On Tuesday morning, all registered attendees are invited to the Oakland Building to enjoy a complimentary breakfast hosted by Anne O’Brien, ACS District I Director and Madeleine M. Joullié, ACS District III Director. Come with your ideas and concerns. Participation and conversation are the goals! On Tuesday afternoon, all are invited to the Women Chemists Committee Luncheon with speaker Jodi Wesemann from the education department at ACS. The luncheon provides a great opportunity for informal networking. Later on Thursday, a free reception in the Oakland building follows the Industrial Innovation Awards Symposium and leads up the Awards banquet.

Shuttle Bus
A complimentary shuttle bus to QCC will be available beginning Sunday morning through the end of programming on Wednesday. Its route will include the nearby Ramada Adria Conference Center and the Anchor Inn, as well as the Bayside Station of the Long Island Rail Road.
### WORKSHOPS & SPECIAL EVENTS at MARM 2008

#### Saturday, May 17

- **POGIL Workshop**  
  8:30 am – 4 pm  
  Library Building, LB-6

- **Spring Meeting of the United States Section of the Royal Society of Chemistry**  
  6 – 10 pm  
  Oakland Cafeteria

#### Sunday, May 18

- **ACS Leadership Development Workshop: Involving Volunteers**  
  8 am – 12 pm  
  Library Building, LB-8

- **ACS Leadership Development Workshop: Leading Change**  
  1 – 5 pm  
  Library Building, LB-8

- **Probeware Workshop and Chemical Demonstrations for pre-college educators**  
  1:30 – 5 pm  
  Science Building, S-405

- **Keynote Address by Dr. Ronald Breslow, Columbia University**  
  5:30 – 6:30 pm  
  Medical Arts Building, M-136

- **Sunday Night Barbecue**  
  6:30 – 8:30pm  
  Student Union Building

#### Monday, May 19

- **ACS Career Management and Development Workshops**  
  9 am – 5 pm  
  Medical Arts Building, MC-28

- **ACS Division of Small Chemical Businesses Workshops**  
  **Tools for Entrepreneurs - from the Kauffman Foundation**  
  8:30 am – 12 pm  
  Medical Arts Building, MC-29

- **Best Practices for the Chemical Entrepreneur**  
  1:30 – 5 pm  
  Medical Arts Building, MC-29

- **Professional Analytical Chemists in Industry: What Does an Analytical Chemist Do?**  
  1 – 5 pm  
  Medical Arts Building, MC-28

- **Probeware Workshop for undergraduate educators**  
  2 – 5 pm  
  Science Building, S-405

- **Keynote Address by Dr. Roald Hoffman, Cornell University**  
  5:30 – 6:30 pm  
  Medical Arts Building, M-136

- **Monday Night Barbecue**  
  6:30 – 8:30pm  
  Student Union Building
Tuesday, May 20

Directors Breakfast 7:30 – 8:30 am Oakland Cafeteria
Women Chemists Committee Luncheon 12 – 1:30 pm Oakland Cafeteria
Industrial Innovation Award Symposium and Reception 4:30 – 7 pm Oakland Cafeteria
Awards Banquet 7 – 9 pm Oakland Cafeteria

UNDERGRADUATE ACTIVITIES at MARM 2008

Saturday, May 17

56th NY-ACS Undergraduate Research Symposium 8 am – 3 pm Student Union Building, Medical Arts Building
Regional Chemagination Competition 1 – 5 pm Medical Arts Building, M-136
Project SEED Poster Session 1 – 5 pm Medical Arts Building, M-136
Making the most of being a Student Affiliate 2 – 4 pm Medical Arts Building, MC-29

Sunday, May 18

Tapping into the excitement: Strategies for building – or rebuilding – a Student Affiliates chapter 9 am – 12 pm Medical Arts Building, MC-29

Monday, May 19

Career Management and Development Workshops 9 am – 12 pm Medical Arts Building, MC-28
Professional Analytical Chemists in Industry: What Does an Analytical Chemist Do? 1 – 5 pm Medical Arts Building, MC-28
Delaware Valley Chromatography Forum 2008 Student Award 1:30 – 5 pm Medical Arts Building, M-140

Tuesday, May 20

Panel Discussion: Traditional and Non-Traditional Careers in Chemistry 9 – 11 am Library Building, LB-16
Women Chemists Committee Luncheon 12 – 1:30 pm Oakland Cafeteria
## CHEMICAL EDUCATORS at MARM 2008

### Saturday, May 17

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<th>Event</th>
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<td>POGIL Workshop</td>
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<td>Regional Chemagination Competition</td>
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<td>Medical Arts Building, M-136</td>
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<td>Project SEED Poster Session</td>
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<tr>
<td>Making the most of being a Student Affiliate</td>
<td>2 – 4 pm</td>
<td>Medical Arts Building, MC-29</td>
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<td>9 am – 12 pm</td>
<td>Medical Arts Building, MC-29</td>
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<tr>
<td>NY Section Nichols Teacher Forum</td>
<td>9 – 11 am</td>
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<td>Chemical Education Sessions I and II</td>
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<td>1:30 – 5 pm</td>
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<td>Analysis of Biomolecules</td>
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<td>Clinical Chemistry II and Clinical Chemistry Workshop</td>
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<td>Metal Complexes in Chemotherapy and Diagnostics</td>
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<td>Plenary Lecture I: Ronald Breslow, Columbia University</td>
<td>Physical Chemistry, I</td>
<td>Polymer II (Material Synthesis)</td>
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<td>Poster Session I</td>
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<td>Spectroscopy of Biological Systems</td>
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PLENARY SPEAKER

SAHA (Vorinostat), An FDA Approved Anticancer Compound with a Novel Mechanism of Action

Ronald Breslow, Columbia University

Sunday, May 18, 2008, 5:30 PM-6:30 PM
Medical Arts Building, Room M-136

The 2008 ACS Middle Atlantic Regional Meeting (MARM) is honored to have Dr. Ronald Breslow, the 2003 Welch and the 2004 Willard Gibbs Medalist, the 1995 President-Elect of the American Chemical Society and 1996 ACS President, presenting a plenary lecture. Dr. Breslow is a distinguished chemist, with research interests in several different physical-/bio-organic chemistry areas: his specialties are the design, synthesis, and study of new molecules with interesting properties. Breslow is noted for his pioneering research in nonbenzenoid aromatic chemistry; enzyme-catalyzed reactions; biomimetic approaches to synthesis of enzymes and complex carbohydrates; and synthesis of simple anticancer compounds.

Breslow has written more than 400 published articles and three books. His numerous honors include the prestigious National Medal of Science, awarded to him in 1991, the American Chemical Society Bader Award in Bioorganic or Bioinorganic Chemistry, the New York City Mayor's Award in Science, the American Chemical Society Priestley Medal, the U.S. National Academy of Sciences Award in Chemical Sciences, the Columbia Alumni Association Great Teacher Award, the British Chemical Society Centenary Medal, and the American Chemical Society Award in Pure Chemistry. He is also a member of the National Academy of Sciences.

His achievements and service to chemistry have been additionally recognized with many honors and awards; the 2003 National Academy of Sciences Award for Chemistry in Service to Society, the 2002 Perkin Medal, and the 1995 E.B. Hershberg Award to name a few.

This plenary lecture will discuss SAHA (Vorinostat), an FDA approved anticancer compound with a novel mechanism of action.
PLENARY SPEAKER

The Chemical Imagination at Work in Very Tight Places

Roald Hoffmann, Cornell University

Monday, May 19, 2008: 5:30 PM-6:30 PM
Medical Arts Building, Room M-136

The 2008 ACS Middle Atlantic Regional Meeting (MARM) is honored to have Dr. Roald Hoffmann present a plenary lecture. Roald Hoffmann was born in 1937 in Zloczow, Poland. Having survived the war, he came to the U. S. in 1949, and studied chemistry at Columbia and Harvard Universities (Ph.D. 1962). Since 1965 he has been at Cornell University, now as the Frank H. T. Rhodes Professor of Humane Letters.

Dr. Hoffmann's research examines transition states in reactions and the electronic structures of stable and unstable molecules. He applies a variety of quantum chemical computational methods as well as qualitative arguments to problems of structure and reactivity of both organic and inorganic molecules of medium size and to extended systems in one-, two-, and three dimensions. "Applied theoretical chemistry" is the way Roald Hoffmann likes to characterize his particular blend of computations, stimulated by experiment and the construction of generalized models of frameworks for understanding. In spite of the amazing science he produces, he believes his major contribution is that "he is a teacher and he is proud of it". At Cornell University he has taught primarily undergraduates, and, almost every year since 1966 he has taught first-year general chemistry. He has also taught chemistry courses to non-scientists and graduate courses in bonding theory and quantum mechanics.

Professor Hoffman received the Nobel Prize in Chemistry with Kenichi Fukui in 1981 for developing a comprehensive theory of pericyclic reactions. He is a member of the National
Academy of Sciences. He has also received five American Chemical Society awards, three in different specific subfields of chemistry - the A.C. Cope Award in Organic Chemistry, the Award in Inorganic Chemistry, and the Pimentel Award in Chemical Education. Notable is his talent in reaching out to the general public; he participated, in the production of a television course "The World of Chemistry," shown widely since 1990. He frequently contributes to the interesting Marginalia column in Sigma Xi's magazine, American Scientist. As a writer, Dr. Hoffmann has carved out a land between science, poetry, and philosophy, through many essays and three books, Chemistry Imagined with artist Vivian Torrence, The Same and Not the Same, and Old Wine, New Flasks: Reflections on Science and Jewish Tradition, with Shira Leibowitz Schmidt. Hoffmann is also an accomplished poet and playwright. He began writing poetry in the mid-1970s and has published The Metamict State (1987), Gaps and Verges (1990), Memory Effects (1999), Soliton (2002), and, in Spanish, Catalista (2002). He has co-written a play with fellow chemist Carl Djerassi, entitled Oxygen, which has been performed worldwide and translated into ten languages. A second play by Roald Hoffmann, Should've, was premiered in Edmonton, Canada in 2006. A monthly cabaret, “Entertaining Science,” at the Cornelia Street Café in Greenwich Village has become the hot cheap ticket in NYC.

In his lecture Dr. Hoffmann will explore how chemistry is different at high pressure and the role that one’s chemical intuition for bonding and structure has in understanding matter at high pressures.
Queensborough Community College (QCC) is one of the six community colleges in the City University of New York (CUNY). Half of its students are foreign born and the ethnic composition consists of 26% African-American, 25% Hispanic, 21% Asian and 27% Caucasian. 57% of its faculty hold doctorates, almost three times the national average for community colleges.

The Chemistry Department at QCC is composed of nine full time Ph.D. faculty, two college laboratory technicians and two dozen adjuncts. Since 2001, it has seen a doubling in the number of registered students, and also full time faculty. Led by the chair Paris Svoronos (Ph.D., Georgetown University, 2003 CASE/Carnegie Foundation Outstanding Professor of the Year), the department has worked as a team to develop into a prime time undergraduate institution. This group of faculty include Irina Rutenburg (Ph.D., CUNY Graduate Center), Sasan Karimi (Ph.D., CUNY Graduate Center), Moni Chauhan (Ph.D., Universite de Montpellier), Daqing Gao (Ph.D., Boston College), Sharon Lall-Ramnarine (Ph.D., CUNY Graduate Center), David Sarno (Ph.D., SUNY Binghamton, Post-doctoral University of Pennsylvania under 2000 Nobel laureate Alan MacDiarmid), Jun Shin (Ph.D., Columbia University) and Mihaela Bojin (Ph.D., Cornell University under 1981 Nobel laureate Roald Hoffmann), as well as college lab technicians Pedro Irigoyen and Bruce Montalbano and adjunct faculty Luis Vargas (Ph.D., University of Madrid), Syamala Ranganathan (M.S., Madras University) and Gopal Subramaniam (Ph.D., Vanderbilt University).

Undergraduate research has expanded from one student in 2000 to thirty in 2008. This gradual progress was also coupled with grants totaling close to $3 million dollars in the last five years that enabled the acquisition of instruments such as a 60-MHz NMR, FT-IR, GC-MS, UV-Vis, C,H,N Analyzer, HPLC, and a tabletop scanning electron microscope, as well as a new laboratory dedicated to student-faculty research. QCC students have made more than 300 presentations in local, regional and national ACS meetings in the last five years.
The E. Emmet Reid Award in Chemistry Teaching at Small Colleges in the ACS Mid-Atlantic Region

Winner for MARM 2008

Dr. Claude Yoder
Franklin & Marshall College

Dr. Claude H. Yoder obtained his BA from Franklin and Marshall College in 1962 and his PhD from Cornell University in 1966. He returned to F&M to teach in 1966, was Chairman of the department from 1974-1982, and was designated Charles A. Dana Professor of Chemistry in 1986. He has written over 120 papers on the organometallic chemistry of the Group IV elements and has recently turned his attention to the characterization of inorganic systems of mineralogical interest. He is the coauthor of several General Chemistry texts, including the first electronic General Chemistry text, and a text on Multinuclear NMR Spectroscopy. His most recent book is Ionic Compounds, Applications of Chemistry to Mineralogy, published by Wiley. He is the recipient of a Dreyfus Teacher-Scholar grant, the CMA Catalyst Award, the ACS Undergraduate Research Award, and was a founding member of the Council on Undergraduate Research. In addition to General and Inorganic Chemistry, he has taught advanced courses on Organometallics, Analytical Chemistry, and Synthesis and Structure Determination.

His favorite part of teaching is working side-by-side with more than 100 undergraduate researchers he has mentored over the last 41 years.
The ACS Division of Chemical Education  
Middle Atlantic Region Award for Excellence in High School Teaching  

Winner for MARM 2008  

Ms. Claire Miller  
Madison High School  
170 Ridgedale Ave  
Madison, NJ 07940  

Ms. Miller received a BS degree from Georgian Court College and an MA from Rutgers University and has been teaching chemistry at Madison High School in New Jersey for 35 years. She has been an inspiration to her students and a role model for other educators.  

When students enter Claire Miller’s chemistry class, they feel excitement, interest and enthusiasm. Her students are highly motivated because they know that something interesting and exciting will happen. It may be that they will be constructing huge balloons to study gas laws or that they will be using the latest technology to gauge the rate of chemical reactions. Her teaching ability is top notch. Her students sense her caring attitude and thoughtfulness and they rise to her standards. A former student describes her as “The Teacher Who Made a Difference. She challenged our formative minds and in turn enabled us to challenge ourselves.”  

Claire is equally respected by her colleagues and she shares her expertise with other members of her department. She has developed professional development activities that use technology and probeware to enhance laboratory investigations in chemistry, biology, physics and earth science. She has created a laboratory safety program that demonstrates safety techniques to the students. She is a regular presenter at the New Jersey Science Teachers Convention and at monthly ChemTAG meetings. Claire stays current with the latest educational trends and scientific information by regularly attending seminars and workshops and she typically earns 60 professional development hours per year.
Regional Industrial Innovation Award

Sponsored by ACS Corporation Associates

Winner for MARM 2008

Dr. Thomas P. Selby
Ms. Charlene G. Sternberg
Dr. James F. Bereznak
Mr. Reed A. Coats
Mr. Eric A. Marshall

Proquinazid Team
DuPont Crop Protection

Among the threats to the human food supply, the devastation of crops by fungal epidemics is one of the worst. Throughout human history, many instances of plant disease causing food shortages and famines have been reported. Perhaps the most devastating of these was the Irish potato famine of the 1840’s. Today, many commercial fungicides are known that help keep fungal diseases in check. However, certain plant pathogens are able to develop immunity to the fungicides which once controlled them. Resistance of the fungus *Blumeria Graminis*, the cause of the plant disease powdery mildew, to many commercial fungicides has made it and related powdery mildews a persistent problem for farmers of wheat, barley, grapes and other crops. In order to protect the food supply from the deleterious effects of the various powdery mildews, chemists at crop protection companies have to continuously come up with new agents to control the fungus and its close relatives.

Chemists at **DuPont’s Stine-Haskell Research Center in Newark, Delaware** have been able to discover and optimize a selective new class of powdery mildew agents that ranks as the most active ever discovered. The result of their labors has been the development and commercialization of the fungicide **Proquinazid**. Proquinazid is currently sold in Europe under the brand names of **Talius and Talendo**.

The story of Proquinzid began in the laboratories of **DuPont Research Fellow Thomas P. Selby**. Selby and **Staff Scientist Reed A. Coats** were working on the synthesis of a novel class of new herbicides when a hint of fungicide activity appeared after several of the analogs were tested against wheat powdery mildew. Selby and his team began an optimization program to increase the fungicidal activity of the class. Over the course of several months the team was able to achieve a several fold jump in activity, eventually far exceeding the activity of commercial standards.

In order to optimize the physical properties of the area, Selby suggested to another **DuPont Chemist Charlene G. Sternberg** that changing the ring system from the pyridopyrimidine system to the quinazoline system might help improve the physical properties of the molecule. Sternberg began a synthesis and optimization program that quickly produced compounds with increased activity and stability. Among these compounds was the compound coded KQ926 which would eventually be chosen for development by DuPont Crop Protection under the common name of Proquinazid.
When Selby later went on to accept new responsibilities at DuPont, the chemical research leadership was carried on by DuPont Group Leader James F. Bereznak. The chemical optimization was continued and eventually over 600 compounds were synthesized by the chemistry team. Bereznak and Staff Scientist Eric A. Marshall discovered and patented alternate ring systems which were just as active as that found in Proquinazid. The exemplary team effort took place over the course of 4 years and produced the most active powdery mildewicide ever discovered.

In addition to tremendous intrinsic activity, there are many other important aspects to the exquisite field activity of Proquinazid. It is unique in crop protection in that it contains an iodine atom which contributes to its excellent field performance. Proquinazid is able to efficiently redistribute under field conditions due to vapor action. By carefully optimizing overall vapor pressure, the chemistry team was able to synthesize a highly active compound which was able to protect new growth. This important characteristic allows Proquinazid to protect the farmer’s plants for an extended period at very low rates without the need for additional spray applications. Another important characteristic of Proquinazid is that the iodine atom also contributes to an increased stability to sunlight allowing field application at even lower rates.

Additionally, the mode of action of Proquinazid is novel and it retains activity against all of the resistant powdery mildew isolates encountered by farmers. Proquinazid inhibits the fungi from establishing an infection by disrupting the formation of appresoria. Fungal appresoria burrow into the plant cells to obtain nutrients to continue the fungal growth cycle. Deprived of nutrients, the fungus never establishes itself on the plant. Because of this Proquinazid acts as a protectant to the plant and is applied by the farmer before the appearance of the disease.

Proquinazid has proved to be an excellent addition to the modern farmer’s arsenal of weapons against the onslaught of fungal borne plant diseases. The low use rates are also a boon to the environment. Proquinazid is able to replace older chemicals which are currently applied at up to 20 times its labeled use rate. The long residual activity also allows farmers to use fewer spray applications in a season further lowering environmental impact.

The first Proquinazid based products reached the European marketplace in 2004 and were an immediate success. The entire production run was sold out during the first years of commercialization. Additionally, each year Talius and Talendo are registered and launched in several new countries. In 2007 sales began in the United Kingdom. Since the 2004 launch, tens of millions of dollars of sales have already been achieved and growth is expected to increase each year as new markets are entered. Worldwide commercialization and registration are continuing.
The Chromatography Forum of Delaware Valley
Student Award Symposium

Winners for MARM 2008

Michael J. Bozym
Casey M. Mulcahy
James D. Vasta
Christopher J. Morrison
Alyson M. Cobb
Sarah A. Schubert
Ranasinghe K. Sampath

The winners will present their work at the DVCF student award symposium on Monday, May 19, from 1:30 pm to 5 pm. The scheduled presentations are:

- **Michael J. Bozym**, Michelle L Owens, Anna Glinko, Karyn M. Usher, West Chester University “Separation of Water Soluble Vitamins by UHPLC”

- **Casey M. Mulcahy**, Scott H. Snyder, Karyn M. Usher, West Chester University “Extra Column Effects as a Function of Flow Rate”


- **Christopher J. Morrison**, Gennaro J. Maffia, Widener University “Lost Protein Technology for Proppant and Catalyst Manufacture”

- **Alyson M. Cobb**, Kyle W. Eckenroad, Gregory A. Manley, David Rovnyak, Timothy G. Strein, Bucknell University “Examining Chiral Separations with Bile Salt Micelles Using MEKC and NMR”

- **Sarah A. Schubert**, John W. Stahl, Timothy G. Strein, Bucknell University, Geneva College “Investigation of Buffering and Mixing Conditions for the Jaffe Reaction with Capillary Electrophoresis”

The E. Ann Nalley Regional Award for Volunteer Service to the American Chemical Society

Winner for MARM 2008

Dr. N. Bhushan Mandava
Mandava Associates, LLC

N. Bhushan Mandava holds B.S., M.S. and Ph.D. degrees in Chemistry and has published over 160 papers, including two patents, several monographs, reviews, and books. He is the Editor-in-Chief of the Ten-Volume CRC Handbook Series on Naturally Occurring Pesticides. Dr. Mandava has been serving in senior management positions for American and foreign companies which are involved in marketing of commercial and agricultural chemicals and health care and consumer products. He consults in health, safety and environmental issues related to agricultural and commercial chemicals, foods, drugs, and biotechnology products. Formerly, he was associated with the U.S. Department of Agriculture and the Environmental Protection Agency as Research Chemist and Senior Science advisor, respectively. He has held several visiting and adjuncts Professorships, and acted as a consultant on pesticides and drugs to various foreign governments. He frequently serves as an expert advisor on pesticides and pharmaceuticals to the Agencies of the United Nations Development Program.

Dr. Mandava has been active in many professional organizations. He has served as President of the Chemical Society of Washington, Councilor of the American Chemical Society, on the Editorial Boards of the Journal of Liquid Chromatography and Regulatory Affairs, on the Board of Advisors to the American Biographical Institute. He was appointed by the Secretary of the United States Department of Transportation to the Chemical Transportation Advisory Committee (CTAC) which advises the U.S. Coast Guard on marine transportation of chemicals.

Dr. Mandava was the 1983 recipient of the USDA Superior Service Award. He received a best publication award from the U.S. Naval Research Laboratory for his research contribution. He has also received the Chemical Society of Washington’s prestigious Hillebrand Prize, Charles Gordon Award and Community Service Award. He is listed, among other citations, in American Man and Women of Science, International Scholars Directory, Who’s Who in North America, Who’s Who in Technology today, Who’s Who in Frontiers of Sciences and Technology, International Leaders in Achievement, and Personalities of America. He is a Certified Chemist (CPC) and a Regulatory Affairs Certified (RAC).

Dr. Mandava’s areas of special expertise include; drugs and pesticides regulation; food, agricultural and pharmaceutical chemistry; plan biotechnology; new product
development and market analysis; good manufacturing practice (GMP) and good laboratory practice (GLP) regulations; biochemistry; environmental chemistry; plant and animal physiology and metabolism; hazard, exposure and, risk assessment; hazardous wastes; and right-to-knows laws.

Dr. Mandava has also been involved in Public Outreach, an American Chemical Society program dedicated to improving the public appreciation of chemistry and chemistry’s central role in our lives. He has been a Career Consultant for more than 15 years, assisting the ACS members in issues related to career management.

MARM AWARDS CRITERIA

The Stanley C. Israel Regional Award for Advancing Diversity in the Chemical Sciences

Nomination Guidelines:

Purpose: To recognize individuals and/or institutions that have advanced diversity in the chemical sciences and significantly stimulated or fostered activities that promote inclusiveness within the region.

Nature: The award consists of a medal and a $1000 grant to support and further the activities for which the award was made. The award also will include funding to cover the recipient’s travel expenses to the ACS regional meeting at which the award will be presented.

Rules of Eligibility: Individuals nominated for the award may come from any professional setting: academia, industry, government, or other independent facility. Nominees may also be organizations, including ACS local sections and divisions. The awardees will have increased the participation and leadership of persons from diverse or underrepresented minority group(s), persons with disabilities, or women.

To Nominate: For nomination of individuals, a letter of nomination of no more than three pages and a CV or resume is required. For institutions or corporations, a brief description of the institution or organization must be included. Nominations may also include up to two supporting letters of no more than three pages and up to five different samples of program materials. For details and most up to date information regarding the award, please refer to the ACS web site: www.acs.org/awards then click on “Other ACS Awards”.

Deadline for receipt of nominations: Spring/Summer Regional Meetings - March 1st; Fall Regional Meetings - May 1st. For information regarding the award, contact Paula Christopher, 800-227-5558, Ext. 6122, or e-mail: p_christopher@acs.org.

Send nominations to: Committee on Minority Affairs
American Chemical Society
1155 16th Street NW
Washington, DC 20036

The E. Emmet Reid Award in Chemistry Teaching at Small Colleges in the ACS Mid-Atlantic Region

Nomination Guidelines:

The E. Emmet Reid Award is administered by the Steering Committee of the Mid-Atlantic Regional Meeting (MARM) of the American Chemical Society for outstanding achievements in teaching chemical sciences at small colleges within the Mid-Atlantic Region.
Purpose: To recognize, encourage and stimulate high quality teaching and research at small colleges.

To nominate: Nominations for the Award are made by the local sections of the Mid-Atlantic Region. The Chairman or Secretary of the Section must sign and transmit the nomination to the MARM Award Committee Chairman. A committee may be appointed to solicit names of candidates for final selection. No special form is required but the Award Chair must receive the nominee's short curriculum vitae, list of publications, and evaluation of the nominee's achievements as a teacher in a small college. This document should clearly demonstrate the candidate's attributes: the quality of the candidate's teaching; organization and efficiency of lab work; research and/or development work; ability to challenge and inspire students; extra-curricular work in chemistry; courses, meetings, presentations, awards, etc. Seconding letters are not essential but as many as three may be included with each nomination. Letters may include careful evaluations of the teacher's abilities by his superiors, associates, or by local section members.

The deadline for the Award is to be announced in any nominee solicitation material, but in no case will it be less than two months before each MARM. The Award committee of the MARM will review the candidates and select the nominee. The candidate need not be a member of the American Chemical Society. The nominee will be presented the Award during the forthcoming MARM. The nominee is expected to deliver a short acceptance speech. The Award will consist of $1000 and a major award plaque.

Unsuccessful candidate's files will be kept active for a period of three years upon receipt of a letter from the nominating section chairman or secretary. Any further updating of the candidates file will be welcomed at that time but are not mandatory.

Please send nominations for 2009 to: Bill Suits, billsuits@earthlink.net.

The ACS Division of Chemical Education Middle Atlantic Region Award for Excellence in High School Teaching

Nomination Guidelines:

ACS Local Section Chairs covered in the MARM geography are invited to nominate an outstanding teacher of high school chemistry for the MARM Award for Excellence in High School Chemistry Teaching.

To nominate, please submit the following application materials for your nominee to the Awards Chair: 1.) A curriculum vitae, 2.) Two letters of support. Unsuccessful candidates' files will be kept active for a period of one year.

Please send nominations for 2009 to: Bill Suits, billsuits@earthlink.net.

The Chromatography Forum of Delaware Valley Student Award Symposium

Nomination Guidelines:

The annual CFDV Student Award Symposium provides graduate and undergraduate students with an opportunity to present their research in the field of separation science at MARM. Presentation of a paper at this symposium enables students to achieve recognition for their accomplishments, as well as developing important career skills and professional contacts.

All students whose papers are accepted for presentation at the Student Award Symposium will receive an honorarium of $250. Each student will also receive a certificate acknowledging his/her accomplishment and commemorating the event, which is sponsored by the Chromatography Forum of Delaware Valley. Though many participants are pursuing separation science as their major course of study, students in the areas of medicine, biochemistry, engineering and organic chemistry have successfully presented papers describing areas of research that involve separations.
Regional Industrial Innovation Award

Nomination Guidelines:

ACS Regional Industrial Innovation Awards Program (RIIA) sponsored by the ACS Corporation Associates celebrates the successful innovations of industrial chemists and chemical engineers that contribute to the health of their local and regional economy and the corporate leadership for its advancement of a healthy economy. Awards are given to individuals and teams whose creative innovations have contributed to the commercial success of their company and, consequently, to the good of the community and society.

Why Place a Nomination?

- To recognize industrial researchers for their creative and valuable contributions
- To promote the importance of the chemical profession and the support of corporate leadership in advancing science
- To enhance the company’s public image by promoting awareness about good science and successful commercialization
- To showcase the advances of industrial companies within your region
- To develop lasting goodwill in the community and higher employee morale within the company

As an added benefit, the honoree's company will enjoy a one-year complimentary membership to the ACS Corporation Associates (CA) if the company is not currently a CA member company. A representative from the company will be invited to attend an upcoming ACS National Meeting and participate in CA's meetings and ACS National Meeting activities. Travel assistance for the appointed representative may be available.

Event

- The event is held during a scheduled ACS Regional Meeting.
- Honoree(s) present a 20-minute talk on their innovation at a special symposium
- Honoree(s) are formally recognized and presented with an official ACS plaque

The event itself, presents a wonderful opportunity for one to peer into the world of industrial research and development. Networking is another important opportunity of the event and key to one's professional development. You will have the unique opportunity to interact with ACS governance, corporate leadership, industrial chemists, and leaders from academe.

What are the criteria?

- The invention or innovation must demonstrate innovation, commercialization of a product or process, commercial success, and be a value to society.
- The work should have been done in the respective region.
- A patent should have been awarded for the product or process, although some commercial process innovations may also qualify if care is taken to explain the nature of the innovation.

Who is eligible?

- Nominees must be chemists or chemical engineers who are ACS members.
- For team nominations, only one member needs to be an ACS member.
- Those who are not ACS members but are employed by an ACS Corporation Associates member company qualify for nomination.
How to place a nomination?
- Any ACS member may submit a nomination for eligible chemists or chemical engineers. Management approval is required.
- A biographical sketch of the nominee(s) is required.
- A letter of not more than 1,000 words containing an evaluation of the nominee's accomplishments, description of the invention or innovation, listing of relevant patents, publications, or reports

Apply online or download a nomination form to mail, fax or e-mail your application. (Nominations will remain valid for three years unless the nominator indicates otherwise). For details, nomination forms, and the most up-to-date information on the award, please refer to the ACS web site: www.acs.org/awards then click on “Industry Awards”.

Completed nomination packages can be sent three ways:

Mail: Attn: Joy Titus-Young
American Chemical Society
Office of Corporation Associates
1155 Sixteenth Street, NW
Washington, D.C. 20036.

E-mail: cheminnovations@acs.org
Fax: (202) 872-6098

The E. Ann Nalley Regional Award for Volunteer Service to the American Chemical Society

Nomination Guidelines:

Purpose: To recognize the volunteer efforts of individuals who have served the American Chemical Society, contributing significantly to the goals and objectives of the Society through their Regional Activities.

Nature and Establishment: This award was instituted in 2006 by ACS President E. Ann Nalley as part of her presidential initiative to recognize ACS volunteerism. It is Dr. Nalley’s wish that the award continue in perpetuity at each regional meeting. The award consists of an ACS Salute to Excellence plaque.

Directions: Any individual, except a member of the award selection committee, may nominate or support only one nominee for this award in any given year.

Rules of Eligibility: A nominee must be a member of the American Chemical Society residing in a local section within the region, and will have made significant contributions to their Region of the American Chemical Society. The volunteerism to be recognized may include a variety of activities, including but not limited to the initiation or sponsorship of a singular endeavor or exemplary leadership in the region. Past and present members of the ACS Board of Directors and staff are ineligible for this award.

Selection of Recipient: Nominations will be solicited from individuals, using the channels customary for other awards in the region. The awards committee of the region, or its equivalent, will select the recipient.

Submittal process: Submit each of the following to the Awards Chair: nomination and support forms, and biographical sketch (or curriculum vitae).

For nomination forms and details on the award, please visit: http://www.marmacs.org/2008/awards.html.

Please send nominations for 2009 to: Bill Suits, billsuits@earthlink.net.
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MARM 2008 Middle Atlantic Regional Meeting
May 17-21, Queensborough Community College

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Saturday, May 17, 2008

Saturday, May 17, 2008, 8:00 AM - 3:00 PM

56th NY-ACS Undergraduate Research Symposium


Student Union Building, Upper

Organizers: Sharon Lall-Ramnarine, Queensborough Community College, CUNY, JaimeLee Rizzo, Pace University, Alison G. Hyslop, St. John's University

Session Overview: The symposium provides an excellent opportunity for undergraduate chemistry students in the New York metropolitan area to present the results of their research. The program includes a keynote address and oral presentations of student papers, followed by a luncheon, award reception, and an expo featuring industry recruitment, research recruitment, and publishing companies.

Saturday, May 17, 2008, 8:30 AM - 4:00 PM

POGIL Workshop

Sponsor: National Science Foundation

Library Building, Rm LB-6

Organizers: David M. Hanson, Stony Brook University, Troy A. Wolfskill, Stony Brook University, Madhu Mahalingam, University of the Sciences in Philadelphia

Session Overview: This workshop introduces the philosophy and methodology of Process Oriented Guided-Inquiry Learning (POGIL). Participants experience the approach from a student's perspective, analyze the design of POGIL activities, and are introduced to various instructional techniques that support a student-centered learning environment. Data documenting the success of this approach are presented, and materials for general, organic, and physical chemistry are available for examination.
Saturday, May 17, 2008, 1:00 PM - 5:00 PM

Chemagination Competition

Medical Arts Building, Medical Arts Well, Rm M-136
Organizer: Vijaya Korlipara, St. John's University

Session Overview: For this competition, high school students are asked to imagine that they are living 25 years in the future and have been invited to write an article for ChemMatters, a magazine for high school students that focuses on the role of chemistry in everyday life. The subject of the article is: “Describe a recent breakthrough or innovation in chemistry and/or its applications that has improved the quality of people’s lives today.” The article is written to fit in one of four categories (Alternative Energy Resources, Environment, Medicine/Health, or New Materials). In addition to the article, students are asked to design a cover for the magazine. The article must be written as if the student is living in the year 2033, looking back at innovations that have occurred since 2008.

Saturday, May 17, 2008, 1:00 PM - 5:00 PM

Project SEED Poster Session

Sponsor: ACS Undergraduate Programs Office

Medical Arts Building, Medical Arts Well, Rm M-136
Organizers: Nadia Makar, Chair for Project SEED (NY Section, ACS), Neil Jespersen, St. John's University

Session Overview: The New York Section is celebrating 40 years of participation in project SEED along with the National Committee on Project SEED. This poster session will present some of the best posters prepared by New York Section students last summer.

Saturday, May 17, 2008, 2:00 PM - 4:00 PM

Making the Most of Being a Student Affiliate

Sponsor: ACS Undergraduate Programs Office

Medical Arts Building, Rm MC-29
Organizer: Neil Jespersen, St. John's University
Workshop Leader: Jodi L. Wesemann, American Chemical Society

Session Overview: The financial benefits of being an ACS Student Affiliate are tangible – reduced meeting registration fees, special student rates on journals and courses, and discounted prices with selected companies. Affiliation also has a wealth of less tangible but more important benefits. This interactive session will highlight ways to benefit both financially and professionally. Participants will explore how they can develop their professional network, explore career options, and position themselves for successful careers.
Saturday, May 17, 2008, 6:00 PM - 10:00 PM

Spring Meeting of the United States Section of the Royal Society of Chemistry

Oakland Building

Organizer: Les McQuire, Novartis Institutes for Biomedical Research

Session Overview: Members of the Royal Society of Chemistry, friends, families and colleagues are invited to participate in an evening which will be instructive, entertaining and a chance to meet old and new friends. Prof. Yorke E. Rhodes of NYU will give the after dinner talk. All are welcome.

6:00 PM: Social Hour and Networking Reception, Open Bar
7:00 PM: Dinner
8:15 PM: What's New In Astrochemistry?, Prof. Yorke E. Rhodes, New York University

If the physical world we know and the universe are described by the same Physics, i.e., if Physics is universal, is Chemistry also universal? Before 1960 that question was rarely raised. Yes, water, CO and CO2 were in Earth's atmosphere, around other planets, and even in spectra of some stars. The spectra were used to measure physical properties of the stars, and one didn't think of those molecules as chemistry. 50 years since Sputnik and with the explorations of the 1960's and on, what discoveries have been made! There are now known over 130 molecules off-earth - extra-solar, interstellar, intergalactic. Is the chemistry similar to Earth's? Three quarters of these molecules are what we would call organic - some are similar to earth chemistry, some exotic - all follow rules of structure/energy that we know. Many are different with unusual structures not found in our more temperate surroundings. Come see what's new and what we can predict.
Sunday, May 18, 2008, 8:00 AM - 12:00 PM

ACS Leadership Development Workshop: Involving Volunteers

Sponsor: ACS Local Section Innovative Project Grant

Library Building, Rm LB-8

Organizer: Ronald D'Amelia, Hofstra University
Workshop Leader: Dale Gaddy, American Chemical Society

Session Overview: One of the greatest challenges facing a volunteer leader is recruiting and engaging volunteers to help accomplish the project/team/committee goals. What’s more, is that a good leader recognizes that engaging volunteers is more involved than signing people up to work on a project. It requires leaders to understand what help is needed, what skills and talents are required to accomplish the project and what form of motivation will truly excite the volunteer to commit to the project. This hands-on, four-hour course will provide ACS leaders with practical tools they need to engage a volunteer in a way that makes the assignment successful and professionally rewarding, so the volunteer will be inclined to participate in future, more ambitious assignments.

Sunday, May 18, 2008, 8:30 AM - 12:00 PM

Chemical Education, I

Sponsor: Pacific Crest

Medical Arts Building, Rm M-133

Organizers: David M. Hanson, Stony Brook University, Judy Lloyd, SUNY College at Old Westbury

Session Overview: The focus is on innovative curriculum materials and instructional strategies that engage students in learning and promote the development of critical learning process skills that are essential for mastery of course content and success in courses, college, and careers. Presentations describe specific implementations along with their successes and challenges. Topics most relevant to introductory and general chemistry are included in Session I, and organic chemistry and more general topics are covered in Session II. Each presentation is expected to have at least one takeaway message or insight.

8:30 1 Introduction to Process-Oriented Guided-Inquiry Learning. David M. Hanson, Stony Brook University

8:50 2 Cooperative Learning in Inorganic Chemistry: Group Activities for Fun and Learning. Elise G. Megehee, St. John's University

9:10 3 LUCID: Measuring and Improving Learning Outcomes in General Chemistry. Troy A. Wolfskill and David M. Hanson, Stony Brook University
Implementing Process Oriented Guided Inquiry in the General Chemistry Course: Introducing New Material Vs Reinforcing Material Already Introduced in Lecture. Terry L. Brack and Sabrina G. Sobel, Hofstra University

POGIL in Recitation and Laboratory at a Community College. Candice J. Foley and Sharadha Sambasivan, Suffolk County Community College

Promoting Learning through Group Problem Solving. Madhu Mahalingam, Fred Schaefer and Elisabeth Morlino, University of the Sciences in Philadelphia

Break.

Linking Analytical Chemistry and Public Policy through Project Based Labs. Charles Hosten, Howard University

Metropolitan Mentors Network: Growing An Urban STEM Talent Pool with An NSF Funded STEP Grant. Pamela A. Brown, New York City College of Technology - CUNY

An “Electronic Dormitory” for Self- and Group-Learning in Chemistry. Harry D. Gafney and Gopal Subramaniam, City University of New York, Queens College,

Industry to Academe: A Practical Perspective on Teaching. Lance D. Silverman, Yeshiva University

Sunday, May 18, 2008, 8:30 AM - 12:00 PM

Clinical Chemistry I

Library Building, Rm LB-14
Organizer: Clive I. Wynter, Nassau Community College

8:30 11 A Brief Overview of Clinical Chemistry. Clive I. Wynter¹, Eugene Brown¹ and Albert Davis², (1)Nassau Community College, (2)Quest Diagnostics

9:00 12 Heavy Metals and Chronic Disease. Christopher Calapai, CC medical Services PC

9:30 13 Relationship Between Lifestyle and Degenerative Health Problems among the Youth. Eugene Brown, Nassau Community College

10:00 Break.

10:30 14 Simplified Physiological Assays Using Filter Photometry. Jerry DeMenna V, Sacred Heart University / FUN-SCience Academics

11:00 15 Inhibition of Intrinsic Peptidase Activity Moderates Sequential Digestion of Human Plasma Peptides. Jizu Yi, Zhaoxia Liu, Gang Ju and Craig A. Gelfand, BD Diagnostics
Sunday, May 18, 2008, 8:30 AM - 12:00 PM

Forensic Chemistry

Library Building, Rm LB-6

8:30  Introductory Remarks.
9:15  17  The Use of Micro-ATR Spectroscopy to Study the Effect of Ph Variation on Changes in Dyed and Non-Dyed Female Hair Exposed to Antipsychotic Agents. **Ali Kocak** and Zann S. Blanchard, John Jay College, CUNY
10:25 Break.
10:50  19  Forensic DNA Testing in New York City. **Noelle J. Umback**, New York City Office of Chief Medical Examiner
11:25  20  Mitochondrial DNA Testing at the New York City Office of Chief Medical Examiner. **Paul Goncharoff**, Jessica Harris, Veronique Bourdon, Kristy Bernard and Eli Shapiro, Office of Chief Medical Examiner

Sunday, May 18, 2008, 8:30 AM - 12:00 PM

Organic Chemistry, General Session I

Sponsor: Mettler-Toledo AUTOCHEM; Pearson Prentice
Science Building, Rm S-112
Organizer: JaimeLee Rizzo, Pace University
Session Overview: This session is for general contributions in the field of organic chemistry.

8:30  Introductory Remarks.
8:35  21  Synthesis of An Oligodeoxyribonucleotide Adduct of Mitomycin C by the Postoligomerization Method, Via a Triamino Mitosene. **Elise Champeil**, John Jay College, Manuel M. Paz, Universidade de Santiago de Compostela and Maria Tomasz, Hunter College
8:55  22  Mechanism for NAD⁺ Hydrolysis at pH 9 as Determined by Kinetic Isotope Effects and Computational Analysis. **Yana Cen** and Anthony A. Sauve, Weill Medical College of Cornell University
9:15  23  Hantzsch Synthesis of 1,4-Dihydropiridines. **Krytsina Ivanova**, New Jersey City University
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<tr>
<td>9:35</td>
<td>Studies toward Total Synthesis of Angelmicin B. <strong>Jialiang Li</strong> and David R. Mootoo, Hunter College</td>
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<td>10:15</td>
<td>Break.</td>
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<tr>
<td>10:30</td>
<td>Use of ReactIR in Studying Fundamental Organic Reactions and Flash Chromatography. <strong>John R. Sowa Jr.</strong>, Seton Hall University and Jian Wang, Mettler-Toledo Autochem</td>
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<td>11:10</td>
<td>Concluding Remarks.</td>
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**Sunday, May 18, 2008, 9:00 AM - 11:00 AM**

**NY Section Nichols Teacher Forum**

Library Building, Rm LB-15  
Organizer: Lew Malchick, Education  
Session Overview: For many years, the New York Section has selected a teacher to receive the Nichols High School Chemistry Teacher of the Year Award. Each has an extensive resume and much experience. A number of recent awardees will speak about their experience and their views of the future of chemistry education. This will be followed by an open forum with questions and discussion from the floor.

**Sunday, May 18, 2008, 9:00 AM - 12:00 PM**

**Tapping into the Excitement: Strategies for Building – or Rebuilding – a Student Affiliates Chapter**

Sponsor: ACS Undergraduate Programs Office  
Medical Arts Building, Rm MC-29  
Organizer: Neil Jespersen, St. John's University  
Workshop Leader: Jodi L. Wesemann, American Chemical Society  
Session Overview: The process of establishing or reactivating a Student Affiliates chapter is an exciting one. Participants in this interactive workshop will explore strategies to help make it successful as well. Ideas for engaging others, conducting business, planning events, and raising funds will be discussed. Approaches for developing leadership skills will also be shared.
**Sunday, May 18, 2008, 1:00 PM - 5:00 PM**

**ACS Leadership Development Workshop: Leading Change**

Sponsor: ACS Local Section Innovative Project Grant

Library Building, Rm LB-8

Organizer: Ronald P. D'Amelia, Hofstra University

Workshop Leader: Dale Gaddy, American Chemical Society

Session Overview: Almost any initiative today in the workplace or within an ACS committee or project team involves change. It could be a change in priorities and direction, people, or goals and objectives. And, with change often comes resistance. It is not easy leading amidst change. It requires leaders to help local section and technical division volunteers, national committee members and regional meeting volunteers move through change by confronting reality, connecting with the vision of the future, designing a new approach, and engaging others to take the steps to move the project ahead. This four-hour course provides leaders with a step-wise process to lead change and guide volunteers more effectively through the change process for greater results and efficiency. Participants will gain a skill that can be used daily in both volunteer leadership roles as well as in your profession.

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**Sunday, May 18, 2008, 1:30 PM - 5:00 PM**

**BioTherapeutics**

Sponsor: Pfizer

Medical Arts Building, Rm M-146

Organizers: Susan A. Rotenberg, Queens College, Regina Sullivan, Queensborough Community College, Barbara Petrak, Drew University

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<tr>
<th>Time</th>
<th>Title</th>
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<tr>
<td>1:30</td>
<td>Introductory Remarks.</td>
<td></td>
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<tr>
<td>1:35</td>
<td>New Therapeutics from Transition State Theory.</td>
<td>Vern L. Schramm, Albert Einstein College of Medicine</td>
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<tr>
<td>1:55</td>
<td>Development of PCK3145, a Novel Multi-Targeted Anti-Tumor Agent for Prostate Cancer.</td>
<td>Susan F. Slovin, Memorial Sloan-Kettering Cancer Center</td>
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<tr>
<td>2:15</td>
<td>DNA Vaccines - Design, Development and Application.</td>
<td>Rangappa Ramachandra, Covance Research Products</td>
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<tr>
<td>2:35</td>
<td>Break.</td>
<td></td>
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<tr>
<td>2:55</td>
<td>Structure-Based Design of An Organoruthenium Phosphatidyl-Insitol-3-Kinase Inhibitor Reveals a Switch Governing Lipid Kinase Potency and Selectivity.</td>
<td>Peng Xie¹, Douglas S. Williams², G. Ekin Atilla-Gokcumen¹, Leslie Milk³, Min Xiao¹, Keiran S.M. Smalley¹, Meenhard Herlyn¹, Eric Meggers² and Ronen Marmorstein⁴, (1)The Wistar Institute, University of Pennsylvania, (2)University of Pennsylvania, (3)Graduate Group in Biochemistry and Molecular Biophysics, School of Medicine, (4)The Wistar Institute</td>
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</table>
3:15  32  Challenges in the Production of Bio-Therapeutics. Amit Banerjee, Pfizer Global Research and Development

3:35  33  Visual Snapshots of Intracellular Kinase Activity at the Onset of Mitosis. Zhaohua Dai¹, Natalya G. Dulyaninova², Sanjai Kumar², Anne R. Bresnick² and David S. Lawrence², (1)Pace University, (2)Albert Einstein College of Medicine

3:55  Concluding Remarks.

Sunday, May 18, 2008, 1:30 PM - 5:00 PM

Chemical Education, II

Sponsor: Cengage Learning

Medical Arts Building, Rm M-133

Organizers: David M. Hanson, Stony Brook University, Judy Lloyd, SUNY College at Old Westbury

Session Overview: The focus is on innovative curriculum materials and instructional strategies that engage students in learning and promote the development of critical learning process skills that are essential for mastery of course content and success in courses, college, and careers. Presentations describe specific implementations along with their successes and challenges. Topics most relevant to introductory and general chemistry are included in Session I, and organic chemistry and more general topics are covered in Session II. Each presentation is expected to have at least one take-home message or insight.

1:30  34  Organic Chemistry for a Thousand. Joseph W. Lauher and Frank W. Fowler, State University of New York at Stony Brook

1:50  35  Using a Combined Lecture/Workshop Model to Improve Student Engagement and Self Confidence in Undergraduate Organic Chemistry. Karen E. S. Phillips, Hunter College of the City University of New York

2:10  36  How I Increased My Organic Chemistry Class Average 20 Percentile Points. Peter J. Wepplo

2:30  37  Anathons in Developing and Solving Ozonolysis Problems. Ray A. Gross Jr., Prince George's Community College

2:50  38  Student Motivation and Reform in the Organic Laboratory. Gail Horowitz, Yeshiva University

3:10  Break

3:20  39  Chemistry in Context Approach to Teaching Allied Health Chemistry. David W. Parkin, Adelphi University


4:00  41  Adding Scientific Process to Chemistry Instruction. Anthony Carpi, John Jay College

4:20  42  Impact of Microcomputer-Based Laboratory Experiences on Content-Related Performance in Science. Fernando Espinoza, SUNY Old Westbury

4:40  43  Student Assessment of Engagement in a “Clicker” Classroom. Daniel B. King, Drexel University
Sunday, May 18, 2008, 1:30 PM - 5:00 PM

Clinical Chemistry II and Clinical Chemistry Workshop

Library Building, Rm LB-14
Organizer: Clive I. Wynter, Nassau Community College
Workshop Leader: Jerry DeMenna, Sacred Heart, Buck Scientific

Session Overview: This will be a continuation of the morning symposium followed by a workshop session on Clinical Chemistry.

1:30  44  Heart Failure: Recent Advances in Diagnosis and Management. **Felix Oviasu**, Garden City Heart Center

2:00  45  Enriching Patient Population in Oncology Drug Development through Proteomic Studies. **Jiwen Chen**, Bristol-Myers Squibb

2:30  46  Oncolytic Herpes Simplex Virus-1 (NV1023) Effectively Treats Anaplastic Thyroid Cancer in An Orthotopic Murine Model. **Vincent Reid**, South Nassau Communities Hospital and Rihahrd Wong, The Memorial Sloan Kettering Cancer Center

3:00  Break.

3:20  47  Treatment of Type 2 Diabetes. **Kenneth H. Hupart**, Nassau University Medical Center

3:50  Discussion.

Sunday, May 18, 2008, 1:30 PM - 5:00 PM

H I V/ AIDS

Medical Arts Building, Rm M-136
Organizer: Rolande R. Hodel, AIDSfreeAFRICA

Session Overview: HIV/AIDS has many faces. On the research side there are new therapies to be invented. New drugs with new mechanisms are needed to beat the ever present threat of drug resistance. Vaccines and microbicides are still not on the market, and antiretroviral drugs that are on the market in western countries are still waiting to get the green light to be produced and made available in developing countries.

1:30  Introductory Remarks.

1:35  48  Development of a Microbicide to Combat HIV. **David Fairhurst**, International Partnership for Microbicides


2:35  Break.

2:55  50  Investigating An Allosteric Binding Site for a New Class of HIV-1 Protease Inhibitors. **Christine L. Shrock**¹, **Ellen L. Shrock**², **Melinda M. Layten**³ and **Carlos Simmerling**³, (1)Ward Melville High School, (2)Long Island School for the Gifted, (3)Stony Brook University


3:55  Concluding Remarks.
Sunday, May 18, 2008, 1:30 PM - 5:00 PM

Ionic Liquids I: Synthesis and Reactions in Ionic Liquids

Sponsor: CEM Corporation

Library Building, Rm LB-6

Organizers: James F. Wishart, Brookhaven National Laboratory, Sharon Lall-Ramnarine, Queensborough Community College, CUNY

Session Overview: Research in ionic liquids (ILs) has exploded in recent years because of their great promise in a broad range of applications in chemistry and chemical technology for process and safety improvement and reduction in overall environmental impact. This three-session symposium features the broad spectrum of ionic liquids research conducted in the Middle Atlantic Region.

1:30 Introductory Remarks.

1:40 52 Manipulating the Properties of Ionic Liquids by Synthetic Design. Sharon Lall-Ramnarine1, Alejandra Castano2, Jasmine Hatcher1, Kijana Kerr1, Xing Li1, Ayisha Munawar1, Ankita Parikh1, Pokay Ma2, Catherine McEntee3 and James F. Wishart4, (1)Queensborough Community College, CUNY, (2)Queens College, CUNY, (3)Kingsborough Community College, (4)Brookhaven National Laboratory

2:20 53 Synthesis and Thermochemical Properties of Racemic Dihydroxy Ammonium Salts. Marie Thomas1, Leah Rothman1, Jasmine Hatcher1, Sharon Lall-Ramnarine2 and Robert Engel3, (1)Queens College, CUNY, (2)Queensborough Community College, CUNY, (3)Queens College of the City University of New York

3:00 Intermission.

3:25 54 Radiation-Induced Reactions in Ionic Liquids. James F. Wishart, Brookhaven National Laboratory

4:05 55 Ionic Liquids: Vehicle for Pharmaceuticals and Therapeutics. Sanjay V. Malhotra, National Cancer Institute-Frederick; SAIC-Inc.

Sunday, May 18, 2008, 1:30 PM - 5:00 PM

Medicinal Chemistry

Sponsor: ACS Division of Medicinal Chemistry

Science Building, Rm S-111

Organizers: Ralph A. Stephani, St John's University, Tanaji Talele, St. John's University, Vijaya Korlipara, St. John's University

1:30 56 Protein-Protein Interactions: Drugability, Design Strategies in Lead Identification and Optimization. Hariprasad Vankayalapati, SuperGen Inc.

2:15 57 Evolution of Selective IGF1R Inhibitors. Kenneth W. Foreman, OSI Pharmaceuticals

3:45 Break.

4:00 59 Fragment Based Design of p53/MDM2/MDM4 Inhibitors Utilizing Multi Component Reaction (MCR) Chemistry. Barbara Beck¹, Stuti Srivastava¹, Balachandran Raghavan¹, Alexander Doemling¹ and Tad Holak², (1)University of Pittsburgh, (2)Max Plank Institute

4:30 60 Potent XIAP Antagonists by a Fragment-Based MCR Approach. Ilaria Monfardini¹, Alexander Doemling¹ and Maurizio Pellecchia², (1)University of Pittsburgh, (2)Burnham Institute for Medical Research

Sunday, May 18, 2008, 1:30 PM - 5:00 PM

Process Chemistry

Science Building, Rm S-112
Organizer: Rick Sidler, Merck & Co.

Session Overview: This session will highlight topics pertaining to the synthesis, optimization, purification and isolation of pharmaceutically interesting compounds or intermediates. Emphasis will be on the development and application of novel and practical solutions to challenges incurred during preparation of these materials.

1:30 61 From the Bench to the Plant: Case Studies in the Development and Scale up of Chemical Processes. Akin H. Davulcu, Bristol-Myers Squibb Company


2:30 63 A Novel and Efficient Cleavage of Silyl Ethers. Daniel Zewge, Rick Sidler and Raymond Cvetovich, Merck

3:00 64 Development of a Scaleable Process for Product Quality Improvement Using Adsorbents. Melodie D. McCain, Jungchul Kim, Jennifer Vance and Thomas Hunter, Schering-Plough

3:30 Break.

3:45 65 Recent Advances in the Use of Preparative Chromatography in the Multikilogram Synthesis of Preclinical Pharmaceutical Candidates. Derek Henderson, Merck Research Laboratories

**Sunday, May 18, 2008, 1.30 PM - 5:00 PM**

**Probeware Workshop and Chemical Demonstrations for Pre-College Educators**

Science Building, Rm S-405

Organizers: Lew Malchick, Education, Pedro Irigoyen, Queensborough Community College

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**Sunday, May 18, 2008, 5:30 PM - 6:30 PM**

**Plenary Lecture I: Ronald Breslow, Columbia University**

Medical Arts Building, Rm M-136

Organizer: Jack Norton, Columbia University

Session Overview: This plenary lecture will discuss SAHA (Vorinostat), an FDA approved anticancer compound with a novel mechanism of action.

**5:30 67** SAHA (Vorinostat), An FDA Approved Anticancer Compound with a Novel Mechanism of Action. **Ronald Breslow**, Columbia University

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**Sunday, May 18, 2008, 6:30 PM - 8:30 PM**

**Sunday Night Barbecue/mixer**

Sponsor: ACS Undergraduate Programs Office

Student Union Building, Upper

This all-you-can-eat dinner follows the evening plenary lecture and takes place adjacent to the poster session.

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**Sunday, May 18, 2008, 7:00 PM - 8:30 PM**

**Poster Session I**

Student Union Building, Upper

Organizers: Irina Rutenburg, Queensborough Community College, Marie Thomas, Queens College, CUNY

**68** Catalase-Peroxidase (M. tuberculosis KatG) Forms a Protein-Based Radical during Catalase Turnover. **Javier Suarez**¹, Shengwei Yu¹, Richard Magliozzo¹ and Kalina Rangelova², (1)Brooklyn College and the Graduate Center of the City University of New York, (2)NIEHS

**69** Predictable Transitive RNA Interference Induced by mRNA Hairpins in C. Elegans. **Jessica Cox** and Matthew Doty, Villa Julie College
Expression and Metal Binding Studies of Tristetrapolin (TTP), a Zinc Finger Protein. Robert DiTargiani1, Sarah L. J. Michel1, Seung Jae Lee2, Sarah Wassink1 and Anab Yusuf3, (1)University of Maryland, (2)University of Maryland School of Pharmacy, (3)Villa Julie College


Bacterial Responses to a Combinatorial Environment. Peter Palenchar and Steven Middler, Rutgers University, Camden

Synthesis and Gp 120 Binding of 1,1-Linked-Disaccharide Mimetics of β Galactosyl Ceramide (GalCer): Potential Entry Inhibitors of HIV. Stewart Bachan and David R. Mootoo, Hunter College

Determining the Role of NO / H-Nox in Colwellia Psychrerythraea. Stephanie A. Georgiou and Elizabeth M. Boon

Engineering Functional Artificial Histone Acetyltransferases. Man Xia Lee, Kinjal Mehta, Susheel Kumar Gunasekar, Zhiqiang Liu, Natalya Voloshchuk, Aye Sandar Moe, Phyllis Frankl, Lisa Hellerstein and Jin K. Montclare, Polytechnic University

Peptides Inhibitors of F11R/JAM-a Adhesion Molecules. Cristina C. Clement and Manfred Philipp, Lehman College, City University of New York (CUNY)

Structure and Stability Analysis of Single-Alanine Mutants of Cartilage Oligomeric Matrix Protein Coiled Coil. Wendy Hom, Hanna Barra, Susheel Gunasekar, Jin Montclare and Jennifer Haghpanah, Polytechnic University

Fluorescence Study of Some Precursors of a Bivalent Src Kinase Inhibitor. Chrystel Dol, Adam Profit and Ruel Z. B. Desamero, York College

Study of in Vitro of Cell Migration. Emily Hughes and Regina Sullivan, Queensborough Community College

Characterization of Fluorinated Histone Acetyl Transferase, tGcn5. Natalya Voloshchuk, Anita Yuhua Zhu and Jin Kim Montclare, Polytechnic University

Hormonal Control of Neuron Development. Christina Dewan and Regina Sullivan, Queensborough Community College

Determination of Breast Cancer Cell Migration Rates. Louis Corradino Jr. and Regina Sullivan, Queensborough Community College

Exploiting Non-Natural Amino Acids to Identify Protein Partners of FnTm2. Yan Mei Chan, Peter James Baker and Jin Kim Montclare, Polytechnic University

Effects of Anti-Androgens on Spinal Cord Motor Nuclei. Sheila Jean-Charles and Regina Sullivan, Queensborough Community College

Effects of Varying Levels of Nitrogen, Potassium and Phosphorus on Plant Growth. Sharisse Lewis and Regina Sullivan, Queensborough Community College

Migration of Rates of Human Breast Cancer Cells. Joseph Mammano and Regina Sullivan, Queensborough Community College

Study of Human Breast Cancer Cell Migration. Sakshi Pasricha-Katyal and Regina Sullivan, Queensborough Community College, CUNY

The Anti-Androgen, Flutamide Causes Organizational Changes in Spinal Cord Motor Nuclei. Marie-Pierre Payen and Regina Sullivan, Queensborough Community College

Human Breast Cancer Cell Migration. Nicole Perrotta and Regina Sullivan, Queensborough Community College
90 The Alu Insert and Human Diversity. **Brooke Rodriguez** and Regina Sullivan, Queensborough Community College

91 Studies of Cell Migration. **Darryl Williams** and Regina Sullivan, Queensborough Community College

92 Comparing the Effects of Anti-Androgens on Two Groups of Nuclei. **Liang Xiang** and Regina Sullivan, Queensborough Community College

93 The Alu Genotype. **Yun Zhao** and Regina Sullivan, Queensborough Community College

94 Synthesis and Study of Nano-Adsorbents. **Philip Botelho**, Christopher Rodriguez and Girija Subramaniam, Penn State University

95 Mechanism Based Inhibitors of Adenylyl Cyclase: Insight into Binding and Reactivity in the Active Site. **Morris Krauss**, Scientist Emeritus, National Institute for Standards and Technology, Rockville, MD 20850

96 Discovery of Substituted Dipiperidine Acids and Alcohols as CC Chemokine Receptor-2 Antagonists. **Mingde Xia**, Cuifen Hou, Duane DeMong, Scott Pollack, Meng Pan, James Brackley, Chrissy Gerchak, Monica Singer, Ravi Malaviya, Michele Matheis, Gil Olini, Druie Cavender and Michael Wachter, Johnson & Johnson Pharmaceutical Research and Development, L.L.C.

97 Biodiesel Synthesis and Characterization in a General Chemistry Laboratory. **Rebecca L. Sanders**, The Pennsylvania State University

98 Teaching Scientific Writing to Second-Language Students. **Mark Kobrak**, Brooklyn College and The Graduate Center of the City University of New York

99 Pokeweed Antiviral Protein: Understanding Its Role in Plant Related Forensics. **Jeannine DeGrazia**¹, Kana Noro² and Diana E. Friedland², (1)John Jay College of Criminal Justice and the Graduate Center of the City University of New York, (2)John Jay College of Criminal Justice and the Graduate Center of the City University of New York

100 Novel and Rapid HPLC Method for the Quantitation of Guaifenesin: Application to Pharmacokinetic Studies. Sangeeta Chavanpatil¹, **Ramesh Reddy Putheti**², K.G Akamanchi³, and R N Okigbo⁴, (1)University of Mumbai, India, (2)Actavis Pharmaceuticals, (3) University of Mumbai, India, (4)Nnamdi Azikiwe University, Nigeria

101 Functional Significance of Protein Kinase Cα And Hsp90 Interaction in a Yeast Model. **Tae Young**¹, Sheila JeanCharles¹, Corinne A. Michels², Susan A. Rotenberg³ and Nidhi Gadura¹, (1)Queensborough Community College, CUNY, (2)Queens College, CUNY, (3)Queens College

102 Synthesis of the Guaifenesin Impurities and Their Spectral Properties. Sangeeta Chavanpatil¹, **Ramesh Reddy Putheti**², Actavis K.G. Akamanchi³, and N. Okigbo⁴, (1)University of Mumbai, India, (2)Actavis Pharmaceuticals, (3)University of Mumbai, India (4)Nnamdi Azikiwe University, Nigeria

103 Environmental Microbiological Monitoring and Source of Contamination in the Pharmaceutical Industry—a Case Study. **Ramesh Reddy Putheti**³, R N Okigbo⁴, Madhusoodan sai Advanapu³, and Radha Leburu⁴, (1)Actavis Pharmaceuticals, (2)Nnamdi Azikiwe University, Nigeria, (3)University of Madras, India (4) S.V University, India

pH-Response of PMAA Hydrogel Multilayer Capsules Crosslinked with Adipic Acid Dihydrazide. **Svetlana Pavlukhina, Veronika Kozlovskaya and Svetlana A. Sukhishvili, Stevens Institute of Technology**

Chemical Shift Modulation by Peptide Bond Distortion. **Adrienne F. Alimasa, Lee Zhang and Ronald L. Koder, The City College of New York**

A Demonstration of Both the Regio- and Stereochemical Outcome of Alkene Hydration. Thomas Lobasso, Christa Iwanoski, Shahrokh Saba and **Donald D. Clarke**, Fordham University

Learning from An Orange Beard. **Brahmadeo Dewprashad** and Latfa Hadir, Borough of Manhattan Community College

Reactions of Hexachloroacetone with Aliphatic Diamines: Syntheses of Bis(trichloroacetamide) Derivatives. **Yoomi Kim** and Jun H. Shin, Queensborough Community College

Reactions of Hexachloroacetone with Aromatic Diamines: Syntheses of N,N'-Phenylenebis(trichloroacetamide). **Emily Hughes** and Jun H. Shin, Queensborough Community College

Determination of Refractive Index of Methanol Solutions Using a Laser Pointer: Relation to Density and Concentrations. **Jeffrey Park**, Crystal Park and Jun H. Shin, Queensborough Community College

Determination of Refractive Index Using a Laser Pointer: Non-Ideal Behavior of Aqueous Solution. **Crystal Park** and Jun H. Shin, Queensborough Community College

Aflatoxin Exposure: Does It Account for Higher Incidence of Liver Cancer. **Joanna Magda** and Angelo Raymond Rossi, York College - City University of New York

Growth Mechanism of Highly Luminescent ZnO Nanoparticles. Alexandra Turner and **Temer S. Ahmadi**, Villanova University

Extraction Methods Used for Fresh Produce (E302 Methods). **Angelo Damanti¹**, Yelena Karaseva¹ and Angelo Rossi², (1) U. S. Food and Drug Administration, (2) York College - City University of New York

Utilization of HPLC-CAD (Charged Aerosol Detection) for Assessing Impurity Profiles in Synthetic Pulmonary Surfactant SURFAXIN® Versus the Current Marketed Animal-Derived Product Surfactant. **Michelle A. De Crosta** and Victoria Scott, Discovery Laboratories, Inc

From SAMs to Drugs: Design and Development of SLx 2101, a Novel PDE5 Inhibitor for the Treatment of Cardiovascular Diseases. **Farah Dhun**, Brian Kirk, Dominick Casalena, Elsa Paradise, Andrew Saati, James Ellis, John Ferkany, Enoch Kim, Stewart Campbell, Michael Grogan, Paul Sweetnam and Bridget Cole, Surface Logix, Inc

How Does the U.S. FDA Test for Pestacides in Produce?. **Yelena Karaseva¹**, Angelo Damanti¹ and Angelo Rossi², (1) U. S. Food and Drug Administration, (2) York College - City University of New York

Distribution of Periodontal Pathogens in the Third Molar Region of Adult Asian Indian Patients. **Darryl Williams**, Dr. Raji Subramaniam and Dr. Patricia Schneider, Queensborough Community College

Effect of Microstructure on Enzymatic Degradation of Polycaprolactone. **Gabriela Sekosan** and Nadarajah Vasanthan, Long Island University

Experimental Design and Inquiry: Exploring the Chemistry of Dental Health Care Products. **Ann E. Shinnar** and Marc Nemetsky, Lander College for Men, Touro College

123 Plant Phenols - Polymer Interactions: Effect on Tyrosinase and Elastase Activities. **Michael Koganov** and **Artyom Duev**, Integrated Botanical Technologies, LLC

124 Stabilization and Continuous Processing Techniques for Manufacturing Phenol/Formaldehyde Resins Used in Making Photoresists. **M. Dalil Rahman**, AZ Electronic Materials USA Corp. and **Stanley F. Wanat**, Union County College

125 Taking the “Nip” out of Catnip: An Undergraduate Experiment Involving Isolation and Identification of Nepetalactone Diastereomers from Commercial Samples of *Nepeta cataria* L.. **James A. Ciaccio**, Rabeka Alam and Christina D’agrosa, Fordham University

126 Metabolic Profiling of the Coral Pathogen *Vibrio Coralliilyticus*. **Elizabeth Pollock**, Sara Lien Huynh, Daniel W. Bearden, Pamela J. Morris and Maria Vizcaino, (1)Stockton College, (2)Mt. Holyoke College, (3)National Institute of Standards and Technology, (4)Medical University of South Carolina

127 A Study of the Ideal Conditions Required for the Uptake of Lawsone from Henna (*Lawsonia Inermis*) as a Greener Approach to Dyeing. **Samuel Ganta** and Kishore K. Bagga, Holy Family University


129 Quinones, Monoradicals and Diradicals from 3- and 4-Mercaptocatechol, and 3,4-Bismercaptocatechol: A Computational Study of a Plausibly Biomimetic Reaction. **Alvaro Castillo**, Joel F. Liebman and Alexander Greer, (1)City University of New York, Brooklyn College, (2)University of Maryland, Baltimore County

130 Structures and Energies of Models for Reduced Symmetrically and Anti-Symmetrically Methylated Arginine Side Chains. **Edward M. Barbieri** and Margaret Mandziuk, Manhattan College

131 The Incorporation of Fluorinated Phenylalanine Analogos into Histone Acetyltransferase. **Anita Y. Zhu**, Polytechnic University

132 Biological Activity of a Water-Insoluble Benzopentasulfane Compound. **Adaickapillai Mahendran**, David Aebisher, Konstantin Astafurov, Rafael Ovalle, Akira Kawamura, Ernest Boamah, Jill Bargonetti and Alexander Greer, (1)City University of New York, Brooklyn College, (2)City University of New York, Brooklyn College

133 Lysine-Triggered β-Lactam Ring Formation of Deoxyguanidinoproclavaminic Acid Which Involves a Rebound of the Phosphate Ion Leaving Group: A Combined DFT and Mutational Analysis. **Mary Raber**, Michael Freeman, Alexander Greer and Craig A. Townsend, (1)Johns Hopkins University, (2)City University of New York, Brooklyn College

134 Asymmetric Transfer Hydrogenation of Allylic Alcohols with Homogeneous Chiral Ruthenium Catalysts. **Marie G. Beauchamps** and John R. Sowa Jr., Seton Hall University

135 Nucleotide Reversible Terminators for Pyrosequencing. **Jian Wu**, Columbia University

136 You Are What You Eat!. **Peter L. Bastos**, Hunter College

137 Synthesis and Application of Water-Soluble Nanocapsules. **Xuejun Liu** and Ralf Warmuth, Rutgers, The State University of New Jersey

138 Morphine as a Mimic of the Backbone of Opioid Peptides. **Zhijun Wu**, ABC Resources
Characterization of Pokeweed Antiviral Protein’s Interaction with Eukaryotic Initiation Factors and a Sarcin/ricin Loop Oligoribonucleotide. **Diana E. Friedland**, Dixie J. Goss, Jeannine DeGrazia and Amy E. Baldwin, (1)John Jay College of Criminal Justice and the Graduate Center of the City University of New York, (2)Hunter College CUNY, (3)Pace University

Detection of rRNA Depurination by Pokeweed Antiviral Protein: Fluorescence Detection of Adenine Release. **Nicole DeLuca**, Ana Sanchez, Eugenia Pontacq, Jacqueline Chaparro and Diana E. Friedland, (1)John Jay College of Criminal Justice, (2)John Jay College of Criminal Justice and the Graduate Center of the City University of New York

Sub-Cloning of Protein Kinase C-alpha3HA in a Yeast Plasmid. **Shih Wei Chiang**, Sakshi Pasricha-Katyal and Nidhi Gadura, Queensborough Community College, CUNY

Analysis of Mycotoxins Using HPLC. **Frandaluz Cuevas**, Paris Svoronos and Barry Mopper, (1)Queensborough Community College, (2)Food and Drug Administration

NMR Studies on the Conformational Exchange in 1-Benzazepines. **Ngai Hin Lo**, Queensborough Community College - CUNY, Gopal Subramaniam, City University of New York, Queens College, Keith Ramig, Baruch College - CUNY and Sasan Karimi, Queensborough Community College

Synthesis of Biologically Active 1-Benzazepines. **Michelle J. Cho**, Queensborough Community College - CUNY, Gopal Subramaniam, City University of New York, Queens College, Keith Ramig, Baruch College - CUNY and Sasan Karimi, Queensborough Community College

The Oxidized LDL/HDL Ratio Test Is An Automated Immunoassay for Identifying Patients with Coronary Artery Disease. **Tod Schild**, Anne McGarrett, Sanford Moos, Marta Moos, Patricia R. Romano and Harold M. Bates, Shiel Medical Laboratory


The Synthesis of Potential Transdermal Pain Killers. **Constance N. Bezankeng**, Susan Caspa, Oyedotun Oyewole and Nadene Houser-Arfield*, Prince George’s Community College

Novel Organosilane Chemistry for Approaches to Bioactive Ether Targets. **Stephen Philip Fearnley**, The City University of New York - York College and Pedro J. Lory, Lamar University


An NMR Demonstration of Nonequivalent Methylene Hydrogens. **Donald D. Clarke** and Shahrokh Saba, Fordham University

Synthesis of Substituted Benzofuran-2-Carboxylic Acid Ethyl Ester. **Luisa Martinez Troncoso** and Dr. Kenneth Yamaguchi, New Jersey City University

The Transition Between the Closed and Semi-Open Form of Apo HIV-1 Protease through the Rearrangement of Hydrophobic Cores. **Fangyu Ding** and Carlos Simmerling, Stony Brook University

Phototoxicity of 2-Substituted Quinoline Analogs. **J. Cobar**, E Milner, D Goodine, T Heady, W McCalmont and G Dow, Walter Reed Army Institute of Research

Synthesis, Anticonvulsant Activity and Neurotoxicity of New N-1',N-3'-Disubstituted, 2'H,3'H,Spiro-(2-benzofuran-1,4'-imidazolidine)-2',3,5'-Triones. **Pallavi Gutta**, Hardik J Patel, István Lengyel and Ralph A. Stephani, St John's University
Layer-by-Layer Surface Engineering Approach for in Vivo Targeting Delivery of siRNA. **Oleh Taratula**, Paul Kirckpatrick¹, Ronak Savla¹, Ipsit Pandya¹, Tamara Minko²,³ and Huixin He¹,³, (1)Department of Chemistry, Rutgers University, (2)The Ernest Mario School of Pharmacy, Rutgers, the State University of New Jersey, (3)Cancer Institute of New Jersey, 195 Little Albany Street, New Brunswick, NJ 08903

Development of 5HT2A Antagonists Based on the Aporphine Alkaloid Nantenine. **Stevan Pecic** and Wayne Harding, Hunter College

Bioassay-Guided Isolation of African Ethnobotanical Anthelmintics. **Carrie Waterman**, University of the Sciences in Philadelphia

Design and Synthesis of De Novo Paclitaxel Mimics Based on REDOR-Taxol Structure. **Liang Sun**, Department of Chemistry, State University of New York at Stony Brook and Iwao Ojima, Department of Chemistry and Institute of Chemical Biology and Drug Discovery, State University of New York at Stony Brook

Synthesis and SAR Study on Novel Benzimidazoles for Antituberculosis Drug Discovery, Targeting FtsZ. **Kunal Kumar**¹, Ilaria Zanardi², Béla Ruzsicska², Richard A. Slayden³ and Iwao Ojima², (1)State University of New York, stony Brook, (2)Institute of Chemical Biology and Drug Discovery, State University of New York, (3)Colorado State University,

Synthesis and Evaluation of Tumor-Targeting Folate-Taxoid Conjugates. **Manisha Das** and Iwao Ojima, State University of New York at Stony Brook

Design, Synthesis and Biological Evaluation of Novel Tumor-Targeting Conjugates. **Edison S. Zuniga**¹, Xianrui Zhao¹, Shuyi Chen¹, Jin Chen¹, Jingyi Chen² and Iwao Ojima³, (1)State University of New York at Stony Brook, (2)Brookhaven National Laboratory, (3)Department of Chemistry and ICB&DD, State University of New York at Stony Brook

Design, Synthesis and Biological Evaluation of a Novel Tumor-Targeting Drug Delivery System Based on Functionalized SWNT. **Edison S. Zuniga**¹, Shuyi Chen¹, Jingyi Chen¹, Xianrui Zhao¹, Stanislaus S. Wong² and Iwao Ojima³, (1)State University of New York at Stony Brook and Materials Science Department, Brookhaven National Laboratory, (3)Department of Chemistry and ICB&DD, State University of New York at Stony Brook

Coulomb's Law and Trends in Sizes of Atoms and Ions. **Parinbam (RAJ) K. Thamburaj**, Ohio University- Zanesville
Monday, May 19, 2008

Monday, May 19, 2008, 8:00 AM - 12:30 PM

Polymer I (Materials Synthesis)

Sponsor: Center for Engineered Polymeric Materials (CePM)

Library Building, Rm LB-6

Organizer: Moni Chauhan, CUNY-Queensborough Community College
Presider: Nan-Loh Yang, CUNY-College of Staten Island

8:00 Breakfast for Speakers.
9:00 Welcoming Remarks.
9:05 164 Nanostructured Functional Materials Via ATRP with Ppm Amounts COPPER. Krzysztof Matyjaszewski, Carnegie Mellon University
9:40 165 Atom Transfer Radical Polymerization Initiated from Surfaces of Ordered Mesoporous Silicas. Michal Kruk¹, Bruno Dufour², Liang Cao¹, Ewa B. Celer³, Tomasz Kowalewski², Mietek Jaroniec³ and Krzysztof Matyjaszewski², (1)College of Staten Island and Graduate Center, City University of New York, (2)Carnegie Mellon University, (3)Kent State University
10:05 166 Synthesis and Assembly of Nanoparticles for Chemical and Biological Applications. Chuan-Jian Zhong, State University of New York at Binghamton
10:30 Break.
10:40 167 Mother NATURE as a Source of NEW Materials: EVERYTHING Old IS NEW Again. James A. Moore, Rensselaer Polytechnic Institute
11:15 168 Nano-Structures of Polyurea Synthesized in Ionic Liquids. Chien-Yueh Huang, NJIT and Center for Engineered Polymeric Materials, College of Staten Island, CUNY and Mu-Ping Nieh, Canadian Neutron Beam Center, National Research Council
11:40 169 Nitroxide-Mediated Copolymerization of Acrylic Acid Derivatives with Styrene. Milan Maric and Benoit Lessard, McGill University
12:05 170 Preparation and Characterization Nanoneedles of Polystyrene, Polyaniline and Polypyrrole from An Interfacial Polymerization. Kai Su¹, Nurxat Nuraje², Lingzhi Zhang³, I-Wei Chu⁴, Hiroshi Matsui² and Nan-Loh Yang⁵, (1)Ciba Specialty Chemicals, (2)CUNY, Hunter College, (3)College of Staten Island, (4)CUNY, College of Staten Island, (5)CUNY-College of Staten Island
**Monday, May 19, 2008, 8:30 AM - 12:10 PM**

**Analysis of Biomolecules**

Sponsor: Novartis Pharmaceuticals Corporation and the ACS Division of Analytical Chemistry

Medical Arts Building, Rm M-136

Organizers: Rosario LoBrutto, Novartis Pharmaceutical Corporation, Richard Thompson, Novartis Pharmaceutical Corporation

Session Overview: Advances in proteomics and genomics have led to a greater emphasis on the analysis and characterization of biomolecules such as phosphopeptides, monoclonal antibodies, proteins, and SiRNA. There are many analytical technologies available for the determination of the chemical purity, aggregation, physical characteristics, and conformational state of biomolecules as well as studying how the folding/stability of these biomolecules impact biological function. This symposium will discuss the current state of application of these technologies and strategies for analysis of biomolecules from both an academic and pharmaceutical perspective.

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<tr>
<th>Time</th>
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<tr>
<td>8:30</td>
<td>Analytical Ultracentrifugation Analysis in the Biopharmaceutical Drug Development Process. <strong>Steven A. Berkowitz</strong>, Biogen Idec</td>
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<td>9:00</td>
<td>Application of Light Scattering for Analysis of Protein-Protein Interaction and Aggregation. <strong>Ewa Folta-Stogniew</strong>, Yale University</td>
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<td>10:00</td>
<td>Phosphopeptide Analysis by Directly Coupling 2D Pec/tlc with MALDI-TOFMS. <strong>Ira S. Krull</strong>, Northeastern University</td>
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<td>10:30</td>
<td>Break.</td>
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<td>10:40</td>
<td>Ultrasonic Storage Modulus as a Novel Parameter for Analyzing Protein-Protein Interactions in High Protein Concentration Solutions. <strong>Devendra Kalonia</strong>, University of Connecticut</td>
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<td>11:40</td>
<td>The Impact of Conformational Fluctuations on the Analysis and Design of Protein Pharmaceuticals. <strong>Vincent J. Hilser</strong>, University of Texas Medical Branch</td>
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**Monday, May 19, 2008, 8:30 AM - 12:00 PM**

**Antimicrobials**

Sponsor: Ciba Corporation

Science Building, Rm S-112

Organizer: Ted Deisenroth, Ciba Specialty Chemicals Corporation

Session Overview: The antimicrobial symposium will cover new technologies that are effective against bacteria, fungi and viruses. Today there is an ever growing concern of pathogenic organisms developing resistance to antibiotics. This is now evident in the current awareness and concern of the general public to MRSA. New antimicrobial technologies are required to be effective against resistance strains of organisms. Infection is not the only concern of these organisms. Both fungi and bacteria attack coatings and materials affecting not only their appearance, but also durability. Technologies will be presented that could have potential application in medicinal, medical and industrial applications.

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<tr>
<th>Time</th>
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<tr>
<td>8:30</td>
<td>Antimicrobial Substituted Bis-Alkylaminopyrimidines and Their Uses. <strong>Todd Elder</strong>, Ted Deisenroth, Sophie Marquais-Bienewald, Werner Hoelzl, Andrea Pruess and Fadi Khawam, Ciba Specialty Chemicals</td>
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<td>8:55</td>
<td>Metal_Loaded Chitosan Nanoparticles with Antibacterial Activities. <strong>Sudeep Banjade, Thong Vo</strong>, Gerhard Haas and Mihaela Leonida, Fairleigh Dickinson University, Metropolitan Campus</td>
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<td>9:20</td>
<td>Novel Penems Bearing a Bicyclic or Tricyclic Heterocycle on Methylidene Linkage as Broad Spectrum B-Lactamase Inhibitors and Their Mechanism of Inactivation. <strong>Aranapakam M. Venkatesan</strong>, Takao Abe, Hideki Ushiroguchi, Atul Agarwal, Itsuka Yamamura, Osvaldo Dos Santos, Yansong Gu, Fuk-Wah Sum, Zhong Li, Lijing Chen, Yang I. Lin, Gulnaz Khafizova, Peter J. Petersen, Youjun Yang, Patricia Bradford, David M Shlaes and Tarek S Mansour, Wyeth Research</td>
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<td>9:45</td>
<td>Antimicrobial Pharmaceuticals without Resistance. <strong>Robert Engel¹</strong>, Cathy Xiong¹, Karin Melkonian², JaimeLee Rizzo³ and Mary Cloninger⁴, (1)Queens College of the City University of New York, (2)C.W. Post College of Long Island University, (3)Pace University, (4)Montana State University</td>
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<td>10:10</td>
<td>Break.</td>
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<td>10:20</td>
<td>Small Talk: Molecules That Control Quorum Sensing in Vibrio Cholerae. <strong>Martin F. Semmelhack¹</strong>, Megan E. Pomianek¹, William E. Brow¹, Shawn R. Campagna¹, Douglas A. Higgins¹ and Bonnie L. Bassler², (1)Princeton University, (2)Howard Hughes Medical Institute</td>
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<td>10:45</td>
<td>Ceragenins: Small Molecule Mimics of Antimicrobial Peptides. <strong>Paul B. Savage</strong>, Yanshu Feng and Jake Pollard, Brigham Young University</td>
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<td>11:10</td>
<td>Antisense Approaches for Antibiotic Discovery, Discovery of Platensimycin and Platencin. <strong>Sheo Singh</strong>, Merck Research Laboratories</td>
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Bioinorganic Chemistry

Library Building, Rm LB-14
Organizer: Roberto A. Sanchez-Delgado, Brooklyn College and The Graduate Center, CUNY

8:30  Introductory Remarks.
9:10  187 Structured Water Facilitates Ligand Binding in M. Tuberculosis Catalase-Peroxidase. Richard S. Magliozzo, Brooklyn College and the Graduate Center of the City University of New York
9:45  188 Fluorescent Probes for Intracellular Manganese(II). James W. Canary¹, Francesca Gruppi¹, Jian Liang¹, Maksim Royzen¹ and Zhaohua Dai², (1)New York University, (2)Pace University
10:20 Break.
11:45 Concluding Remarks.

Monday, May 19, 2008, 8:30 AM - 12:00 PM

Frontiers in Nanoscience and Nanotechnology – I

Sponsor: Momentive Performance Materials

Medical Arts Building, Rm M-142
Organizers: Bhanu P. S. Chauhan, William Paterson University, Kenrick Lewis, Momentive Performance Materials
Presiders: Bhanu P. S. Chauhan, William Paterson University, Kenrick Lewis, Momentive Performance Materials
Session Overview: The presentations will cover all fundamental aspects of nanoscience

8:30 Welcoming Remarks.
8:35 191 Complex Particles and Patterned Substrates: Opportunities in Life Sciences and Material Science. Joseph M. DeSimone, University of North Carolina at Chapel Hill
9:10 192 Distance and Orientation Effects at Chomophore/Semiconductor Interfaces. Elena Galoppini, Rutgers-Newark

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10:00 Break.

10:08 Presider: Kenrick Lewis.

10:10 194 Characterization Methods for Nanoparticle Properties for Biosystems. Alamgir Karim, National Institute of Standards and Technology

10:45 195 Synthesis of SBA-15 Silica with Very Large Mesopores. Liang Cao¹, Tiffany Man² and Michal Kruk¹, (1)College of Staten Island and Graduate Center, City University of New York, (2)College of Staten Island, City University of New York

11:10 196 The Advantages of Nanoparticulate MRI Contrast Agents, a Review. Marc Walters, New York University

11:35 197 Silylation of Single-Walled Carbon Nanotubes. Tirandai Hemraj-Benny, SUNY@Old Westbury and Stanislaus S. Wong, State University of New York at Stony Brook

Monday, May 19, 2008, 8:30 AM - 12:00 PM

Green Chemistry

Sponsor: The Green Chemistry Institute Pharmaceutical Roundtable

Science Building, Rm S-111

Organizer: John Leazer, Merck & Co.

8:30 198 Copper-Catalyzed Air Oxidation of Cyclopentadienes to Cyclopentadienones. Brian S. Hickory and Paul A. Deck, Virginia Tech

9:00 199 Green Chemistry and Green Workflows at Merck. Roy Helmy, John Leazer, Tim Rhodes, Wes Schafer, David Tellers, Steve Weissman and Jia Zang, Merck & Co., Inc.


10:20 Break.


11:00 202 Supercritical Fluid Chromatography (SFC) as a Green Chromatography Technique for Support in Rapid Development of Pharmaceutical Candidates. Jimmy DaSilva, Henry Shiuhang Yip, Vinod Hegde PhD and Alex Zaks PhD, Schering-Plough Research Institute

11:30 203 An Efficient Asymmetric Synthesis of the Tricyclic Indole Prostaglandin D2 Receptor Antagonist Laropiprant. Peter Maligres, Merck & Co., Inc
Monday, May 19, 2008, 8:30 AM - 12:00 PM

Ionic Liquids II: Properties and Applications

Sponsor: CEM Corporation

Medical Arts Building, Rm M-143

Organizers: James F. Wishart, Brookhaven National Laboratory, Sharon Lall-Ramnarine, Queensborough Community College, CUNY

Session Overview: Research in ionic liquids (ILs) has exploded in recent years because of their great promise in a broad range of applications in chemistry and chemical technology for process and safety improvement and reduction in overall environmental impact. This three-session symposium features the broad spectrum of ionic liquids research conducted in the Middle Atlantic Region.

8:30 204 Ionic Liquids in Extreme Cold: Proposed 100 Meter Lunar Liquid Mirror Telescope. Gregory A. Konesky, SGK Nanostructures, Inc.


9:20 206 Induced Amphotropic and Thermotropic Ionic Liquid Crystallinity in Phosphonium Halides: "Lubrication" by Hydroxyl Groups. Kefeng Ma¹, B. S. Somashekhar², G. a. Nagana Gowda³, C. L. Khetrapal² and Richard G. Weiss¹, (1)Georgetown University, (2)Sanjay Gandhi Post Graduate Institute of Medical Sciences, (3)Purdue University

9:45 207 Exploring the Potential of Amphotropic Liquid Crystals as Orienting Media for NMR Spectroscopy. Astghik A. Shahkhatuni¹,², Kefeng Ma² and Richard G. Weiss², (1)National Academy of Sciences, Armenia, (2)Georgetown University

10:10 Intermission.

10:25 208 Enzyme Electrodes Using Lactate Dehydrogenase Modified with Ionic Liquids. Sujan Shrestha, Amol Kafle and Mihaela Leonida, Fairleigh Dickinson University, Metropolitan Campus

10:50 209 Assessing the Toxic Effects of Ionic Liquids: More Concerns for Environmental Safety. Catherine McEntee¹, Placide Bisangwa¹, Majid Sahin², Xing Li³, James F. Wishart¹, Jinhee Gwon³ and Sharon Lall-Ramnarine³, (1)Kingsborough Community College, (2)Brooklyn College, (3)Queensborough Community College, CUNY, (4)Brookhaven National Laboratory

11:30 210 Use of Zebrafish Embryos in Assessing Ionic Liquid Toxicity. PoKay Ma¹, Ayisha Munawar², Ankita Parikh², Hughton R. Walker¹, Jee-Un Lee¹ and Sharon Lall-Ramnarine², (1)Queens College, CUNY, (2)Queensborough Community College, CUNY
Monday, May 19, 2008, 8:30 AM - 12:00 PM

Physical Chemistry, I

Medical Arts Building, Rm MC-41
Organizers: Jianbo Liu, Queens College of the City University of New York, Ruben Gonzalez, Columbia University

Session Overview: This session will focus on experimental physical chemistry, particularly on spectroscopy and reaction dynamics.

8:30 211 Cosolvent Effects on Hydrophobic Surfaces: Salts and Sugars. Joseph M. Serafin, Jeff Stepan, Abdul Waheed and Jonathan Patete, St. John’s University
8:55 212 Explaining "Temperature"-Dependent Vibrational Spectra of Gas-Phase Proton-Bound Complexes. Xiaohu Li¹, David T. Moore² and Srinivasan S. Iyengar¹, (1)University of Indiana, (2)Lehigh University
9:55 Break.
10:15 214 Flipping Electron Spin without Touching: Collision Induced Intersystem Crossing in CH₂. Gregory E. Hall, Brookhaven National Laboratory
10:50 215 Injecting Single Charges into Nanoscale Molecular Wires. John R. Miller¹, Andrew R Cook¹, Paiboon Sreearunothai¹, Sadayuki Asaoka², Kirk S. Schanze³, Norihiko Takeda¹, Tomokazu Iyoda² and Julia M. Keller³, (1)Brookhaven National Laboratory, (2)Tokyo Institute of Technology, (3)University of Florida
11:25 216 The Electronic Spectroscopy and Anomalous Photophysics of Phenylacetylene. Philip M. Johnson, Stony Brook University

Monday, May 19, 2008, 8:30 AM - 12:00 PM

Tools for Entrepreneurs- from the Kauffman Foundation.

Sponsor: ACS Division of Small Chemical Businesses

Medical Arts Building, Rm MC-29

Session Overview: Representatives of the Kauffman Foundation, the largest foundation dedicated to advancing entrepreneurship in America, will facilitate a variety of exercises that are relevant, practical "just-in-time" information, tools, and resources—designed specifically to assist aspiring and existing entrepreneurs in building companies that innovate and create jobs and wealth.
Monday, May 19, 2008, 9:00 AM - 12:00 PM

ACS Career Management and Development Workshops

Sponsor: ACS Department of Career Management & Development

Medical Arts Building, Rm MC-28

Organizer: Ronald P. D'Amelia, Hofstra University
Workshop Leaders: Valerie J. Kuck, Seton Hall University, Warren Bush, Mm

Session Overview: An array of career services workshops and individual resume reviews will be offered.
9:00 AM: Resume Preparation and Targeting the Job Market for Undergraduates
10:00 AM: Interviewing Skills
11:00 AM: Managing an Effective Job Search

Monday, May 19, 2008, 1:00 PM - 5:00 PM

ACS Resume Reviews

Sponsor: ACS Department of Career Management & Development

Medical Arts Building, Rm MC-28

Organizer: Ronald P. D'Amelia, Hofstra University
Workshop Leaders: Valerie J. Kuck, Seton Hall University, Warren Bush, Mm

Session Overview:
1:00 PM: Resume Preparation for Experienced Chemists
2:00 PM: Individual resume reviews

Monday, May 19, 2008, 1:00 PM - 5:00 PM

Professional Analytical Chemists in Industry: What Does An Analytical Chemist Do?

Sponsor: Procter & Gamble

Medical Arts Building, Rm MC-21

Organizer: Ronald P. D'Amelia, Hofstra University
Workshop Leader: Alan Ullman, Procter and Gamble Company

Session Overview: This Course begins with a discussion of the education requirements and salaries that an analytical chemist may expect in industry. The different roles (including scientific consultant, methods developer, and problem solver) of the industrial analytical chemist are explained. A majority of time is spent on problem solving, both the process and solving real-world problems. Students will learn a “framework” for approaching problems. Time will be available to ask questions on these topics and other related subjects. The Course Notebook includes supplementary material on finding a job, summer employment, etc. The entire course, especially the problem solving, is structured for extensive participation and interaction. It is intended primarily for undergraduate students, but all are welcome.
Monday, May 19, 2008, 1:30 PM - 5:00 PM

Analytical Chemistry, General Session I

Medical Arts Building, Rm M-136
Organizers: Rosario LoBrutto, Novartis Pharmaceutical Corporation, Richard Thompson, Novartis Pharmaceutical Corporation
Session Overview: This session is for general contributions in the field of analytical chemistry.

1:30  217 Development and Validation of HPLC Method for Related Compounds Test in USP Norethynodrel Monograph. Zarema Kassymbek, Shane X. Tan, MinLi Liu and Samir Wahab, US Pharmacopeia


2:10  219 A Stepwise Strategy for Developing a Robust HPLC Separation for a Novel Diabetes Compound. Karthik Jayaraman, Frank Hu, Frank Tomasella and Merill Davies, Bristol Myers Squibb Company

2:30  Break.

2:50  220 Development of DBTAA Grafted Macroporous Monolithic Stationary Phases for HPLC. Kathleen M. Ford and J. Faye Rubinson, Georgetown University

3:10  221 Characterization of Major Degradation Products of An Adenosine 2a Receptor Antagonist Under Stressed Conditions by LC Tandem MS Analysis. Li-Kang Zhang and Birendra Pramanik, Schering-Plough Research Institute

3:30  222 Enhancing the Selective Detection of Dipicolinic Acid (DPA) with a Fluorescent Dye Using a Molecular Imprinting Method. Anne Okafor, Enju Wang, Neil Jespersen and Mostafa Sadoqi, St. John's University

Monday, May 19, 2008, 1:30 PM - 5:00 PM

Best Practices for the Chemical Entrepreneur

Sponsor: ACS Division of Small Chemical Businesses

Medical Arts Building, Rm MC-29
Session Overview: Join our wide spectrum of experienced panelists for a facilitated discussion as to best steps for the chemical entrepreneur. Topics include intellectual property as strategic business assets; alternative forms of financing; and, factors relating to enterprise success.
Monday, May 19, 2008, 1:30 PM - 5:00 PM

Biocatalysis and Biomimetic Catalysis

Medical Arts Building, Rm M-146
Organizer: Kent Kirshenbaum, New York University

1:30  223  Thiamine Inspired Catalysis: Not Just for Breakfast Anymore!. Jeffrey W. Bode, University of Pennsylvania

2:10  224  Organocatalytic Activation Modes for the Asymmetric Alpha-Functionalization of Aldehydes and Ketones. Teresa D. Beeson and David W. C. MacMillan, Merck Center for Catalysis, Princeton University

2:35  225  Folded Peptides for Asymmetric Catalysis: Some Structures and Some Functions. Scott J. Miller, Yale University

3:15  Break.


4:15  228  Biomimetic Catalysis. Ronald Breslow, Columbia University

Monday, May 19, 2008, 1:30 PM - 5:00 PM

Delaware Valley Chromatography Forum Student Award

Sponsor: Chromatography Forum of Delaware Valley

Medical Arts Building, Rm M-140

Session Overview: The annual CFDV Student Award Symposium provides graduate and undergraduate students with an opportunity to present their research in the field of separation science. Though many participants are pursuing separation science as their major course of study, students in the areas of medicine, biochemistry, engineering and organic chemistry have successfully presented papers describing areas of research that involve separations.

1:30  Introductory Remarks.

1:35  229  Separation of Water Soluble Vitamins by UHPLC. Michael J. Bozym, Michelle L Owens, Anna Glinko and Karyn M. Usher, West Chester University

1:55  230  Extra Column Effects as a Function of Flow Rate. Casey M. Mulcahy, Scott H. Snyder and Karyn M. Usher, West Chester University

2:35  Intermission.

2:55  232 Lost Protein Technology for Proppant and Catalyst Manufacture. Christopher J. Morrison and Gennaro J. Maffia, Widener University

3:15  233 Examining Chiral Separations with Bile Salt Micelles Using MEKC and NMR. Alyson M. Cobb, Kyle W. Eckenroad, Gregory A. Manley, David Rovnyak and Timothy G. Strein, Bucknell University

3:35  234 Investigation of Buffering and Mixing Conditions for the Jaffe Reaction with Capillary Electrophoresis. Sarah A. Schubert¹, John W. Stahl² and Timothy G. Strein¹, (1)Bucknell University, (2)Geneva College

3:55  235 Improving the Sensitivity of Electrophoretically Mediated Micro Analysis (EMMA) for the Determination of Creatinine. Ranasinghe K. Sampath¹, John W. Stahl² and Timothy G. Strein¹, (1)Bucknell University, (2)Geneva College

Monday, May 19, 2008, 1:30 PM - 5:00 PM

Frontiers in Nanoscience and Nanotechnology - Nanoscience, II

Sponsor: Momentive Performance Materials

Medical Arts Building, Rm M-142

Organizers: Bhanu P. S. Chauhan, William Paterson University, Kenrick Lewis, Momentive Performance Materials

Presiders: Michal Kruk, College of Staten Island and Graduate Center, City University of New York, Moni Chauhan, CUNY-Queensborough Community College, Frieder Jäkle, Rutgers University-Newark

1:30  Presiders: Moni Chauhan, Frieder Jäkle, Michal Kruk.


2:10  237 Molecular Network Reinforcement of Sol-Gel Glasses. Geraud Dubois¹, Willi Volkser¹, Teddie Magbitang¹, Robert D. Miller¹, David M. Gage² and Reinhold H. Dauskardt², (1)IBM, (2)Stanford University

2:35  238 Organic Rigid-Rods with Para- and Meta- Conjugated Bridges for Semiconductor Nanoparticles Sensitization. Olena Taratula and Elena Galoppini, Rutgers-Newark

3:00  Break.

3:15  239 Nano-Size Particles of Porous Metal Oxides and Their Applications. Steven L. Suib, University of Connecticut

3:50  240 Molecular Grafting of Metallic Solutions. Moni Chauhan, Devindra Tilakdhari and Maninder Kaur, CUNY-Queensborough Community College

4:15  241 Nanostructured Organoboron Block Copolymers. Frieder Jäkle¹, Chengzhong Cui¹, Yang Qin¹ and Edward M. Bonder Sr.², (1)Rutgers University, (2)Rutgers University-Newark

4:35  242 Lab on a Chip: The Role of ProteinChip Arrays in the Discovery of Cardiovascular Biomarkers. Bishambar Dayal, William Paterson University and Norman H. Ertel, University of Medicine and Dentistry of New Jersey
Monday, May 19, 2008, 1:30 PM - 5:00 PM

Ionic Liquids III: Dynamical Effects in Ionic Liquids

Sponsor: CEM Corporation

Medical Arts Building, Rm M-143

Organizers: James F. Wishart, Brookhaven National Laboratory, Sharon Lall-Ramnarine, Queensborough Community College, CUNY

Session Overview: Research in ionic liquids (ILs) has exploded in recent years because of their great promise in a broad range of applications in chemistry and chemical technology for process and safety improvement and reduction in overall environmental impact. This three-session symposium features the broad spectrum of ionic liquids research conducted in the Middle Atlantic Region.

1:30  243  Electric Field Responsive Ionic Liquid Polymers. Arthur W. Snow and Holly Ricks-Laskoski, Naval Research Laboratory

1:50  244  Understanding Solvent Polarity in Ionic Liquids. Mark Kobrak, Brooklyn College and The Graduate Center of the City University of New York

2:30  245  Intermolecular Dynamics and Solvation in Ionic Liquids. Edward W. Castner Jr.¹, Tatiana A. Fadeeva¹, Heather Y Lee¹, Hideaki Shirota² and James F. Wishart³, (1)Rutgers, The State University of New Jersey, (2)Chiba University, (3)Brookhaven National Laboratory

3:10  Intermission.


4:00  247  Heterogeneous Solute Kinetics in Ionic Liquids. Mark Maroncelli, Hui Jin, Xiang Li and Sergei Arzhantsev, The Pennsylvania State University

4:40  248  Carbon Dioxide and Molecular Nitrogen as Switches Between Ionic and Uncharged Room-Temperature Liquids. Tao Yu, Georgetown University

Monday, May 19, 2008, 1:30 PM - 5:00 PM

Metal Complexes in Chemotherapy and Diagnostics

Library Building, Rm LB-14

Organizer: Roberto A. Sanchez-Delgado, Brooklyn College and The Graduate Center, CUNY

1:30  Introductory Remarks.

1:35  249  Platinum Complexes as Anticancer Agents. Nicholas Farrell, Virginia Commonwealth University

2:15  250  Inorganic Radioisotopes for Molecular Imaging and Radiotherapy. Lynn C. Francesconi, Hunter College and the Graduate Center of the City University of New York

2:55  Break.
Chemically Inert Metal Complexes as Anticancer Agents. **Eric Meggers**, Phillips-Universitat

Ruthenium Complexes as Potential Antiparasitic and Antitumor Agents. **Roberto A. Sanchez-Delgado**, Brooklyn College and The Graduate Center, CUNY

Concluding Remarks.

**Monday, May 19, 2008, 1:30 PM - 5:00 PM**

**Physical Chemistry, II**

Medical Arts Building, Rm MC-41

Organizers: Ruben Gonzalez, Columbia University, Jianbo Liu, Queens College of the City University of New York

Session Overview: This session will bring together experimental biophysical chemists who are using advanced spectroscopies and microscopies in order to gain mechanistic insights into complex biological systems.


2:00 254 Biophysical Insights into the Mechanism of Viral Protein Synthesis. **Dixie J. Goss**, Mateen A. Khan, Artem Domashevskiy and Hasan Yumak, Hunter College CUNY

2:30 255 How Does a Bacterium Secrete Folded Proteins across the Outer Membrane - a Cryo-EM Study. Chunyan Tang¹, Nadine Henderson², David G. Thanassi² and **Huilin Li¹**, (1)Brookhaven National Laboratory, (2)Stony Brook University

3:00 256 NMR Studies of Protein Dynamics. **Ann E. McDermott**, Columbia University

3:30 Break.


4:10 258 Coupled Proton Diffusion and Binding within Bacterial Spore Nanocompartments. **Sergey V. Kazakov** and Elizabeth M. Bonvouloir, Pace University

4:35 259 Binding of Modified Alkane Polymers to Human Recombinant TLR-2 Receptor Monitored by Intrinsic Tyr Fluorescence. **Cristina C. Clement**, Albert Einstein College of Medicine (AECOM)

**Monday, May 19, 2008, 1:30 PM - 5:30 PM**

**Polymer II (Material Synthesis)**

Sponsor: Center for Engineered Polymeric Material (CePM)

Library Building, Rm LB-6

Organizer: Moni Chauhan, CUNY-Queensborough Community College

Presider: Chwen-Yang Shew, CUNY-College of Staten Island

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1:30  260  Complex Particles and Patterned Substrates: Future Opportunities in Life Sciences and Material Science. **Joseph M. DeSimone**, University of North Carolina at Chapel Hill

2:05  261  Carbon Nanostructures Made by Focused Ion Beams on Carbonaceous Substrates. **Alexander Zaitsev**, College of Staten Island

2:25  262  Effect of Semiflexibility on the Conformational Hysteresis of a Giant DNA. **Chwen-Yang Shew**, CUNY-College of Staten Island and Higuchi Yuji, Kyoto University

2:45  263  ADMET (acyclic diene metathesis) Synthesis of Heteroatom Containing Polymers. **Ralf M. Peetz** and Narayan Mukherjee, CUNY-College of Staten Island

3:05  265  Synthesis of Protein-Polymer Hybrids. **Krishnaswami Raja**, Department of Chemistry, College of Staten Island, CUNY

3:20  264  Engineering Nanoparticles for Rendering Polymer Blends Flame Retardant:. S. Pack, SUNY Stony Brook, **M. H. Rafailovich**, Stony Brook University, E. Weil, University of Akron and T. Kashiwagi, NIST

3:55  266  Soft-Template Synthesis of Conducting Polymer Hollow-Nano-Spheres and the Study of Release Control Via pH Value. **I-Wei Chu**, Kai Su and Nan-Loh Yang, (1)CUNY-College of Staten Island, (2)Ciba Specialty Chemicals

4:15  267  From Oligo(phenylene vinylene)S to Conjugated Polyazines. **Narayan Mukherjee** and Ralf M. Peetz, CUNY-College of Staten Island

4:35  268  Luminescent Polystyrene: Synthesis and Characterization. **Kshitij Parab** and Frieder Jäkle, Rutgers University

**Monday, May 19, 2008, 1:30 PM - 5:00 PM**

**Synthesis of Complex Biologically Active Molecules**

Sponsor: ACS Division of Organic Chemistry

Science Building, Rm S-112

Organizers: Christian Rojas, Barnard College, David R. Mootoo, Hunter College, CUNY

Session Overview: Complex biologically active molecules have traditionally attracted the attention of synthetic chemists because they provide a showcase for new synthetic methodology, raise the necessity for analogs for biological studies, or simply present compelling synthetic challenges. This symposium will feature new technologies that enable the preparation of complex molecules as well as syntheses of specific molecular targets. Presentations from both academic and industrial research will provide an opportunity to compare the interests and strategies in these settings.

1:30  269  Total Synthesis Complex Galbulimima Alkaloids. Discovery of a Himbacine Based Antithrombotic Agent SCH 530348. **Samuel Chackalamannil**, Schering-Plough Research Institute

2:10  270  Strategies and Methods for the Synthesis of Natural Products. **Kathlyn A. Parker**, Stony Brook University

2:45  271  Multicatalysis: A Platform for Increasing Synthetic Efficiency and Inspiring Discovery. **Tristan H. Lambert**, Columbia University
3:20 Break.

3:40 272 COPPER-Promoted C-Heteroatom Bond Cross-Coupling Via Boronic Acids: Chan-Lam Coupling Reaction. Patrick Y. S. Lam, Bristol-Myers Squibb

4:15 273 Exploring Hetero-Annulation Strategies for Complex Alkaloid Synthesis. David Y. Gin, Memorial Sloan-Kettering Cancer Center

Monday, May 19, 2008, 2:00 PM - 5:00 PM

Probeware Workshop for Undergraduate Educators

Science Building, Rm S-405
Organizers: Lew Malchick, Education, Pedro Irigoyen, Queensborough Community College

Monday, May 19, 2008, 5:30 PM - 6:30 PM

Plenary Lecture II: Roald Hoffmann, Cornell University

Medical Arts Building, Rm M-136
Organizer: John R. Sowa, Seton Hall University

Session Overview: Diamond anvil cell and shock-wave technologies now permit the study of matter under multimegabar (i.e. several hundreds GPa) pressures. The properties of matter in this pressure regime differ drastically from those known at 1 atm. Just how different chemistry is at high pressure and the role that a chemical intuition for bonding and structure can have in understanding matter at high pressures will be explored in this lecture. I will discuss in detail an overlapping hierarchy of responses to increased density, consisting of (a) squeezing out van der Waals space (for molecular crystals); (b) increasing coordination; (c) decreasing the bond length of covalent bonds and the size of anions; and (d) an extreme regime of electrons moving off atoms and new modes of correlation. Examples of the startling chemistry and physics that emerge under such extreme conditions will alternate in this account with qualitative chemical ideas about the bonding involved.

5:30 274 The Chemical Imagination at Work in Very Tight Places. Roald Hoffmann, Cornell University

Monday, May 19, 2008, 6:30 PM - 8:30 PM

Monday Night Barbecue/mixer

Student Union Building, Upper

Session Overview: This all-you-can-eat dinner follows the evening plenary lecture and takes place adjacent to the poster session.
Monday, May 19, 2008, 7:00 PM - 8:30 PM

Poster Session II

Student Union Building, Upper

Organizers: Irina Rutenburg, Queensborough Community College, Marie Thomas, Queens College, CUNY

275 Structural Effects of Interstrand Crosslinks on DNA through Molecular Dynamic Simulations. Arthur J. Campbell, Angelo Guainazzi, Orlando D. Scharer and Carlos L. Simmerling, Stony Brook University

276 Exploring Structure and Biochemistry of Nitrogen Mustard Interstrand Crosslinks through Synthetic Analogs. Angelo Guainazzi and Orlando Schärer, SUNY Stony Brook

277 The Relationship Between the Ionic Structure and Viscosity in the Room-Temperature Ionic Liquids. Hualin Li, Mufat Ibrahim, Ismail Ageremi and Mark Kobrak, Brooklyn College and The Graduate Center of the City University of New York

278 Synthesis of Imidazolium and Pyridinium Ionic Liquids for Toxicity Studies. Xing Li, Jinhee Gwon, James F. Wishart, Catherine McEntee and Sharon Lall-Ramnarine, (1)Queensborough Community College, CUNY, (2)Brookhaven National Laboratory, (3)Kingsborough Community College

279 An Electrospray Ionization Guided-Ion-Beam Tandem Mass Spectrometer for Studying Gas-Phase Biological Ion-Molecule Reactions. Fang He, Yigang Fang and Jianbo Liu, Queens College of the City University of New York

280 Synthesis of Pyrrolidinium Ionic Liquids for Toxicity Studies. Jinhee Gwon, Xing Li, James F. Wishart, Catherine McEntee and Sharon Lall-Ramnarine, (1)Queensborough Community College, CUNY, (2)Brookhaven National Laboratory, (3)Kingsborough Community College

281 Instrument Control and Data Acquisition for a Guided-Ion-Beam Tandem Mass Spectrometer. Yigang Fang, Fang He and Jianbo Liu, Queens College, City University of New York

282 Synthesis and Toxicity to Zebra Fish of Mono- and Diammonium Phosphate and Bis(trifyl)Imide Ionic Liquids. Ayisha Munawar, Ankita Parikh, Houghton Walker, Jasmine Hatcher, Xing Li, Sofya Penkhasova, Kijana Kerr, Pokay Ma and Sharon Lall-Ramnarine, (1)Queensborough Community College, CUNY, (2)Brooklyn National Laboratory, (3)Kingsborough Community College

283 Nitroxide-Mediated Polymerization of Poly(ethylene glycol) Acrylate Comb-Like Polymers. Milan Maric and Benoit Lessard, McGill University

284 Synthesis of Mixed-Valence Compounds with Metal-Metal Bonds. Amy Schauss and Jack Lu, University of Houston-Clear Lake

285 Determination of Methamphetamine and Amphetamine in Urine Using Ionic Liquid Based Headspace Solid-Phase Microextraction (HS-SPME) and Gas Chromatography-Mass Spectrometry (GC-MS). Yi He, Jeremy Pohl and Stephanie Petch, John Jay College, City University of New York

286 Properties of DABCO Containing Ionic Liquids. Kijana Kerr, Marie Thomas, Gopal Subramaniam, James F. Wishart and Sharon Lall-Ramnarine, (1)Queensborough Community College, CUNY, (2)Queens College, CUNY, (3)Brookhaven National Laboratory

287 The Quantitative Determination of the Minimum Inhibitory Concentration of Silver Ions to Bacterial Growth. David E. Marx and John J. Mercuri, The University of Scranton

Carbon Nanotubes Filled with Copper Nanoparticles. James Giammarco¹, Patricia Valenzuela¹, Sebastian Oswald¹, Vadym Mochalin¹, Farhad Forohar² and Yury Gogotsi¹, (1)Drexel University, (2)NSWC, Indian Head Division

Synthesis and Characterization of Transition Metal Complexes of Pendant Arm Macroycles and Tripodal Ligands. Savitri Chandrasekhar, Rick Chen, Jeff Chan and Amanda Lee, University of Toronto Scarborough

Ruthenium(II) Complexes of Some Tripodal Amine Ligands. GorDan T. Reeves¹, Anthony W. Addison¹, Vitaly V. Pavlishchuk², Allen Hunter³ and Matthias Zeller³, (1)Drexel University, (2)Institute of Physical Chemistry, (3)Youngstown State University

Colloidosomes:"Smart" Materials for Biomedical Applications. Rachel Rosenberg, Drexel University

Organogold (III) Iniminophosphorane Complexes and Study of Their Cytotoxicity against Solid Tumor Cells. Neha Shaik, Idline Augustin and Maria Contel, Brooklyn College and the Graduate Center, The City University of New York

Ground State Association of Benzo[B]Fluorenone with Ethanol and Trifluoroethanol. Aaron Halpern and Brian Williams, Bucknell University


Arene-Ru-Chloroquine Complexes as Potential Antimalarial Agents. Chandima S.K. Rajapakse¹, Alberto Martinez², Becky Naoulou² and Roberto A. Sanchez-Delgado², (1)Brooklyn College, CUNY, (2)Brooklyn College

Greening the Organic Chemistry Laboratory at Widener University. Kaitlyn Gerhart and Loyd D. Bastin, Widener University

Mechanism of Antimalarial Action of the Ruthenium(II)-Chloroquine Complex [RuCl₂(CQ)]₂. Alberto Martinez¹, Chandima S.K. Rajapakse², Becky Naoulou¹ and Roberto A. Sanchez-Delgado³, (1)Brooklyn College, (2)Brooklyn College, CUNY, (3)Brooklyn College and The Graduate Center, CUNY

Incorporation of Cisplatin, Carboplatin and Oxaliplatin into a Trinuclear Iron-Platinum Intervalent Charge Transfer Complex: Options for the Photochemical Delivery of Drug to Targeted Sites. Kate Keets and Andrew Bocarsly, Princeton University

Parvalbumin in Fish Muscle: Cation Binding Properties and Its Role in Muscle Relaxation. Mohit Sirohi, Steven Youseff, Kristen Sands, David Coughlin and Loyd D. Bastin, Widener University

Trinculear Iron-Platinum Complexes as Chemotherapeutic Agents: Increasing Water Solubility. Amanda Tricarico and Andrew B. Bocarsly, Princeton University

Light Activated De Novo Proteins Using Phthalocyanines. Andrew C. Mutter and Ronald L. Koder, The City College of New York


The Properties of the Amyloid Beta Protein Coated Gold Colloidal NANOPARTICLES. Sophia H. Hahn, Hyunah Cho, Nicole Briglio and Kazushige Yokoyama, State University of New York at Geneseo (SUNY Geneseo)

Benzyl Imidazolium Porphyrins. Weici Fang, Maung-Tin Htoo Kyaw, Rukya Ali, Virginia Seng, Xiulan Wang and Alison Hyslop, St. John's University

307 Synthesis of Porphyrin-Heterocycle-Osmium Complexes for Use as Light Harvesting Compounds. **Elissa Ramcharitar**, Samantha Blondel, Carina Hernandez, Elise Megehee and Alison Hyslop, St. John's University

308 Theoretical Calculations of C60 Isomers: A New Stable? or Unstable? Isomer C60[3,4,5]. **John R. Sowa Jr.,** Jacqueline Rodriguez, Johnna Campbell and Theresa Wertheimer, Seton Hall University

309 Does the Chain Length of Alkyl 4-Hydroxybenzoates Alter Phenolic Pka Values?. **John J. Sczepanski**1,2, Leopold May1, Jason R. Kinder2 and Fransis B. Pedersen2, (1)The Catholic University of America, (2)Hood College

310 Polyaniline Nanofibers and Composites with Polymer-Stabilized Gold Nanoparticles. **Asifa Noreen**1, William L'Amoreaux2 and David M. Sarno1, (1)Queensborough Community College - CUNY, (2)College of Staten Island - CUNY

311 Morphological Effects of Ring-Substitution on Polyaniline Nanomaterials. **Carolina Chaves Prado** and David M. Sarno, Queensborough Community College - CUNY

312 Effects of Commonly Used Cosmetic Industry Preservatives on Water Activity. Karen Root Caldwell1, **Michael A. Lull**2 and Janet R. Bass2, (1)Pace University -- Westchester, (2)San-Mar Laboratories, Inc.

313 Identification of Clinical Candidate OSI-906 as a Potent, Selective and Orally Bioavailable IGF-1R Inhibitor. **Brian Volk**, Mark J. Mulvihill, Elizabeth Buck, Andrew Cooke, Andrew Crew, Hanqing Dong, Alexandra Eyzaguirre, Maryland Franklin, Lixin Feng, Kenneth W. Foreman, Qun-Sheng Ji, Darla Landfair, Yunyu Mao, Matthew O'Connor, Caroline Pirritt, Stacia Silva, Kam Siu, Arno Steinig, Kathryn Stolz, Paula Tavares and Doug Werner, OSI Pharmaceuticals

314 Synthesis of C-Glycosides of Glycoinositols Pseudodisaccharides. **Sunej Hans** and David Mootoo*, City University of New York, Hunter College


316 Absolute Configuration Determination of a Light Harvesting Porphyrin by Circular Dichroism Tweezer Methodology. **Troy, M. McCord**1, Alicia Canzian1, Gloria Proni1, Ana G. Petrovic2, Nina Berova2 and Teodor S. Balaban3, (1)John Jay College of Criminal Justice, (2)Columbia University, (3)Karlsruhe Institute of Technology, Forschungszentrum Karlsruhe

317 Analysis of Vitamin "C" in Fruits and Vegetableas. **Rana Said**, Syamala Ranganathan, and Pedro Irigoyen, Queensborough Community College

318 Analysis Of Vitamin "C" in Commercial Juices. **Shaun Bruney**, Syamala Ranganathan, and Pedro Irigoyen, Queensborough Community College

319 Comparison of Hemoglobin in Thin Films and in Hydrogels Formed by Photo Initiated Polymerization on Glassy Carbon. **Amos Mugweru** and Christian Schnarr, Rowan University


321 Design, Synthesis and Applications of Metal Oxide Nanocomposites. **Christopher P. Avanzato**1, Marsiyana M. Henricus1, Karl R. Fath2 and Ipsita A. Banerjee1, (1)Fordham University, (2)Queens College

322 Design and Synthesis of Nanotube Bound Biocompatible Hydrogels. **Evan M. Smoak** and Ipsita A. Banerjee, Fordham University

83

324 Xanes Study of Cross Sectional Distribution of Charge States and Local Structural Environments of Iron in Porous Vycor Glass. S. Amarasinghe, D Sunil and H.D Gafney, Queens College

325 Hf(IV) and Zr(IV) Porphyrins as Dyes on Semiconductor Surfaces. Ivana Radivojevic¹, Alexander Falber¹, Benjamin P. Burton-Pye² and Charles Drain¹, (1)Hunter College and Graduate Center of the City University of New York, (2)Hunter College

326 Porphyrinoid Derivatives and Fullerene C60 for Light Harvesting Materials. Alessandro Varotto, Charles Drain and Joao Tome, Hunter College and Graduate Center of the City University of New York

327 The Analysis of the Interactions and Complexation of Polycyclic Aromatic Hydrocarbons and Cyclodextrin Using Electrospray Ionization Mass Spectrometry. Andrew Harron¹, Catherine Bentzley¹, Preston Moore¹, Zhiwei Liu¹, Jhenny Galan¹ and Darryl Davis², (1)University of the Sciences in Philadelphia, (2)Cenocore

328 New Approach to 3,5-diamino-sugars from 4,6-dodeoxy-1,2-O-isopropylidene-D-glycero-pent-4-enopyranos-3-ulose. Zbigniew J. Witczak, Arthur Jankowski and David Lorchak, Wilkes University, Nesbitt School of Pharmacy

329 Synthesis of 3-Substituted Coumarins by the Knoevenagel Condensation Reaction. Mariam N. Israiel, New Jersey City University

330 The Synthesis of Biodiesel. Shane E. Smith¹, Josh M. Gesford¹, Kathleen M. Halligan¹, Gregory P. Foy¹ and Gary A. Sigel², (1)York College of Pennsylvania, (2)Armstrong World Industries

331 New Synthetic Probes for Understanding Molecular Recognition during Olfaction. Yadi Li¹, Zita Peterlin², Stuart Firestein², Grant Sun¹ and Kevin Ryan¹, (1)City College of New York, CUNY, (2)Columbia University

332 Formation of Novel Fused-Ring System by Rhodium-Catalyzed Cycloaddition Reactions. Yu Han Gary Teng, Joseph Jr. Kaloko and Iwao Ojima, State University of New York at Stony Brook

333 The Synthesis and Rearrangement of Carbazole Sulfonamide and Imidobenzyl Sulfonamide to the Corresponding Sulfones. Taylor W. Meek, James R. Mckee and Murray Zanger, University of the Sciences in Philadelphia

334 Sodium Ion Dependence and Deuterium Solvent Isotope Effect Studies of the Inhibition of Human á-Thrombin by Hirudin and NAPAP. Ildiko M. Kovach, John Paul Sheehy and Krystal Dole, The Catholic University of America

335 Determination of Conditions for the Dimerization of Pokeweed Antiviral Protein. Alexia Tussay¹, Amy E. Baldwin², and Diana E. Friedland³, (1)John Jay College of Criminal Justice, (2) Pace University, (3)John Jay College of Criminal Justice and the Graduate Center of the City University of New York

336 Expression Levels of PKC Substrates in Human Breast Cancer Cells. Guy Surpris¹, Susan A. Rotenberg² and Regina Sullivan¹, (1)Queensborough Community College, (2)Queens College

337 Investigations into the Conversion of Cellulose to Simple Sugars for Ethanol Production. Lisa A. Williams, York College of Pennsylvania

338 Study of the Characteristics of Modified PF Resins from Microwave Synthesis. Meghan M. MacIntyre, David Irwin and Adango Miadonye, Cape Breton University

339 Sugarcane as an Energy Crop for USA. Sohan L. Jindal, Punjab Agricultural University
Engineering Fluorinated Phosphotriesterases to Detoxify Organophosphates. Peter James Baker and Jin Kim Montclare, Polytechnic University

Modified Gum Acacia in Emulsions and Spraydried Flavors. Florian M. Ward and Stephen A. Andon, TIC GUUMS, Inc.

Protection of Enzymes in Harsh Aqueous and Organic Environments. Andreas Mylonakis, Indranil Mukherjee, Sudipto Das, Shuxi Li and Yen Wei*, Drexel University

Platinum and Palladium Metallic Solutions. Moni Chauhan and Devindra Tilakdhari, CUNY-Queensborough Community College

The NYSTAR Sponsored Center for Engineered Polymeric Materials. Andrew Auerbach, CUNY-College of Staten Island

Rational Design Methodology for Porphyrin Binding Proteins. Christopher Negron, Christian Fufezan and Ronald Koder, The City College of New York

Synthesis and Self-Assembly of Boron-Containing Block Copolymers. Chengzhong Cui, Yang Qin, Edward M. Bonder and Frieder Jäkle, Rutgers University-Newark

When Is the Histone Protein Bound to a Chain End of a Giant DNA Molecule?. Chwen-Yang Shew and Andy Khoo, CUNY-College of Staten Island

A New Catalyst for Efficient and Selective Conversion of Silanes to Silanols. Moni Chauhan*, Abhshek Roka1, Alok Sarkar2 and Bhanu P. S. Chauhan*, (1)CUNY-Queensborough Community College, (2)William Paterson University

Synthesis and Characterization of Chromophore-Grafted Polybutadienes. Bhanu P. S. Chauhan*, Alok Sarkar, Esra Cinar and Mauhanad (George) A. Bittar, William Paterson University

Chemical/Thermal Reduction of Gold and Silver Salts: A New Route to in-Situ Nanoparticle Synthesis and Stabilization. Moni Chauhan and Maninder Kaur, CUNY-Queensborough Community College

Synthesis and Characterization of Polystyrene Supported Borane Complexes PS-BH2•D. Ami Doshi, Yang Qin and Frieder Jäkle, Rutgers University

High-Yield Acyclic Diene Metathesis (ADMET) Synthesis of Easily Accessible PPV Oligomers. Narayan Mukherjee and Ralf M. Peetz, CUNY-College of Staten Island

Formation and Characterization of Donor-Acceptor Complexes of Polyamide 6 as a Mean to Modify the Morphology and Extensibility. Hsin Ho and Nadarajah Vasanthan, Long Island University

Cationic Polymerization of Norbornadiene. Narmandakh Mijd-Taylor and Ralf M. Peetz, CUNY-College of Staten Island

Functionalization of Si(100) Surfaces with Rigid-Rod Oligo(p-phenylenevinylene)S. Chivin Sun and Ralf M. Peetz, CUNY-College of Staten Island

n-Stacking of Soluble N-Type Semi-Conductors. Min Zhi Chen, Yingfeng Tu and Shi Jin, CUNY-College of Staten Island

Synthesis and Characterization of Oxazoline Block Copolymers for Photovoltaic Devices. Hongmei Li and Morton Litt, Case Western Reserve University

High Performance Size-Exclusion Chromatography (SEC) Column for Water Soluble Polymers. Ken Tseng1, Ryuji Takahashi2, Ritsuko Ohno2 and Masatoshi Murakami2, (1)Shodex, (2)Showa Denko, K.K.
DNA Functionalized Carbon Nanotubes as Active Stabilizers: Conducting Polymer Nanocomposites with Enhanced Stability. **William Cheung**, Yufeng Ma, Guangru Mao and Huixin He, (1)Rutgers University, (2)Rutgers University, Newark Campus

Synthesis and Characterization of Fluorene-Based Organoboron Quinolate Polymers. **Haiyan Li** and Frieder Jäkle, Rutgers University

Preparation and Characterization of Nano-Hollow Spheres of Conducting Polymer by “Micro-Interfacial Polymerization” and the Study of Controlled Release from Them. **I-Wei Chu**, College of Staten Island/CUNY, Kai Su, Ciba Specialty Chemicals and Nan-Loh Yang, CUNY-College of Staten Island

Biocompatible, Hydrogen-Bonded Multilayers of a Polyphenol with High pH-Stability. **Irem Erel Unal** and Svetlana Sukhishvili, Stevens Institute of Technology

An Odd Couple: A Designed Protein:Natural Protein Chimera. **Jessica A. Norman**, Andrew C. Mutter and Ronald L. Koder, The City College of New York

De Novo Designed Safranine Enzymes. **Gheevarghese Raju**, Graduate Student and Ronald L. Koder, The City College of New York

Multi-Responsive Polyelectrolyte Diblock Copolymer Micelles. **Zhichen Zhu**, Li Xu and Svetlana Sukhishvili, Stevens Institute of Technology

Rheology and Confocal Reflectance Microscopy as Complementary Probes of the Kinetics of Collagen and Collagen/hyaluronan Gelation. **Yali Yang** and Laura J. Kaufman, Columbia University
Tuesday, May 20, 2008

Tuesday, May 20, 2008, 7:30 AM - 8:30 AM

Directors Breakfast

Sponsor: American Chemical Society

Oakland Cafeteria

Organizer: Madeleine M. Joullie, University of Pennsylvania

Session Overview: Your District Directors (Madeleine Joullie, District III and Anne O’Brien, District I) invite you to complimentary breakfast and a conversation about ACS. You’ll hear up-to-date ACS news but, more importantly, have an opportunity to give your views and suggestions. How should ACS best respond to globalization? How can ACS best create a community of scientists addressing world problems? Come with your ideas and questions. Participation and conversation are the goals!

Tuesday, May 20, 2008, 8:00 AM - 12:30 PM

Polymer III (Functional Materials)

Sponsor: Center for Engineered Polymeric Materials (CePM)

Library Building, Rm LB-6

Organizer: Moni Chauhan, CUNY-Queensborough Community College

Presider: Frieder Jaekle, Rutgers University

8:00 Breakfast for Invited Speakers.

9:00 Welcoming Remarks.

9:05 367 Living Photocontrolled and Living Supramolecular Polymerizations as Routes to Functional Metallopolymers. **Ian Manners**, University of Bristol

9:40 368 Tightening the Belt. **Colin Nuckolls**, Columbia University

10:00 369 In-Situ Polymerization of a Thin Skin of Self-Doped Conducting Polymer to Improve the Electronic Performance of Carbon Nanotube Networks. **Huixin He**, Rutgers University, Newark Campus

10:20 Break.

10:30 370 Poly(ferrocenylenes) with Three- and Four-Coordinate Boron Bridges. **Matthias Wagner**, J. W. Goethe-Universität

11:05 371 Iridium Containing Phosphorescent Polymers for OLED Applications. **Marcus Weck**, New York University and Alpay Kimyonok, Georgia Institute of Technology

11:25 372 Selective Olefin and Polyolefin Stiching to Silicon. **Bhanu P. S. Chauhan***, Alok Sarkar and Bharthi Balagam, Engineered Nanomaterials Laboratory, William Paterson University

11:45 373 Nanoparticle Applications to Wool Part I: Synthesis and Characterization. **Justin J. Martin**, Jeanette M. Cardamone and Peter Irwin, USDA ARS Eastern Regional Research Center
**Tuesday, May 20, 2008, 8:30 AM - 12:00 PM**

**Applications of Organometallic Chemistry**

Sponsor: Strem Chemicals, Air Products, Boulder Scientific

Medical Arts Building, Rm M-134

Organizer: Chip Nataro, Lafayette College

Session Overview: Organometallic chemists from inorganic and organic backgrounds will discuss how organometallic compounds are being used to solve new and interesting problems in their labs.

8:30 374 Tuning the Electronic and Structural Properties of a Ferrocene Based Bifunctional Lewis Acid. **Thilagar Pakkirisamy**, Krishnan VenkataSubbaiah and Frieder Jäkle, Rutgers The State University Newark

8:50 375 Anchored Wilkinson's Catalyst: Comparison with the Homogeneous Catalyst and Supported Rhodium with Respect to Reaction Selectivity. **Robert L. Augustine**, Setrak K Tanielyan, Norman Marin and Gabriela Alvez, Seton Hall University

9:10 376 Novel Approaches to the Cross-Coupling Reactions. Jing Liu, Yingsheng Zhao, Xiancai Luo and **Aiwen Lei**, Wuhan, China

9:30 377 Regioselectivity of Platinum-Catalyzed Hydrosilylation of Alkynes in Silyl-Substituted Ferrocenes and Related Sandwich Compounds. **John B. Sheridan** and Rhyan Terrado, Rutgers University


10:10 Intermission.


10:45 380 Catalysis as Means to Perform Organic Synthesis: Cheaper, Cleaner and Greener. **John R. Sowa Jr.**, Seton Hall University

11:10 381 Tandem Asymmetric C-C Bond-Forming Reactions. **Patrick J. Walsh**, University of Pennsylvania

11:35 382 Use of Vanadium Hydrides to Effect Radical Cyclizations. **Jack Norton**, Mary E. Pulling and Deborah M. Smith, Columbia University

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**Tuesday, May 20, 2008, 8:30 AM - 12:00 PM**

**Chemistry and the Arts**

Medical Arts Building, Rm M-143

Organizer: Sasan Karimi, Queensborough Community College

8:30 Introductory Remarks.

8:35 383 Color Science Laboratory Exercises in Art and Theatre. **Maria C. Gelabert** and Christopher Mustakas, Wagner College

88
8:55 384 Chemical and Materials Analysis of Copper-Alloy Artifacts from High Status Burials at the Pyramids at Moche Site, Peru. **Marc L. Richard**, Elizabeth Myers Cooney² and Heather Lechtman², (1)The Richard Stockton College of New Jersey, (2)Massachusetts Institute of Technology


9:35 386 Teaching Science of Art in Italy. **Robert Richman**, Mount Saint Mary's University


10:15 Break.

10:30 388 Chemistry in Art: Seventeen Years of Courses and Workshops. **Patricia S. Hill**, Millersville University

10:50 389 Why Chemistry and Art?: **Michael Henchman**, Brandeis University

11:10 390 Uncovering the Secrets of Ancient and Medieval Artists through Chemistry. **Mary Virginia Orna**, College of New Rochelle

**Tuesday, May 20, 2008, 8:30 AM - 12:00 PM**

**Computational Chemistry for the Health of Humanity and the Planet, I - Kinetics and Dynamics**

Sponsor: Healthcare & Life Sciences Department, Dell, Inc.; Chemistry Department, Brookhaven National Laboratory

Medical Arts Building, Rm M-146

Organizers: Daqing Gao, Queensborough Community College, Seogjoo Jang, Queens College of the City University of New York

Session Overview: Computational chemistry has become an essential tool for biomedical research (health of humanity) and renewable energy research (health of the planet). This session discusses recent advances and key issues in understanding the kinetics and the dynamics of important systems in these research areas.

8:30 391 Reaction Coordinates in Enzymes - Promoting Vibrations. **Steven D. Schwartz**, Albert Einstein College of Medicine

9:10 392 A Computational Study of Changing Intramolecular Interactions in Serine and Threonine, at Different Phs. **Mihaela D. Bojin**, Queensborough Community College, CUNY


10:10 Break.

10:20 394 The Transition State for Formation of the Peptide Bond in the Ribosome. **Lou Massa**, Hunter College, City University of New York

11:00 395 Efficient, Transformation-Free, Conformational Sampling Via Driven Adiabatic Free Energy Dynamics. **Jerry B. Abrams** and **Mark E. Tuckerman**, New York University

Tuesday, May 20, 2008, 8:30 AM - 12:00 PM

Frontiers in Nanoscience and Nanotechnology – Bioapplications

Sponsor: Momentive Performance Materials

Medical Arts Building, Rm M-142
Organizers: Bhanu P. S. Chauhan, William Paterson University, Kenrick Lewis, Momentive Performance Materials

8:30  Introduction and Welcome Remarks- Bhanu P. S. Chauhan.
8:33  Presider: Bhanu P. S. Chauhan.
8:35  397  DNA: Not Merely the Secret of Life. Nadrian C. Seeman, New York University
9:15  398  Nanoparticle Based Therapeutic Agents for Brain (Rhabdoid ) Tumor. Bhaskar C. Das, Albert Einstein College of Medicine
9:40  399  Target Co-Delivery of Nanoheaters and siRNAs for Cancer Therapy. Oleh Taratula¹, Ronak Savla¹, Ipsit Pandya¹, Andrew Wang², Tamara Minko³ and Huixin He¹, (1)Department of Chemistry, Rutgers University, (2)Ocean NanoTech, (3)The Ernest Mario School of Pharmacy, Rutgers, the State University of New Jersey
10:05  Break.
10:18  Presider: Kenrick Lewis.
10:20  400  Controlling Self-Assembly Reactivity in DNA- and Protein-Nanoparticle Systems. Mathew M. Maye, Brookhaven National Laboratory
10:45  401  GdDTPA-TAA Functionalized Nanoparticles as MRI Contrast Agents. Talha S. Siddiqui and Marc Walters, New York University
11:10  402  Towards a SERS-Based Nanobiosensor for Organophosphorus Compounds. Melek Erol, Henry Du and Svetlana A. Sukhishvili, Stevens Institute of Technology
11:35  403  Tailored Bionanocomposites for Applications in Tissue Engineering, Drug Delivery and Bone Materials. Karen T. Johnson and Ipsita A. Banerjee, Fordham University

Tuesday, May 20, 2008, 8:30 AM - 12:00 PM

HPLC Methods Development

Sponsor: Novartis Pharmaceuticals Corporation and the ACS Division of Analytical Chemistry

Medical Arts Building, Rm M-136
Organizers: Rosario LoBrutto, Novartis Pharmaceutical Corporation, Richard Thompson, Novartis Pharmaceutical Corporation

Session Overview: HPLC separations are accomplished when there are significant differences in the interactions of analytes with the stationary and mobile phases. There are numerous options that can be undertaken in accomplishing a successful separation with respect to choice of separation mode, mobile phase components, and particularly stationary phase. However, the availability of so many options can in itself be an encumbrance. This symposium will address current means to facilitate, expedite, and optimize both chiral and achiral separations including the use of high throughput screening methodology and the implementation of software optimization and peak tracking tools.
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>8:30</td>
<td><strong>404</strong> Comprehensive LCxLC for the Analysis of Semi-Volatile Compounds. Luigi Mondello, University of Messina</td>
</tr>
<tr>
<td>10:05</td>
<td>Break.</td>
</tr>
<tr>
<td>10:15</td>
<td><strong>407</strong> Computerized Design of Robust Gradient HPLC Methods. Imre Molnar and Hans-Jürgen Rieger, Institute for Applied Chromatography</td>
</tr>
<tr>
<td>10:40</td>
<td><strong>408</strong> Rapid Automated HPLC Method Development. Ahmed Aced, Iris Technologies International Ltd /The ChromSword Group and Sergey Galushko, Dr. Galushko Software Entwicklung/ The ChromSword Group</td>
</tr>
<tr>
<td>11:05</td>
<td><strong>409</strong> Strategies and Systematic Processes to Develop Efficient, Sensitive and Robust HPLC Methods for Pharmaceutical Analyses. Jinjian Zheng and Abu Rustum, Schering-Plough Corporation</td>
</tr>
<tr>
<td>11:30</td>
<td><strong>410</strong> Automated Chiral Application, Databasing, Evaluation and Selection (ACADES). Frank Riley, Pfizer</td>
</tr>
</tbody>
</table>

**Tuesday, May 20, 2008, 8:30 AM - 12:00 PM**

**Industrial Chemistry Symposium, I**

Medical Arts Building, Rm M-133

Organizer: Steven R. Carlo, Exponent

Session Overview: A forum for industrial or government chemists from any chemistry discipline, to present their work. The emphasis will be on the applicability of chemistry and your work to the real world.

<table>
<thead>
<tr>
<th>Time</th>
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<tbody>
<tr>
<td>8:30</td>
<td>Break.</td>
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<tr>
<td>8:55</td>
<td>Introductory Remarks.</td>
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<tr>
<td>9:00</td>
<td><strong>411</strong> Sugarcane Extract-- An Excellent Phytochemical Functional Foods. Chung Chi Chou, Dr Chou Technologies, Inc and Wen Hong Gao, South China University of Technology, China</td>
</tr>
<tr>
<td>9:20</td>
<td><strong>412</strong> The “WOW” Factor Secret behind Retail Cosmetics. John Gormley, Grant Industries Inc.</td>
</tr>
<tr>
<td>9:40</td>
<td><strong>413</strong> Creating Controlled and Sustainable Innovation for the Cosmetic Industry. Laurence Dryer, BASF Beauty Care Solutions</td>
</tr>
<tr>
<td>10:00</td>
<td><strong>414</strong> Application of Rheology and in-Vitro SPF Testing to Optimize Sunscreen Emulsion Formulation. Laura A. Spaulding and A. Christopher Pattillo, Energizer Personal Care</td>
</tr>
<tr>
<td>10:20</td>
<td>Intermission.</td>
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<tr>
<td>10:40</td>
<td><strong>415</strong> Adventure in Product Development - Water-Based Primer for Coatings. T. Page McAndrew, Arkema Inc.</td>
</tr>
</tbody>
</table>
11:00 416 Forensic Chemistry in the Investigation of Product Tampering. Jason E. Schaff, FBI Laboratory

11:20 417 Consultancy: A Prospective Career for Scientists and Engineers. Jennifer Vondran, PA Consulting Group


Tuesday, May 20, 2008, 8:30 AM - 12:00 PM

Photochemistry, I

Sponsor: Boston Electronics Corporation; Edinburgh Instruments Ltd.; HORIBA Jobin Yvon Inc.; Coherent Inc.

Medical Arts Building, Rm M-133
Organizer: Steffen Jockusch, Columbia University

Session Overview: Photochemistry is an interdisciplinary research area, which includes aspects of organic and inorganic chemistry, material sciences, biochemistry, spectroscopy, physics and chemical engineering. The involvement of light brings these diverse fields together. The morning session of this photochemistry symposium focusses on environmental topics, luminescence sensors, and biological systems.

8:30 Welcoming Remarks.

8:35 419 Photophysical and Photochemical Investigations of CO₂-Soluble Catalysts for the Reduction of CO₂ to CO in Supercritical CO₂. David C. Grills, Mark D. Doherty and Etsuko Fujita, Brookhaven National Laboratory

8:55 420 Photocatalytic Reduction of Organic and Inorganic Compounds. Miguel Valenzuela, Sergio Flores and Omar Rios, Instituto Politecnico Nacional

9:25 421 Optical Switches for Affinity-Switchable Molecular Interaction and Fluorescence Tracking. Jochen Mattay, Bielefeld University

10:05 Coffee Break.

10:20 422 An Exploration into the Structure and Photophysics of Hemilabile Coordination Complexes. Anthony Tomcykoski and Wayne E. Jones, State University of New York at Binghamton

10:40 423 Use of Luminescence Resonance Energy Transfer to Identify Locations of Site-Bound Metal Ions in the Spliceosomal U2–U6 snRNA Complex. Nancy L. Greenbaum, Hunter College, City University of New York and Faqing Yuan, Florida State University

11:20 424 New Chromophore Systems and Photoactive Compounds Arising from Chlorophyll Breakdown in Plants. Bernhard Kraeutler, University of Innsbruck
Tuesday, May 20, 2008, 8:30 AM - 12:00 PM

Spectroscopy of Biological Systems

Library Building, Rm LB-15

Organizers: Ruel Desamero, York College, Emmanuel Chang, York College

Session Overview: Advances in instrumental techniques are pushing the analytical boundaries for the spectroscopic study of biological macromolecules. Both the structure and dynamics of biomacromolecular assemblies are being probed with unprecedented detail using optical, NMR and mass spectrosopies. This symposium highlights some recent developments in the application of these cutting edge technologies to important problems in basic and disease-related biochemistry. The session will be headlined by Dr. David Cowburn of the NY Structural Biology consortium, and Dr. Bob Callender of Albert Einstein College of Medicine, and will include other leading speakers from industry and academia.

8:30 425 Mass Spectrometry and the Bioprocessing of Vaccines and Therapeutic Proteins. Steven L. Cohen, Merck Research Laboratories

9:10 426 Dynamic Processes. David Cowburn, New York Structural Biology Center

10:00 427 EPR Measurements of Distances and Electronic Couplings in Biological Macromolecules. Dr. Donald J. Hirsh, Ryan Biczo, Xi Jun Chen and Steven Wisniewski, The College of New Jersey

10:20 Break.

10:30 428 The Dynamical Nature of Proteins: Understanding the Physics of Enzymes. Robert Callender, Albert Einstein College of Medicine, Yeshiva University

11:20 429 Q-Space NMR Imaging Studies of Water in Elastin. Gregory Boutis, York College of CUNY


Tuesday, May 20, 2008, 9:00 AM - 11:00 AM

Panel Discussion: Traditional and Non-Traditional Careers in Chemistry

Library Building, Rm LB-16

Organizer: Ronald P. D'Amelia, Hofstra University

Session Overview: A panel of various traditional and non-traditional career chemists will provide real case histories on the many different options available to chemists as second and/or alternate careers in Chemistry. A discussion will follow.
Tuesday, May 20, 2008, 12:00 PM - 1:30 PM

Women Chemists Committee Luncheon

Sponsor: Metrowomen Chemists Topical Group of the New York and North Jersey ACS Sections, Metropolitan New York Chapter of the Association for Women in Science, ACS Women Chemists Committee

Oakland Cafeteria

Organizers: Hiroko Karan, Medgar Evers College, Nancy Tooney, Women Chemists Committee

Session Overview: Students and regular meeting attendees are invited to join us for a luncheon with speaker Jodi Wesemann from the education department at ACS. The luncheon provides a great opportunity for informal networking. All are welcome.

12:00 PM Luncheon
12:30 PM Fostering Access, Success, and Excellence. Jodi Wesemann, ACS Department of Higher Education

Tuesday, May 20, 2008, 1:30 PM - 5:00 PM

Analytical Chemistry, General Session II

Library Building, Rm LB-14

Organizers: Rosario LoBrutto, Novartis Pharmaceutical Corporation, Richard Thompson, Novartis Pharmaceutical Corporation

1:30 431 Use of the Quartz Crystal Microbalance to Monitor Deposition from Organic Solvent. **Hyun-Su Lee** and Lynn S. Penn, Drexel University

1:50 432 Silver Coated Barium Titanate Beads as Surface-Enhanced Raman Scattering (SERS) Substrates for the Detection of Aromatic Thols. **Jonathan Onuegbu**¹, Charles Hosten¹, Angie Fu², Orest Glembocki² and Sharka Prokes², (1)Howard University, (2)Naval Research Laboratory

2:10 433 Impedance Behavior of Conducting Polymer Electrodes in Vivo and in Vitro. **Yohani Kayinamura** and J. Faye Rubinson, Georgetown University

2:30 Break.

2:50 434 POLY(2,2'-BITIOPHENE) –Modified Electrodes for Detection of Neurotransmitters in the Presence of Interferents. **Justyna Widera** and Natana Podlubnaya, Adelphi University

3:10 435 Enhancement in Teaching and Learning IR, UV-Visible and Fluorescence Spectroscopy through Animation and Virtual Experiments. **Savitri Chandrasekhar**, Michael Murphy Boyer, Julia Bronfenbrener and Amanda Peruzza, University of Toronto Scarborough

Tuesday, May 20, 2008, 1:30 PM - 5:00 PM

Arthur C. Cope Scholar Symposium

Sponsor: ACS Division of Organic Chemistry

Medical Arts Building, Rm M-136

Organizer: Christian Rojas, Barnard College

Session Overview: This symposium honors Cope Scholar Awardee Colin Nuckolls of Columbia University for fundamental studies toward molecular-scale electronic components and devices. Achievements from the Nuckolls group include self-assembled columnar structures having supramolecular dipoles and methodology for oxidatively cutting nanotubes and bridging the gaps with conducting organic fragments.

1:30 Welcoming Remarks.
1:35 437 Glycal Metallanitrenes for 2-Amino Sugar Synthesis. Christian Rojas, Barnard College
2:15 438 Through-Bond Interactions "beyond the Molecule". Ling Yuan¹, Yan Li¹, Andrew J. Lampkins¹, Jennifer K. Mattler¹, Khalil A. Abboud¹, Bobby G. Sumpter² and Ronald K. Castellano¹, (1) University of Florida, (2) Oak Ridge National Laboratory
2:55 439 Stretching the Limits of Chemical Reactivity through Mechanochemistry. Stephen L. Craig, Duke University
3:35 Break.
3:55 440 Reaction Chemistry Meets Lithography. Colin Nuckolls, Columbia University

Tuesday, May 20, 2008, 1:30 PM - 5:30 PM

Computational Chemistry for the Health of Humanity and the Planet, II - Energetics, Structure, and Functionality

Sponsor: Healthcare & Life Sciences Department, Dell, Inc.; Chemistry Department, Brookhaven National Laboratory

Medical Arts Building, Rm M-146

Organizers: Daqing Gao, Queensborough Community College, Seogjoo Jang, Queens College of the City University of New York

Session Overview: Computational chemistry has become an essential tool for biomedical research (health of humanity) and renewable energy research (health of the planet). This session discusses recent advances in understanding how the energetics and the structure are related to the functionality of important systems in these research areas.

1:30 441 Computational Studies of Artificial Photosynthesis. James T. Muckerman and Etsuko Fujita, Brookhaven National Laboratory
2:10 442 Solvent Structure on Surfaces and Its Relation to Protein-Ligand Binding. Tom Young¹, Robert Abel², Richard A. Friesner² and Bruce Berne², (1) Yeshiva University, (2) Columbia University
<table>
<thead>
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</tr>
</thead>
<tbody>
<tr>
<td>2:30</td>
<td>443</td>
<td>Characterization of the Solvation Dynamics of Ionic Liquids.</td>
<td>Mark N. Kobrak, Brooklyn College -- CUNY</td>
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<tr>
<td>3:00</td>
<td>Break.</td>
<td></td>
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<tr>
<td>3:10</td>
<td>444</td>
<td>An Electrostatic/Geometric Mechanism for Compact Chromatin Stabilization.</td>
<td>Tamar Schlick, New York University and Gaurav Arya, University of California, San Diego</td>
</tr>
<tr>
<td>3:50</td>
<td>445</td>
<td>Characterizing Drug Resistance Using All-Atom Molecular Dynamics Simulations.</td>
<td>Robert C. Rizzo, Trent E. Balius, Rashi Goyal, Brian E. McGillick and Sudipto Mukherjee, Stony Brook University</td>
</tr>
<tr>
<td>4:20</td>
<td>446</td>
<td>Quantum Calculations as a Tool in Structural Biology: Protons and Water in Biological Molecules.</td>
<td>Michael E. Green, City College of the City University of New York</td>
</tr>
<tr>
<td>5:00</td>
<td>447</td>
<td>The Role of Modeling and Simulation in Bringing Drugs to Market.</td>
<td>August Calhoun and Stefan Unger, Dell, Inc.</td>
</tr>
</tbody>
</table>

**Tuesday, May 20, 2008, 1:30 PM - 5:00 PM**

**Environmental Chemistry – in Honor of Frances S. Sterrett**

Medical Arts Building, Rm M-143

Organizers: John Gibbs, Medgar Evers College of The City University of New York, B. Hillery, SUNY Old Westbury

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Number</th>
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<tbody>
<tr>
<td>1:30</td>
<td>Welcoming Remarks.</td>
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<td>1:35</td>
<td>448</td>
<td>Occurrence and Fate of Pharmaceutically Active Contaminants in the Hudson Basin.</td>
<td>Bruce Brownawell, Xiaolin Li, Mark Benotti and Joseph Ruggieri, Stony Brook University</td>
</tr>
<tr>
<td>1:55</td>
<td>449</td>
<td>Biomagnetic Microcapsules for Environmental Applications.</td>
<td>Silvana Andreescu, Matthew T. Ravalli and Cristina R. Ispas, Clarkson University</td>
</tr>
<tr>
<td>2:35</td>
<td>451</td>
<td>Temporal Trend of Perchlorate in Arctic Snow.</td>
<td>Vasile Furdui and Frank Tomassini, Ontario Ministry of the Environment</td>
</tr>
<tr>
<td>2:55</td>
<td>Break.</td>
<td></td>
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<tr>
<td>3:15</td>
<td>452</td>
<td>Surge in NOx Emissions on High Ozone, High Electric Demand Days.</td>
<td>Thomas F. McNevin, New Jersey Department of Environmental Protection</td>
</tr>
<tr>
<td>3:35</td>
<td>453</td>
<td>Hydroperoxide Measurements in Mexico City.</td>
<td>Judith Weinstein-Lloyd¹, Barbara Hillery², Linda Nunnermacker³, Lawrence Kleinman³ and Brian Giebel⁴, (1)State University of New York, (2)State University of New York / Old Westbury, (3)Brookhaven National Laboratory, (4)Rosenstiel School of Marine and Atmospheric Sciences</td>
</tr>
<tr>
<td>3:55</td>
<td>454</td>
<td>Spatial Distribution of Mercury Vapor in Homes in Brooklyn, New York.</td>
<td>Clyde Johnson, Ramapo College of New Jersey</td>
</tr>
<tr>
<td>4:15</td>
<td>455</td>
<td>Oil Sector Complex at An Old Salt-Chlorine Industrial Site.</td>
<td>Abdul Rehman Khan¹, Layla Al-Awadi¹, Mohammad Al-Ramadhan¹, Awadh Saeed², Abdulraheem Al-Rashidi² and Fatimah Al-Shatti², (1)Environment and Urban Development Division, (2)Kuwait Petroleum Corporation</td>
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Tuesday, May 20, 2008, 1:30 PM - 5:00 PM

Frontiers in Nanoscience and Nanotechnology – Fabrication

Sponsor: Momentive Performance Materials

Medical Arts Building, Rm M-142

Organizers: Bhanu P. S. Chauhan, William Paterson University, Kenrick Lewis, Momentive Performance Materials
Presiders: Geraud Dubois, IBM, Gilbert K. Min, Agilent Technologies, Inc., Vinod M. Menon, Queens College of CUNY

1:30 456 Welcome Remarks. Geraud Dubois, IBM

1:33

1:35 457 Device Fabrication and Materials Synthesis in Bionanotechnology Approach; Biomimetic Assemblies of Peptide Nanowires and Nanoparticles and Their Controlled Mineralization at Room Temperature. Hiroshi Matsui, City University of New York, Hunter College

2:10 458 Biocompatibility Testing of a Novel Nanoporous Hemodialysis Membrane. Loyd D. Bastin, Mark Schneider and Robert Morris, Widener University

2:35 450 Carbon Nanostructures Made by Focused Ion Beams. Alexander Zaitsev, College of Staten Island

3:00 Break.

3:10 Presider: Gilbert K. Min.

3:15 460 Hybrid Photonic Devices Based on Colloidal Quantum Dot Composites. Vinod M. Menon, Queens College of CUNY

3:40 461 Synthesis and Self-Assembly of Smart Hydrogel Nanoparticles into Soft Opals. Xihua Lu, Northwestern University and Gao Qiu, Donghua University

4:05 Presider: Vinod Menon.

4:10 462 Solvent and Concentration Effects on the Two-Dimensional Network Formation of Benzene Carboxylic Acids. Gina M. Florio, Kimberly A. Stiso and Joseph S. Campanelli, St. John's University

Tuesday, May 20, 2008, 1:30 PM - 5:00 PM

Industrial Chemistry Symposium, II

Medical Arts Building, Rm M-133
Organizer: Steven R. Carlo, Exponent
Session Overview: A panel discussion to allow conference attendees to find out everything they wanted to know about life in industry, but were too afraid to ask.

1:30 Break.
2:00 Panel Discussion.
4:00 464 John Gormley's Bio. John Gormley, Grant Industries Inc.
4:02 466 Page McAndrew's Bio. T. Page McAndrew, Arkema Inc.
4:03 467 Jason Schaff's Bio. Jason E. Schaff, FBI Laboratory

Tuesday, May 20, 2008, 1:30 PM - 5:00 PM

Inorganic Chemistry, General Session

Medical Arts Building, Rm M-134
Organizers: Roberto A. Sanchez-Delgado, Brooklyn College and The Graduate Center, CUNY, William H. Hersh, Queens College of the City University of New York, Zhaohua Dai, Pace University

1:30 Introductory Remarks.
1:35 469 Further Study of Dr. Frankenstein's Reaction. Stephen A. Koch, State University of New York at Stony Brook
2:05 470 Effect of Solvent Environment on the CO Band Position in the Infrared Spectrum of [Fe(CN)₄(CO)₂]²⁻. R. Viswanathan, A.M. Etra and J. Jiang, Yeshiva University
2:35 471 Chemistry of Ruthenium and Osmium Cyanide Compounds. Daniel Amarante, Stony Brook University
3:05 Break.
3:20 472 Tailoring Tripodal Ligands for Zinc Sensing. Zhaohua Dai, Pace University and James W. Canary, New York University
3:50 473 Kinetic and Equilibrium Studies of Small Molecule Binding to (PCP)Rh Pincer Complexes. Mark D. Doherty¹, David C. Grills¹, Kuo-Wei Huang², Dmitry Polyansky¹ and Etsuko Fujita¹, (1)Brookhaven National Laboratory, (2)National University of Singapore
4:20 474 Reactions of Inorganic Tin (IV) and Lead (II) Compounds with Mono- and Bi-Dentate Ligands Having Nitrogen and Oxygen Donors. Burl C. Yearwood, Emily Bouret and Ronke Alo, LaGuardia Community College (CUNY)
4:50 Concluding Remarks.
Tuesday, May 20, 2008, 1:30 PM - 5:00 PM

Photochemistry, II

Sponsor: Boston Electronics Corporation; Edinburgh Instruments Ltd.; HORIBA Jobin Yvon Inc.; Coherent Inc.
Library Building, Rm LB-15

Organizer: Steffen Jockusch, Columbia University

Session Overview: Photochemistry is an interdisciplinary research area, which includes aspects of organic and inorganic chemistry, material sciences, biochemistry, spectroscopy, physics and chemical engineering. The involvement of light brings these diverse fields together. The afternoon session of this photochemistry symposium focusses on supramolecular photochemistry.

1:30 475 Supramolecular Photochirogenesis with Biomolecules. **Yoshihisa Inoue**, Osaka University

2:10 476 Singlet Oxygen Generation at the Porous Glass-Water Interface. **Alexander Greer**, City University of New York, Brooklyn College

2:35 477 Photo-Fries Rearrangements of O-Cresyl Acetates in Isotropic Solutions and in Polyethylene Films. the Role of Reaction Cavities. **Yuzhe Chen** and **Richard G. Weiss**, Georgetown University

2:55 Break.

3:10 478 Controlling Photochemistry with Weak Non-Covalent Forces and Confined Spaces. **Vaidhyanathan Ramamurthy**, University of Miami

3:50 479 Controlling Photoreactivity of Coumarins in Water Soluble Nano-Cavities. **Sivaguru Jayaraman** and **Nilotpal Barooah**, North Dakota State University

4:20 480 From Molecular to Supramolecular to Superdupermolecular Organic Photochemistry. **Nicholas Turro**, Columbia University

Tuesday, May 20, 2008, 1:30 PM - 5:30 PM

Polymer IV (Functional Polymers)

Sponsor: Center for Engineered Polymeric Materials(CePM)

Library Building, Rm LB-6

Organizer: Moni Chauhan, CUNY-Queensborough Community College
Presider: Ralf. M Peetz, College of Staten Island, City University of NY

1:30 481 Polycarbosilanes as Ceramic Precursors and Low-K Dielectric Materials. **Leonard V. Interrante**, Rensselaer Polytechnic Institute

2:05 482 Organic Electronics for Early Detection/Diagnostics. **Kalle M. Levon**, Polytechnic University

2:25 483 Metal Ion Affinity of Polymer-Supported Phosphoryl Oxygen in Nitric Acid Solution. **Xiaoping Zhu** and **Spiro D. Alexandratos**, Hunter College

99
2:45  484  Ultrathin Responsive Polymer Films and Capsules. Svetlana Sukhishvili, Stevens Institute of Technology

3:05  Break.

3:20  485  Polymer-Supported Reagents and Their Application to Environmental Remediation. Spiro D. Alexandratos, Hunter College

3:55  486  Controlling Porphyrin Affinity in Designed Proteins. Ronald L. Koder, Christopher Negron and Andrew C. Mutter, The City College of New York

4:15  487  Organoborane Functionalized Conjugated Polymers as Optoelectronic Materials. Frieder Jäkle, Haiyan Li and Anand Sundararaman, Rutgers University

4:35  488  Guided Self-Assembly of Block Copolymer Thin Films. Alamgir Karim, National Institute of Standards and Technology

Tuesday, May 20, 2008, 4:30 PM - 7:00 PM

Industrial Innovation Award Symposium and Reception

Sponsor: ACS Corporate Associates
Oakland Cafeteria

Session Overview: This session honors the recipient of the 2008 Regional Industrial Innovation Award. The Awardee will present an overview of the efforts that led to the process/product innovation.
4:30 PM: Symposium
5:30 PM: Reception

Tuesday, May 20, 2008, 5:30 PM - 7:00 PM

Poster Session III

Student Union Building, Upper

Organizers: Irina Rutenburg, Queensborough Community College, Marie Thomas, Queens College, CUNY

489  Determination of the Ionization Constant of Carboxylic Acids Using Microscale Freezing Point Depression Measurements. Junior Gonzales¹, Gopal Subramaniam², Paris Svoronos¹, David M. Sarno¹ and Pedro Irigoyen¹, (1)Queensborough Community College, (2)Queens College

490  Influence of Cation Size and Charge in Ion-Pair Formation. Thomas Kim¹, Paris Svoronos¹, Gopal Subramaniam², David M. Sarno¹ and Pedro Irigoyen¹, (1)Queensborough Community College - CUNY, (2)City University of New York, Queens College

491  Studies on the Anion Size, Charge and Nature in the Dissociation of Salts in Aqueous Solutions. Tayyaba Nasar¹, Gopal Subramaniam², David M. Sarno¹ and Pedro Irigoyen¹, (1)Queensborough Community College, (2)City University of New York, Queens College

492  Thermal Intramolecular H-Atom Transfer across Hydrogen Bonds in Radicals. Theodore S. Dibble¹, Keith T. Kuwata², Emily Sliz² and Erin B. Petersen², (1)SUNY-ESF, (2)Macalester College

494 An EPR and NMR Study of Supramolecular Effects on Spin-Spin Coupling Between a Nitroxide Incarcerated within a Nanocapsule with a Nitroxide in Bulk Aqueous Media. Judy Y. -C. Chen¹, Nicholas Turro¹, Steffen Jockusch¹, Vaidhyanathan Ramamurthy², Francesca Ottaviani³ and Jayaraj Nithyanandhan², (1)Columbia University, (2)University of Miami, (3)University of Urbino

495 Investigation of Mono- and Bimetallic Ruthenium Complexes with the Facial Terminal Ligand Tris(1-pyrazolyl)Methane. Theresa Yi and Matthew T. Mongelli, Kean University

496 ANALYSIS of the Alternation of Vibration Modes on the Ring STRUCTURE of Mono-Substituted and Di-Substituted Benzene. Sharmaine Lewis, Yi Da and Ruel Desamero, City University of New York - York College


498 Computational Study of Structural Modifications to a Novel Class of Paramagnetic Chemical Exchange Saturation Transfer Agents. Whelton A. Miller III, Zhiwei Liu and Vojislava Pophristic, University of the Sciences in Philadelphia


500 Reactivity of Tris(trimethylsilyl) Phosphite (TMSP): Reactions with Halo-Chloroformates. Jeong-hoon Ham and Luis Vargas, Queensborough Community College

501 Reactivity of Tris(trimethylsilyl)Phosphite (TMSP): Reactions with Haloacetyl Chlorides. Jazmin Garduno and Luis Vargas, Queensborough Community College

502 Reactivity of Tris(trimethylsilyl)Phosphite (TMSP): Reactions with Chloroformates. Joseph Mammano and Luis Vargas, Queensborough Community College

503 Structural Determination of a Process Impurity and Control of Its Formation in Support of Development of Brivanib, An Oral Dual Inhibitor of VEGFR and FGFR Tyrosine Kinases. Qingmei Ye, Zhongmin Xu, George Crull, Vera Leshcinskaya, Yande Huang and V Palaniswamy, Bristol-Myers Squibb


505 Progress on Determining the Active Site of Cytochrome P450 BMP. Jaclyn I. Catalano, Michael J. Harris and Ann E. McDermott, Columbia University

506 Elastic Network Molecular Dynamics Simulations of Coarse-Grained Molecular Systems. Marco Cavalli, Yi He and Marco Ceruso, The City College of New York

507 Coarse-Grain Molecular Dynamics of Tetrapeptides. Kenny Nguyen¹, Russell DeVane², Zhiwei Liu¹ and Preston B. Moore¹, (1)University of the Sciences in Philadelphia, (2)University of Pennsylvania

508 Undergraduate Research at PSU Abington: IR Prediction of Methylarsine and Methylstibine Using HF Method. Mitalben K. Patel and Hae-Won Kim, Abington College Penn State

509 Fourier-Transform Infrared Analysis of Some Amino Acids and Peptides That Are Precursors of a Bivalent Src Kinase Inhibitor. Justina Chinwong, Adam Profit and Ruel Z. B. Desamero, York College of CUNY
Conformational Dynamics of Ionotropic Glutamate Receptors: Apo Vs Holo, Monomers Vs. Dimers. Rodney Versace and Marco Ceruso, The City College of New York

Structural and Chemical Effects of Alkylation in Nickel Thiolate Dimers. Gerard Davidson, Michael J. Maroney and Seleena Rashid, (1)St. Francis College, (2)University of Massachusetts

Success Rates by Protein Family in Small Molecule Docking. Sudipto Mukherjee and Robert C. Rizzo, Stony Brook University

Synthesis and Characterization of Bis-(Diimine)Carbonylalkyllosium(II) Complexes. Vennessa O. Williams, Sarswati Ramoutar, Viet Tran and Elise G. Megehee, St. John's University

Synthesis and Characterization of Bis-(Diimine)Carbonylpurindineosmium(II) Complexes. Carina Hernandez, Ryan Mahabir, Carmen Leung and Elise G. Megehee, St. John's University

Computational Analysis of Intramolecular Interactions in Serine and Threonine, at Their Isoelectronic Points. Elizabeth Cipriana, Alexandru Pestesi and Mihaela D. Bojin, Queensborough Community College, CUNY

The Nature and Distribution of Tungsten Oxide Photocatalysts. Edward G. Look and Harry D. Gafney, Queens College, City University of New York

Energetic and Structural Analysis of EGFR Inhibition Using Molecular Dynamics Simulations. Trent E. Balius and Robert C. Rizzo, Stony Brook University

Excited State Coordination Chemistry: Synthesis, Characterization and Acid-Base and Coordination Chemistry of a Ruthenium (II) Diimine – [Ru (bpy)2(ppz)] 2+ (ppz- 4′7′-phenanthroline-5′,6′:5,6-pyrazine). Anthony Perri and Harry D. Gafney, Queens College, City University of New York

Theoretical Studies of Basic and Acidic Serine and Threonine – An Exploration of Hydrogen Bonding Patterns. Alexandru Pestesi, Elizabeth Cipriana and Mihaela D. Bojin, Queensborough Community College, CUNY

Using Computation to Elicit the Structure of HIVgp41 in Lipid Membranes. Brian E. McGillick and Robert C. Rizzo, Stony Brook University

Targeted Drug Design for Pandemic Influenza Strain H5N1. Rashi Goyal and Robert C. Rizzo, Stony Brook University

Assessment of a Service-Learning Chemistry Course for Widener Students. Louise M. Liable-Sands, Mark G. Bradley, Nadine McHenry, Steven Menden, Stephanie Nilan, Heaven Pokorny, Jillian Filewicz, Carly Graffeo and Jennifer Pinel, Widener University

Tetraphenylporphyrin Photosensitizer Covalently-Bonded by a Urea Linkage Onto Porous Vycor Glass. Matibur Zamadar, David Aebisher, Steven Greenbaum and Alexander Greer, (1)City University of New York, Brooklyn College, (2)City University of New York, Hunter College

Computations of Singlet Oxygen Release from 1,4-Polymethylene Linked Naphthalene Endoperoxides. Alvaro Castillo and Alexander Greer, City University of New York, Brooklyn College

Spin-Forbidden Resonance Energy Transfer Probes for DNA Detection. Angel Martí, Columbia University

Tin-Free and Catalytic Radical Cyclizations. Mary E. Pulling, Deborah M. Smith, Jong Wook Choi and Jack Norton, Columbia University

528 Enantioselective Carboalumination of Olefins. James M. Camara, Robby A. Petros and Jack R. Norton, Columbia University

529 LCMS Analysis of Drug Molecules in Serum by Restricted Access Material Column. Ken Tseng¹, Junji Sasuga², Kei Oide², Eiji Kagawa² and Hideyuki Kondo², (1)Shodex, (2)Showa Denko, K.K.


531 Complexation Behavior, Photoluminescence Properties and Supramolecular Structures of Pentafluorophenylcopper. Ami Doshi¹, Krishnan Venkatasubbaiah¹, Anand Sundararaman¹, Lev N. Zakharov², Arnold L. Rheingold² and Frieder Jäkle¹, (1)Rutgers University, (2)University of California - San Diego

532 Ruthenium Complexes with Non-Innocent O-Quinonoid Ligands. Jonathan Rochford and Etsuko Fujita, Brookhaven National Laboratory

533 Non-Radiative Deactivation of Singlet Oxygen (¹O₂) by Cubane and Its Derivatives. Jeffrey R. Lancaster¹, Angel A. Martí¹, Juan Lopez-Gejo², Steffen Jockusch¹, Naphtali O'Connor¹, Philip E. Eaton³ and Nicholas J. Turro¹, (1)Columbia University, (2)Universidad Complutense de Madrid, (3)University of Chicago

534 The Synthesis of Diaryl Sulfones Via Rearrangement of Sulfonanilides. Lisa Marie Neuls Meseroll, James R. McKe and Murray Zanger, University of the Sciences in Philadelphia

535 Novel Chiral Biphenol-Based Monodentate Phosphoramidite Ligands and Their Application to Asymmetric Allylic Substitution Reactions. Stephen J. Chaterpaul¹, Ce Shi² and Iwao Ojima², (1)State University of New York at Stony Brook, (2)Institute of Chemical Biology and Drug Discovery, State University of New York

536 Conformational Equilibria of Simple Organic Molecules in the Gas Phase and Solution. Ermir Pjetri, Yinjuan Cui, Eza Chikashvili and Daqing Gao, Queensborough Community College

537 Molecular Interactions of Amino Acids and Water. Athanasia Pavlou, Yinjuan Cui, Anibal Davalos and Daqing Gao, Queensborough Community College

538 Ab Initio Computation of the Pka Values of Neutral Molecules and Anions in Water. Yinjuan Cui, Athanasia Pavlou, Anibal Davalos and Daqing Gao, Queensborough Community College

539 Phase II Stormwater Management. Lorraine J. Kuhn, Village of Ardsley

540 Optical Study of Src Kinase Inhibitors. Jeonghee Kang, Adam A. Profit, Jong I. Lee and Ruel Z. B. Desamero, York College- City University of New York, the Graduate Center and the Institute of Macromolecular Assembly of CUNY

541 Studies into the Gas Phase Chemistry of Phosphorylated Peptide Ions Using Mass Spectrometry. Teresa Allen-Michaud, York College/Queens College, the City University of New York and Emmanuel Chang, York College


543 Novel DNA Staining Technique Employing Gold Phosphine Salts: Application for Nanowire Synthesis. Jacopo Samson¹, Charles Michael Drain¹ and Patrick Nahirney², (1)Hunter College of City University of New York, (2)Rockefeller University

544 Molecular Delivery Systems: Synthesis of [(bpy)²RudppW(CO)₄]²⁺. Julie C. Colis, Melissa D'Souza and Harry D. Gafney, City University of New York, Queens College

545 Triggered Protein Derived Scaffold as Self-Assembled Materials. Susheel Kumar Gunasekar and Jin Montclare, Polytechnic University
A Low-Cost Stable Metabolic Stable Isotope Labeling Method for Quantifying in Vivo Protein Phosphorylation. **Emmanuel Chang**, York College

A Novel Photobioreactor for Algae Production. **Arthur T. Poulos**, Alex Angilella, Ester Byram, Andrew Flood, Joe Liu, Timothy McMichael, Spenser Reilly and Amanda Vangeli, SciCore Research Institute

Toward Photochemical CO\(_2\) Reduction by Rhenium Complexes. **Sean E. Hightower**\(^1\), David C. Grills\(^1\), Jinzhu Chen\(^1\), Koji Tanaka\(^2\) and Etsuko Fujita\(^1\), (1)Brookhaven National Laboratory, (2)Institute for Molecular Science and CREST

Determination of Electron Transfer Rate Contant Between Congo Red and Selected Organic Fluorescence Quenchers. **Maurice Iwunze**, Morgan State University

Growth Inhibition of Retinoic Acid Treated MCF-7 Breast Cancer Cells-Identification of Sox 9 and Other Proteins. **Tiffany Remsen**, P. Kessler, A. Stern, H. Samuels and P. Pevsner, New York University School of Medicine

IMAGING MALDI of Colorectal Carcinoma - Field Defects in SatelliteTissue. **Tiffany Remsen**\(^1\), P. Kessler\(^1\), F. Francois\(^1\), A. Stern\(^1\), S. Anand\(^2\) and P. Pevsner\(^1\), (1)New York University School of Medicine, (2)Brooklyn Hospital Center


Synthesis of Novel Tetrasubstituted Phthalocyanines with Dibenzazepine Frames as Potential PDT Agents. **Matteo Parravicini**, Stefano Tollari and Giovanni Palmisano, Universita’ dell’Insubria

Validation of Analytical Procedures for the Determination of Some Pharmaceutical Products. **Hilmi Ibar** and Özlem Bayram Basdag, Trakya University

Purification of Vitamine E from Waste Oil. **H.R. Ferhat Karabulut** and Omar Zaim, University of Trakya

Extractive-Spectrophotometric Investigations on Ternary Ion-Associated Vanadium(V) Complexes. **M. Türkyilmaz**\(^1\), O. Altun\(^1\) and K. B. Gavazov\(^2\), (1)University of Trakya, (2)University of Plovdiv


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**Tuesday, May 20, 2008, 7:00 PM - 9:00 PM**

**Awards Banquet**

Oakland Cafeteria

Organizer: Mihaela D. Bojin, Queensborough Community College, CUNY
Organizer: Jane Pepper, Novartis

Session Overview: This banquet is in honor of the recipients of MARM 2008 Awards. It immediately follows the Industrial Innovation Award Reception.
Computational Chemistry for the Health of Humanity and the Planet, III - Complexity and Accuracy

Sponsor: Healthcare & Life Sciences Department, Dell, Inc.; Chemistry Department Brookhaven National Laboratory

Medical Arts Building, Rm M-146

Organizers: Daqing Gao, Queensborough Community College, Seogjoo Jang, Queens College of the City University of New York

Session Overview: Computational chemistry has become an essential tool for biomedical research (health of humanity) and renewable energy research (health of the planet). This session discusses recent advances in how the issues of complexity and accuracy can be overcome in these research areas.

8:30  558  Desulfurization Reactions on Metal Carbides and Phosphides: Complex Role of C and P Sites. **Jose A. Rodriguez**, Ping Liu and James T. Muckerman, Brookhaven National Laboratory


10:10  Break.

10:20   561  Towards Computational Simulation of Receptor-Mediated Transmembrane Signaling Events in Realistic Environments. **Marco Ceruso**, The City College of New York


11:10   563  Computational Design of Small Molecular Inhibitors to Promote Induction of Bone Growth by BMPs. **Boojala Vijay B. Reddy**¹, Sreedhara Sangadala², Raghu Prasad Rao Metpally¹, Shaila Ahmed³ and Pooja Makkar³, (1)Queens College of City University New York, (2)Atlanta VA Medical Center, (3)Graduate Center, The City University New York

11:40   564  Network Approach for Analysis of Residue Packing in Helical Membrane Proteins and Its Application in Membrane Protein Structure Prediction. **Vagmita Pabuwal** and Zhijun Li, University of the Sciences in Philadelphia
Wednesday, May 21, 2008, 8:30 AM - 12:00 PM

Infrared Spectroscopy

Sponsor: MicroLab, Inc.; Smith Detection

Medical Arts Building, Rm M-140

Organizers: Luis Avila, Columbia University, Leonard Fine, Columbia University

Session Overview: Infrared Spectroscopists have moved their spectrometers from their benchtops into the fields of homeland security and environmental remediation. They have also refocused IR photons of all ranges into tissue imaging, looking at two-dimensional time-evolving structures. In this symposium we would like to invite you to share your work with us and highlight the versatility of infrared spectroscopy. Fiat Lux!

8:30 Introductory Remarks.
8:40 Planar-Array Infrared (PA-IR) Spectroscopy: Evolution, Revolution or Back to the Future???. John F. Rabolt, University of Delaware
9:10 Intermission.
9:20 Membrane Catalyzed hIAPP Folding Followed by 2DIR SPECTROSCOPY. Yun L. Ling, Dave B. Strasfeld, Sang-Hee Shim and Martin T. Zanni, University of Wisconsin-Madison
9:50 Saint Wolfgang's Secret Past: A Microspectroscopic Analysis of Paints Removed from a Medieval Sculpture. Patricia Lang, Ball State University
10:20 Break.
11:20 Discussion.
11:40 Concluding Remarks.

Wednesday, May 21, 2008, 8:30 AM - 12:00 PM

Materials, General Session

Sponsor: Momentive Performance Materials

Medical Arts Building, Rm M-142

Organizer: Bhanu P. S. Chauhan, William Paterson University
Presiders: Bhanu P. S. Chauhan, William Paterson University, Elena Galoppini, Rutgers-Newark

8:30 Welcome and Introductory Remarks: Bhanu P. S. Chauhan.
8:35 Functional Polycarbonates. James A. Moore, Rensselaer Polytechnic Institute
8:55 Design of Nitrogen-Containing, Low Molecular-Mass Organogelators Based on (R)-12-Hydroxyoctadecanoic Acid and the Properties of Their Organogels. V. Ajay Mallia and Richard G. Weiss, Georgetown University
9:15 571 Direct White Light from a Single Semiconductor Material: A Unique Approach. **Wooseok Ki** and Jing Li, Rutgers, The State University of New Jersey

9:35 572 Aggregation Studies of Tripodal Linkers on Semiconductor Surfaces. **Sujatha Thyagarajan** and Elena Galoppini, Rutgers-Newark

9:55 Break.

10:15 Presider: Elena Galoppini.

10:20 573 The Role of Aqueous Chemistry in Subcritical Hydrothermal Crystal Growth. **Maria C. Gelabert**, Wagner College

10:40 574 Nanoscale Morphology of Polyaniline and Its Analogs. **David M. Sarno¹**, Steve Da Silva¹, Carolina Chaves Prado¹ and William L'Amoreaux², (1)Queensborough Community College - CUNY, (2)College of Staten Island - CUNY


11:20 576 Luminescence, the Instrumental Key to the Future of Nanotechnology. **Adam M. Gilmore**, HORIBA Jobin Yvon Inc.

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**Wednesday, May 21, 2008, 8:30 AM - 12:00 PM**

**Polymers in Medicine/ Bio-Inspired Polymers**

Medical Arts Building, Rm M-143

Organizers: Jin Montclare, SUNY Downstate Medical Center, Richard Gross, Polytechnic University

8:30 577 Nanostructured Tri-Block Copolymer Gels for Pain Management. **Benjamin Chu**, Fen Wan, Chirakkal V. Krishnan and Benjamin S. Hsiao, Stony Brook University

9:00 578 Side-Chain Functionalized Supramolecular Polymers. **Marcus Weck**, New York University

9:30 579 Inherent Antibacterial Activity of a Peptide-Based β-Hairpin Hydrogel. **Daphne A. Salick**, Juliana K. Kretsinger, Lisa A. Haines-Butterick, Darrin J. Pochan and Joel P. Schneider, University of Delaware

10:00 580 Multilayer Multifunctional Magnetic Polymeric Nanoparticles for Imaging and Therapy. **Mostafa Sadoqi¹**, Shah Chintan², Emilio Squillante², Sunil Kumar³ and Richard A. Gross³, (1)St. John's University, (2)St John's University, (3)Polytechnic University

10:30 581 Morphology, Dynamics, and Mechanics of Cells on Electrospun Scaffolds. Ying Liu, Zhi Pan, Richard Clark, Nadine Pernodet and **Miriam Rafailovich**, Stony Brook University

11:00 582 Functional Nanofibrous Scaffolds for Biomedical Applications. **Benjamin S. Hsiao** and Benjamin Chu, Stony Brook University

11:30 583 Self-Assembling Protein Polymers. **Jin Montclare**, Polytechnic University
Wednesday, May 21, 2008, 9:00 AM - 12:00 PM

Organic Chemistry, General Session II

Medical Arts Building, Rm M-136
Organizer: JaimeLee Rizzo, Pace University
Session Overview: This session is for general contributions in the field of organic chemistry.

9:00 Introductory Remarks.

9:05 584 Preparation, Antibacterial Activity and Absorption Spectra of Pyrazolo-Oxadiazine Derivatives. **Fayez M. Eissa**, Awan Faculty of Science

9:25 585 Oxazolone Cycloadducts as Versatile Scaffolds for Alkaloid Synthesis. Charnsak Thongsornkleeb and **Stephen Philip Fearnley**, The City University of New York - York College

9:45 586 Conformational Analysis of cADPR and cADPR Analog Agonists and Antagonists Using PSEUROT, Molecular Mechanics, and Ab Inito Calculations. **Steven M. Graham**, St. John's University

10:05 587 Cognitive Organization and Learning in Organic Chemistry: The See-Think-Predict Method. **Steven M. Graham**, St. John's University and Debra A. Swoboda, York College of the City University of New York

10:25 Concluding Remarks.
Chemical Education, I

Sponsor: Pacific Crest
Organizer: David M. Hanson Stony Brook University, Stony Brook, NY
Organizer: Judy Lloyd SUNY College at Old Westbury

Session Overview: The focus is on innovative curriculum materials and instructional strategies that engage students in learning and promote the development of critical learning process skills that are essential for mastery of course content and success in courses, college, and careers. Presentations describe specific implementations along with their successes and challenges. Topics most relevant to introductory and general chemistry are included in Session I, and organic chemistry and more general topics are covered in Session II. Each presentation is expected to have at least one take-home message or insight.

1. Introduction to Process-Oriented Guided-Inquiry Learning
David M. Hanson, Stony Brook University, Stony Brook, NY

POGIL is both a philosophy and a strategy for teaching and learning. It is a philosophy because it encompasses specific ideas about the nature of the learning process and the expected outcomes. It is a strategy because it provides a specific methodology and structure to achieve these outcomes that are consistent with the way people learn. The motivation for implementing POGIL, the research base that supports it, and the design of POGIL activities will be described. Student outcomes data that document the success of POGIL will be presented.

2. Cooperative Learning in Inorganic Chemistry: Group Activities for Fun and Learning
Elise G. Megehee, St. John's University, Queens, NY

Over the past five years I have developed and implemented 20-25 group exercises in the classroom setting in a senior level inorganic chemistry lecture without appreciable loss of course content. These exercises allow the students to try the calculations or apply a theory and discover what they do and don't understand in the classroom setting. It also has allowed me to understand and quickly correct errors in student understanding of the material. I will discuss the range of activities such as Jeopardy games to make reviewing more interesting, strategies for implementing the activities into the lecture and the observed outcomes.

3. LUCID: Measuring and Improving Learning Outcomes in General Chemistry
Troy A. Wolfskill and David M. Hanson, Stony Brook University, Stony Brook, NY

LUCID is a web-based assessment system that provides many novel features, including POGIL activities with interactive models, support for teams in a computer classroom, peer review, computer analysis of symbolic responses such as molecular structures, and import of form-based responses from examinations. This presentation will focus on LUCID's multidimensional assessment model. Multidimensional assessment goes beyond common score-based assessment by scoring responses with respect to learning objectives. A single response can be associated with one or more objectives and analyzed to determine which have and have not been demonstrated. Taxonomies for classifying
objectives by topic and educational objective (e.g., Bloom’s taxonomy) enable students and instructors to review learning outcomes in multiple dimensions and at varying levels of resolution. Measures of learning outcomes in General Chemistry at Stony Brook will be presented and issues in using such measures to improve student learning will be discussed.

4. Implementing Process Oriented Guided Inquiry in the General Chemistry Course: Introducing New Material Vs Reinforcing Material Already Introduced in Lecture

Terry L. Brack and Sabrina G. Sobel, Hofstra University, Hempstead, NY

As a result of the dual restrictions of using a fixed set of POGIL activities and a fixed recitation time for POGIL work, POGIL sessions introduce some material for the first time and some material after it is presented in the lecture. Similarities in student behavior and their responses to Key Questions in the POGIL activities suggest that student interaction with the material is independent of this temporal modality. This implies that the kind of leaning the student experiences at the POGIL session is, indeed, different from the learning occurring during lecture. The POGIL activities force the student to experience the dissonance between what they think they understand and what they do understand. In order to complete the POGIL Key Questions the student must reorganize the information presented in the Model presented and develop connections between the new concepts and prior conceptual frameworks. Does this carry over into the lecture class as the content of the POGIL session is further developed in lecture?

5. POGIL in Recitation and Laboratory at a Community College

Candice J. Foley and Sharadha Sambasivan, Suffolk County Community College, Selden, NY

The General Chemistry curriculum at Suffolk Community College has implemented POGIL methodology into the laboratory and recitation components through activities developed at national POGIL workshops. We will share our observations regarding the usage of POGIL techniques in the smaller classroom size afforded in a community college setting.

6. Promoting Learning through Group Problem Solving

Madhu Mahalingam, Fred Schaefer and Elisabeth Morlino, University of the Sciences in Philadelphia, Philadelphia, PA

We describe the implementation of group problem solving in recitation sections associated with the general chemistry course at the University of the Sciences in Philadelphia and discuss the impact on exam averages as a result of the structured group work. To supplement the lecture portion of the course, recitation sections limited to approximately 45 students are utilized with the primary goal of having students solve problems in small groups. Students are placed in groups of mixed ability based on math SAT scores in their first semester and regrouped based on their first semester course grades for the second half of the course. The groups provide opportunity for students to interact in solving problems that are specifically designed to foster collaboration and discussion among group members. Students are assigned homework through WebAssign™ prior to the recitation sessions to prepare them for the group activity. In addition, students rate their level of participation and preparation for the group activity and that of their peers twice a semester. The peer evaluation system was modeled after that of Barbara Oakley [Journal of Student Centered Learning, 2 (1) 2004, 9-34]. The students’ recitation scores are adjusted based on the peer evaluation. The effect of this structured group work on exam averages will be presented. We show that it is possible to enhance student learning through implementation of structured group work in the course with minimal changes in faculty hours.
7. Linking Analytical Chemistry and Public Policy through Project Based Labs

Charles Hosten, Howard University, Washington, DC

Project based labs have been introduced into the Analytical Laboratory. The projects were chosen so as to be relevant to our students and bear on their career interests. The projects are divided into two broad areas covering human health issues and environmental issues. The lab also includes a service learning component which is meant to make students examine the relationship between chemistry and societal needs. As an example one project has students conduct test for lead in drinking water and paint samples form old houses in close proximity to the Howard University campus. Washington DC lead poisoning rates are among the highest in the nation and the incident rates for Wards 1, 4, and 5 (located near to Howard University) exceed those of other Wards in the District of Columbia. This revised curriculum results in students who are more aware of precision, accuracy, and error in measurements. It also broadens the horizons of minority students entering the field of chemistry so that they can make connections with human needs outside the classroom.

8. Metropolitan Mentors Network: Growing An Urban STEM Talent Pool with An NSF Funded STEP Grant

Pamela A. Brown, New York City College of Technology - CUNY, Brooklyn, NY

This presentation will focus on how data was used to identify some of the factors contributing to poor retention and graduation rates, and develop a strategy to address the problems. This data-driven approach resulted in a funded National Science Foundation STEP Grant, "MMNet: Growing an Urban STEM Talent Pool Across New York City" (award ID 0622493). Through grant funded activities, combined with coordination of existing efforts, well-marked pathways from high school through the associate and bachelor's degrees to employment or graduate education, and a safety net of academic, social, and economic supports are being created. Activities include creation of unique summer bridge courses, mentoring by City Tech alumni now in graduate school, opportunities for research and internships, and peer-led team learning. This presentation will provide suggestions on preparing successful grants, project implementation, and using assessment to gauge the effectiveness of the program.


Harry D. Gafney and Gopal Subramaniam, City University of New York, Queens College,, Flushing, NY

Pedagogically, commuter students differ from residential students in the time spent on campus and their access to available support systems. The problem is compounded in urban commuter schools where differences in ethnicity, language, religion and different learning styles further separate the students away from campus. This necessitates systems capable of providing support 24/7 and accessible from both on and off the campus. For the past three years, we have been using online homework system, group learning activities based on LUCID, and Chemistry Honor Society tutors to help our students learn the material. These systems are valuable to some students, but fail to reach all students. This presentation will describe a web-based, self-help system that is available to all students at all times. This approach mixes conventional web-based materials with video taped hints, to lead the student through exam-level problems. This approach (1) is not book-specific, (ii) addresses problems that are generally multi-concept and not addressed by commercial online programs, (iii) instructor-led solution broken down to steps starting with a strategic discussion of the problem statement, and (iv) digitized step-wise solution available as sequential video hints only when the student fails to give a correct answer on their own at each step. The self-help tool is evolving further with more content and communication features that allows students to talk to each other and with their instructor. The development of the project as it attempts to connect learning outside-the-classroom with an active in-class learning environment will be presented.
10. Industry to Academe: A Practical Perspective on Teaching
Lance D. Silverman, Yeshiva University, New York, NY

The speaker will share his experiences teaching college chemistry after a productive and varied career in corporate R&D. Dr. Silverman will highlight how student learning can be enhanced by taking advantage of a broad corporate background and bringing many aspects of his earlier career into the classroom. His diverse experiences include inventing and developing products for oil refining, semiconductor manufacturing, forensic analysis, and pharmaceutical development. Teaching in the private sector included training police officers and criminologists in forensic analyses, instructing international customers and sales representatives in the use of analytical instruments, and teaching laboratory technicians analytical procedures. Nonetheless, a career change into teaching brought many challenges, especially how to teach effectively despite students' highly varied technical backgrounds and levels of interest. Taking advantage of the practical, results-orientated perspective gained in industry helps to engage students. Classroom examples drawn from personal experiences in forensics, pharmaceutical manufacturing, and energy production bring home the importance of the knowledge and skills that the students are learning. Measurement of a contaminant and purification of a product take on new meaning, when you are the sole supplier of a lifesaving drug and a test animal just died from an unknown contaminant. The traceability of analytical standards and validation of the procedures become critical issues when you testify as an expert witness in a vehicular homicide-DUI trial. This talk will expand on the speaker's experiences in becoming a teacher after a varied career in corporate R&D, and emphasize what this perspective can bring to enhancing students' learning.

Clinical Chemistry I
Organizer: Clive I. Wynter Nassau Community College, Garden City, NY

11. A Brief Overview of Clinical Chemistry
Clive I. Wynter¹, Eugene Brown¹ and Albert Davis², (1)Nassau Community College, Garden City, NY, (2)Quest Diagnostics, Miramar, FL

Clinical chemistry in its most basic sense relates abnormal values of chemical parameters to one or more disease state(s). With the recent rise in new methodologies due to the discovery of new proteins and their antibodies, clinical chemistry is in a state of flux where new information from the new methodologies are being integrated with old information.

The present talk is a brief overview of the foundation of classical clinical chemistry parameters with the known disease states. It is a review of clinical chemistry 101 and it is intended to be informative of our annual physical biochemical test.

12. Heavy Metals and Chronic Disease
Christopher Calapai, CC medical Services PC, East Meadow, NY

Heavy metals play a significant negative role in human health and well-being. A variety of these metals are in common exposure and most individuals are unaware of their complications. This discussion will include the most common types, occurrence and medical concerns therein. Substances such as aluminum, arsenic, cadmium, mercury, lead, nickel, and copper are associated with a variety of disorders including Parkinson's Disease, MS, ALS, Alzheimer's Disease, Lupus, cardiovascular compromise including heart failure and cardiomyopathy, immune dysfunction, cancer, and developmental disorders including autism. Abstracts from the medical literature have supported these correlations and will be referenced at the presentation.
13. Relationship Between Lifestyle and Degenerative Health Problems among the Youth
Eugene Brown, Nassau Community College, Garden City, NY
This presentation will look at one of the many facets of Complementary Alternative Medicine (CAM). It will involve the relationship between lifestyle and the tremendous growth in the rate and level at which degenerative health problems are reacting. Although this is a general problem, special attention will be given to that which is happening to our youth. That which used to be accepted as problems of aging is now growing like prairie fire amongst our youth. What was the lifestyle of the child then and now? What within the changed lifestyle has become so detrimental to everyone's health? It is not limited to children because our modern day lifestyle is an equal opportunity killer.

14. Simplified Physiological Assays Using Filter Photometry
Jerry DeMenna V, Sacred Heart University / FUN-SCience Academics, Bronx, NY
Most of the World's Technologies depend on ANALYTICAL Science to characterize materials, refine a process or solve a problem. Whether it is an Environmental Application off the Long Island Sound or a Clinical Assay at Nassau County Medical Center... it is critical to have the correct Analytical Instrument to accurately do that job. Many of the routine test procedures in a Medical Technology Laboratory can be done with fairly simple, often automated Instrumentation... either Electro-Chemistry, Spectroscopy or Chromatography. Based on the defined “Standard Methods of Analysis” from NIH, NCCLS and other Regulatory agencies, a number of simplified Clinical Lab tests can be done with compact, economical Filter-based Photometer systems, instead of the more expensive and complex Diffraction Grating-based Spectrophotometer Instrumentation.

The inherently more rugged and smaller design of a Filter Photometer makes it ideal for the high-throughput Clinical / Med Tech Lab; and the simple operation of these units are well-suited for use by multiple personnel with varying backgrounds and expertise.

This talk will review some Assays that can be performed with a Filter UV-Fluorescence Photometer for Free Amino Acids, Vitamins and Drug Screening; and also a Flame Emission Photometer which is a quick and accurate procedure for determining the Electrolyte Metals (Na, K, Mg & Ca) and some of the more common Drug & Metabolite precursors (Li & P). Examples of Calibration and Sample Analyses will be shown, and Instruments will be demonstrated in the Exhibitions area.

15. Inhibition of Intrinsic Peptidase Activity Moderates Sequential Digestion of Human Plasma Peptides
Jizu Yi, Zhaoxia Liu, Gang Ju and Craig A. Gelfand, BD Diagnostics, Franklin Lakes, NJ
We have previously reported that intrinsic protease activity in plasma and serum samples cause ex vivo variability and instability of samples (Yi et al, J. Proteome Res. (2007) 6: 1768-1781). In this study, we investigated stability of peptide biomarkers in human plasma and serum. Biomarkers were tested in five blood samples: serum or plasma with either citrate, heparin, or EDTA as anticoagulant, or EDTA plus protease inhibitors (BD P100*). After incubation of the sample spiked with a peptide (FPA, GLP-1, BNP, C3 and C4) for a specified period ranging from 0 minute to 72 hours, the peptides were extracted and analyzed by MALDI-TOF MS. The results indicate that all tested biomarkers are decreasing over time, demonstrating their proteolytic instability in these different blood products. Within the same serum or plasma sample, each peptide shows a unique half life, suggesting that the peptidase specificity differs between peptides. However, the spiked peptides are the most stable in the protease-inhibited plasma by inhibition of intrinsic proteolysis. The stability of the peptides in different collected samples is as following order: P100 plasma > EDTA > Citrate & Heparin > Serum. Furthermore, kinetic analysis of the fragments of digested FPA suggests that the intrinsic peptidase activity cause a first-order, sequential multiple step reaction (SMSR). The modeling analysis of the SMSR indicates a significant contribution of the end leaving reside on the stability of the peptide. The applications of these observations to plasma proteome research will be further discussed.

Footnote: * For research use only.
**Forensic Chemistry**

**Organizers:** Anthony Carpi John Jay College of Criminal Justice, CUNY, New York, NY  
**Organizer:** Lawrence Kobilinsky John Jay College of Criminal Justice, CUNY, New York, NY

**Gloria Proni**, Donna Wilson and Elise Champeil, John Jay College of Criminal Justice, New York, NY

In this preliminary report we explore the possibility of using 1H nuclear magnetic resonance (1H NMR) spectroscopy for the detection of opioids in urine.

Several techniques are currently available to detect opioids in this biological fluid. High performance liquid chromatography (HPLC) and gas chromatography - mass spectrometry (GC-MS) are the most frequently used. Nevertheless, these methods require a labor intensive sample preparation, extraction of the drugs, and in the case of GC/MS, derivatization.

Without any pretreatment, the presence of opioids in artificial urine was confirmed by characteristic resonance peaks in the NMR spectra. Data for few members of the opioid family and the limits of the technique are also presented.

17. The Use of Micro-ATR Spectroscopy to Study the Effect of PH Variation on Changes in Dyed and Non-Dyed Female Hair Exposed to Antipsychotic Agents  
**Ali Kocak** and Zann S. Blanchard, John Jay College, CUNY, New York, NY

Antipsychotic drugs are one of the mostly used medications and, similar to drugs of abuse, are usually administrated for a long period of time. Due to accumulation and trap of drugs, hair provides a useful indication of long-term exposure to drugs. Micro-ATR spectroscopic methods can examine the structural changes of the hair sample by applying sufficient pressure and without microtoming the hair sample.

In this investigation, female hair samples (before and after dyed) were spiked externally with two different antipsychotic drugs, Clozapine and Haloperidol and their respective effect at different PH ranges (PH: 2.0, 7.0, 9.0) on the structure of the hair samples was observed.

**Mark Gil**¹, Mario Louis² and **Nicholas D. K. Petraco**², (1)New York City Police Crime Laboratory, Jamaica, NY, (2)John Jay College of Criminal Justice, New York, NY

The intention of this study was to differentiate liquid gasoline samples from casework as well as different brands of liquid gasoline purchased from local gas stations by utilizing multivariate pattern recognition methods on data from gas chromatography-mass spectrometry. A supervised learning approach was undertaken to achieve this goal employing the methods of principal component analysis, canonical variate analysis, orthogonal canonical variate analysis, linear discriminant analysis, support vector machines and neural networks. The study revealed that the variability in the sample of gasolines form casework was sufficient enough to distinguish all the samples from one another using the classical methods of discrimination. New results using support vector machines and neural networks will be presented.
19. Forensic DNA Testing in New York City

Noelle J. Umback, New York City Office of Chief Medical Examiner, New York, NY

The Department of Forensic Biology of the New York City Office of Chief Medical Examiner (OCME) performs the DNA testing for thousands of cases each year from all five boroughs of New York City. Cases range from homicides and sexual assaults to burglaries and robberies to the identification of unknown persons; the samples tested are typically blood and other body fluids, as well as epithelial cells or bone. The results of such testing can be used to link people to other people, people to crime scenes, or people to evidence. The majority of DNA cases are tested using short tandem repeat (STR) polymerase chain reaction (PCR) testing at 13 or more locations of nuclear DNA. When eligible, the DNA profiles generated are submitted to the national DNA database, to be compared to results from forensic labs across the state and across the country. Analysts from OCME provide expert witness testimony at court when necessary, to interpret their results for jurors. A review of the science involved in creating DNA profiles will be offered, as well as some cases which were solved using DNA testing.

20. Mitochondrial DNA Testing at the New York City Office of Chief Medical Examiner

Paul Goncharoff, Jessica Harris, Veronique Bourdon, Kristy Bernard and Eli Shapiro, Office of Chief Medical Examiner, New York, NY

The Department of Forensic Biology, New York City Office of Chief Medical Examiner, is responsible for all of the City's DNA testing in all criminal cases, such as homicides, sexual assaults, and property crimes. DNA testing is also conducted for body identification and missing persons cases. The DNA testing methodologies used include short tandem repeat (STR) analysis of human nuclear genomic DNA and DNA sequencing of mitochondrial DNA (mtDNA). Generally, mtDNA analysis is many orders of magnitude less discriminative than is STR nuclear DNA testing. Yet occasions and sample types do arise where nuclear DNA testing is inconclusive while mtDNA testing provides a conclusive result. Therefore mtDNA testing is used as supporting evidence for STR nuclear results and in cases where STR nuclear DNA testing fails to give results. This talk will review the current methodologies for mtDNA testing at the NYC Office of Chief Medical Examiner in addition to presenting several case examples where mtDNA testing provided useful results.

**Organic Chemistry, General Session I**

**Sponsor:** Mettler-Toledo AUTOCHEM; Pearson Prentice

**Organizer:** JaimeLee Rizzo, Pace University

**Session Overview:** This session is for general contributions in the field of organic chemistry.

21. Synthesis of An Oligodeoxyribonucleotide Adduct of Mitomycin C by the Postoligomerization Method, Via a Triamino Mitosene

Elise Champeil, John Jay College, New York, NY, Manuel M. Paz, Universidade de Santiago de Compostela, Lugo, Spain and Maria Tomasz, Hunter College, New York, NY

We report here the first alternative access to one of the DNA adducts of Mitomycin C, an antitumor antibiotic used in clinical cancer chemotherapy (MC), based on organic synthetic methods, featuring a postoligomerization. Specifically, we describe a synthesis of monoaadduct 8 on both the nucleoside
and oligonucleotide levels. MC has numerous sensitive functional groups and the adduct described herein is, to the best of our knowledge, the most complex DNA adduct synthesized by the post-oligomerization strategy to date. Adduct 8 is a major adduct in MC-treated tumor cells. However, in biomimetic reactions in vitro it is formed only in trace quantities. We present now definitive 1H NMR characterization of adduct 8. The present synthetic approach to the previously unavailable sister adduct 8 will provide a substrate to examine the biological and structural properties of 8 in parallel with its major groove adduct counterpart and the other minor groove guanine-N2 monoadducts of MC.

22. Mechanism for NAD⁺ Hydrolysis at pH 9 as Determined by Kinetic Isotope Effects and Computational Analysis

Yana Cen and Anthony A. Sauve, Weill Medical College of Cornell University, New York, NY

There has been long interest in understanding the chemical mechanisms of NAD⁺ hydrolysis. These mechanisms are characterized by pH independent and pH dependent regimes. Below pH 6 hydrolysis reaction rate is pH-independent and complete KIE analysis has determined a transition state involving an oxocarbenium ion, which has low bond orders to the nicotinamide leaving group and the incoming water nucleophile. Between pH 7 and 11 the log of the rate constant is linearly dependent on pH, and becomes pH independent at pH values above 11. This profile suggests a mechanism dependent on sugar ionization, although to date the specific mechanism by which NAD⁺ hydrolysis is accelerated by sugar ionization is unexplained. To determine the role of sugar ionization on hydrolysis, we investigated the transition state structure of NAD⁺ hydrolysis at pH 9 using competitive kinetic isotope effects and density functional calculations (Gaussian03, ISOEFF07). A family of KIEs was determined for the hydrolysis reaction at pH 9, using competitive-radiolabel method. Primary isotope effects were 1.15 for 1'N-C¹⁴-NAD⁺ and 1.024 for 1N-N¹⁵-NAD⁺. Secondary KIEs were 1.22 for 1'N-H³- and 1.09 for 2'N-H³-NAD⁺, respectively. The KIEs suggest strong nucleophile participation at the transition state in the hydrolysis reaction. However, vibrationally less constrained environments for both the 1'N- and 2'N-hydrogens suggest that sugar ionization leads to an epoxide-product like transition state.

23. Hantzsch Synthesis of 1,4-Dihydropyridines

Krystsina Ivanova, New Jersey City University, Jersey city, NJ

A family of 1,4-dihydropyridines (1,4-DHP) were synthesized via the Hantzsch condensation reaction using microwave energy. The synthesis of this 1,4-DHP compounds was optimized from a variety of aldehydes, urea and ethylacetoacetate. Most of these products commercially synthesized and serve as a main ingredient in drugs for treatment of high blood pressure. It also function as a “calcium channel blockers” to prevent heart failure and arterial aneurysm.

24. Studies toward Total Synthesis of Angelmicin B

Jialiang Li and David R. Mootoo, Hunter College, New York, NY

Angelmicin B (hibarimicin B) has been shown to be a highly specific inhibitor of ν-Src type protein tyrosine kinase (IC₅₀: 23 μM). It has also been shown to inhibit the growth of tumor cells and to induce differentiation in human myeloid leukemia cell lines HL-60 (IC₅₀: 57 nM). The complexity and the intriguing bioactivity make it an important synthetic target. We have previously described a Ring
Closing Eneyne Metathesis/Intramolecular Diels-Alder, and tandem alkoxy radical fragmentation-etherification sequence for the synthesis of AB subunit synthon. Herein we present the further advances toward the total synthesis of Anglemicin B.

25. A New Type of Karplus Equation? Dependence of Phosphorus-Hydrogen Coupling Constants on Lone-Pair Conformation

William H. Hersh, Sherrell T. Lam, Daniel J. Moskovic and Antonios J. Panagiotakis, Queens College of the City University of New York, Flushing, NY

In contrast to literature reports of a Karplus-type curve that correlates $^{3}J_{PH}$ with phosphorus-hydrogen dihedral angle, the recently-reported glycine-derived phosphorus heterocycle shown has two hydrogen atoms on the ring with identical PNCH dihedral angles but measured coupling constants of $\sim 6$ Hz and 1.5 Hz. DFT calculations suggested that the smaller coupling constant is negative. Experimental evidence of the sign of the coupling constant was obtained by analysis of the ABX NMR spectrum of a new glycine-derived $N$-p-toluenesulfonyl analogue. Calculation of the phosphorus-hydrogen coupling constants of $(\text{CH}_3)_nYPH_2$ ($Y = C, n=3$; $N, n=2$; $O, n=1$) both as a function of the PYCH dihedral angle ($\theta$) and the lone pair-YPY dihedral angle ($\omega$) showed similar $\theta, \omega$ surfaces for $^{3}J_{PH}$, and a range of $^{3}J_{PH}$ from $-4.4$ Hz to $+51$ Hz. While a modified Karplus equation as a function of $\theta$ and $\omega$ can be derived and provides qualitative agreement, no single equation can suffice to provide quantitative predictions for a range of atoms. DFT calculations provide a simpler means to accurately determine $^{3}J_{PH}$.

26. Use of ReactIR in Studying Fundamental Organic Reactions and Flash Chromatography

John R. Sowa Jr., Seton Hall University, South Orange, NJ and Jian Wang, Mettler-Toledo Autochem, Columbia, MD

In this presentation we will present our studies of fundamental organic reactions and separations by in situ IR spectroscopy. This type of analysis allows deeper insight into spectroscopy, reaction analysis, kinetics and dynamics of these fundamental processes. There is potential benefit for research as well as education. So far, we have investigated standard sophomore organic
experiments such as acetylation of aniline and the Williamson ether reactions. We have also developed a flash chromatography procedure monitored by ReactIR which wonderfully illustrates the dynamics of a flash chromatography separation.

27. Regioselective Acylations of Isosorbide: Synthesis, Characterization and Radical Polymerization of Isosorbide (Meth)Acrylate Esters

Liliana Craciun, Orest Polishchuk, George W. Schriver and Ronald Rodebaugh, Ciba Specialty Chemicals, Tarrytown, NY

1,4:3,5-Dianhydro-D-glucitol (isosorbide) is a chiral, thermally stable, biomass-derived bicyclic diol with a conformationally rigid structure made of two tetrahydrofuran rings fused in a cis junction. Catalytic hydrogenation of glucose to sorbitol followed by acid-catalyzed dehydration easily yields enantiopure isosorbide. Numerous isosorbide-containing thermoplastic polymers were prepared and characterized, showing high temperature performance, good impact strength, optical clarity, and biodegradability. The two hydroxy groups in isosorbide, one oriented exo- (C2) and the other endo- (C5), are diastereotopic and exhibit different reactivities. Herein, we report our efforts to efficiently and selectively synthesize isosorbide mono-exo, mono-endo and di- (meth)acrylates. The synthesis, characterization and polymerization kinetics of isosorbide (meth)acrylic esters are presented. The observed selectivities of various acylation procedures are discussed in relation to isosorbide stereochemistry and esterification mechanisms. All isosorbide (meth)acrylate esters were found to polymerize easily, and furnished hard, colorless, and infusible resins. Thermal properties of several isosorbide-containing acrylic polymers and co-polymers, i.e. glass transition temperature and decomposition behavior, are described. The carbohydrate-derived core could potentially make these monomers suitable for applications from chiral auxiliaries in cholesteric color filters, asymmetric reactions, or chromatography columns, to biodegradable building blocks in template-imprinting polymers.
**BioTherapeutics**

**Sponsor:** Pfizer  
**Organizer:** Susan A. Rotenberg Queens College, Flushing, NY  
**Organizer:** Regina Sullivan Queensborough Community College, Bayside, NY  
**Organizer:** Barbara Petrak Drew University

28. New Therapeutics from Transition State Theory  

**Vern L. Schramm,** Albert Einstein College of Medicine, Bronx, NY

Computational chemistry combined with experimentally determined multiple intrinsic kinetic isotope effects provide atomic maps of substrates at their enzymatic transition states. The transition state structures of bovine and human purine nucleoside phosphorylases (PNPs) are distinct, despite homologous catalytic sites. Specific transition state analogues have been synthesized as isozyme-specific enzymatic inhibitors. Immucillin-H is similar to the transition state of inosine in bovine PNP and has Kd values of 23 and 56 pM for bovine and human PNPs, respectively. DADMe-Immuclllin-H was designed to mimic the transition state structure of 2'-deoxyinosine at the transition state of human PNP and has Kd values of 9 and 110 pM for human and bovine PNPs, respectively. These compounds are in clinical trials for leukemia and autoimmune diseases. A transition state analogue of Plasmodium falciparum PNP shows 112-fold specificity for parasite PNP relative to human PNP and kills cultured parasites. The transition state structure of human 5'-methylthioadenosine phosphorylase (MTAP) has led to pM transition state analogues with activity against solid tumors. Inhibitors designed to match the transition state structures of bacterial 5'-methylthioadenosine nucleosidases (MTANs) are active in blocking quorum sensing in cultured bacteria. Powerful inhibitors designed from transition state theory are demonstrating promise as new therapeutics for several diseases.

29. Development of PCK3145, a Novel Multi-Targeted Anti-Tumor Agent for Prostate Cancer  

**Susan F. Slovin,** Memorial Sloan-Kettering Cancer Center, New York, NY

PCK3145 is a synthetic 15-mer peptide derived from Prostate Secretory Protein (PSP94), a protein found in human seminal fluid, which has been shown to inhibit extracellular matrix (ECM) degradation by MMP-9, a matrix metalloproteinase involved in prostate cancer progression. PSP94 is one of three predominant proteins found in human seminal fluid along with PSA and prostate acid phosphatase. Prostate cancer cells express receptors on their surface that selectively binds to PSP94. Exogenous PSP94 inhibits tumor cell growth through an unknown mechanism. Its mode of action may involve activation of apoptosis via a receptor-mediated signal transduction pathway. PCK3145 subserves several functions and appears to work in animal models as an inhibitor of angiogenesis by rapid onset of binding to the laminin receptor in a “hit-and-run” fashion to downregulate Erk, and to reduce plasma MMP-9 levels, as well as the expression of MMP-9 within tumor. In a phase I dose escalating study, patients (pts) with castrate metastatic prostate cancer who failed hormones and chemotherapy were treated at different dose levels and schedules. Pts treated at all dose-levels had precipitous declines in plasma MMP-9 levels while on the drug; these rose once the drug was discontinued. While safe, pts with disease to bone and/or lymph nodes who progressed despite prior treatment with hormones and chemotherapy have radiographically stable disease and lengthening of PSA doubling times for close to two years. These results were unexpected given the natural history of progression for those patients who have failed prior treatment with hormones and/or chemotherapy.
30. DNA Vaccines - Design, Development and Application

Rangappa Ramachandra, Covance Research Products, Denver, PA

The discovery and advances in molecular biology and biotechnology resulted in the newest generations of biologics – DNA vaccines to prevent infectious diseases. DNA vaccines mediate both humoral and cellular immune response and are efficacious even in the presence of maternal antibodies in young individuals. DNA vaccines work by introducing genes of the infectious agents into host cells that encode for an antigen that induces protective immune responses. DNA vaccines can contain one or more antigenic epitope either from virus or bacteria structural proteins. The DNA vaccines can be delivered in various ways: naked DNA injected intramuscularly, attached to a microscopic gold or tungsten beads and pushed into the skin a helium blast, using electric field, or incorporated into live, attenuated non-pathogenic viruses or bacteria. Another exciting aspect of DNA vaccines is their potential use as a therapeutic vaccine. The presentation will highlight the current status of DNA vaccine development, molecular designs, delivery methods, adjuvants, and development and testing of vaccines.

31. Structure-Based Design of An Organoruthenium Phosphatidyl-Inositol-3-Kinase Inhibitor Reveals a Switch Governing Lipid Kinase Potency and Selectivity

Peng Xie¹, Douglas S. Williams², G. Ekin Atilla-Gokcen⁴, Leslie Milk³, Min Xiao¹, Keiran S.M. Smalley¹, Meenhard Herlyn¹, Eric Meggers² and Ronen Marmorstein⁴, (¹)The Wistar Institute, University of Pennsylvania, Philadelphia, PA, (²)University of Pennsylvania, Philadelphia, PA, (³)Graduate Group in Biochemistry and Molecular Biophysics, School of Medicine, Philadelphia, PA, (⁴)The Wistar Institute, N/a, PA

Mutations that constitutively activate the PI3K signaling pathway, including alterations in PI3K, PTEN and AKT are found in a variety of human cancers, implicating the PI3K lipid kinase as an attractive target for the development of therapeutic agents to treat cancer and other related diseases. In this study, we report on the combination of a novel organometallic kinase inhibitor scaffold with structure-based design to develop a PI3K inhibitor, called E5E2, with an IC50 potency in the mid-low-nanomolar range and selectivity against a panel of protein kinases. We also show that E5E2 inhibits phospho-AKT in human melanoma cells and leads to growth inhibition. Consistent with a role for the PI3K pathway in tumor cell invasion, E5E2 treatment also inhibits the migration of melanoma cells in a 3D spheroid assay. The structure of the PI3Kα/E5E2 complex reveals the molecular features that give rise to this potency and selectivity towards lipid kinases with implications for the design of a subsequent generation of PI3K-isoform specific organometallic inhibitors.
Chemical Education, II

Sponsor: Cengage Learning
Organizer: David M. Hanson Stony Brook University, Stony Brook, NY
Organizer: Judy Lloyd SUNY College at Old Westbury

Session Overview: The focus is on innovative curriculum materials and instructional strategies that engage students in learning and promote the development of critical learning process skills that are essential for mastery of course content and success in courses, college, and careers. Presentations describe specific implementations along with their successes and challenges. Topics most relevant to introductory and general chemistry are included in Session I, and organic chemistry and more general topics are covered in Session II. Each presentation is expected to have at least one take-home message or insight.

34. Organic Chemistry for a Thousand
Joseph W. Lauher and Frank W. Fowler, State University of New York at Stony Brook, Stony Brook, NY

This academic year the organic chemistry course at Stony Brook reached an important milestone when the fall enrollment passed the thousand student mark for the first time. An advanced course of such a large size requires special teaching strategies. During the last few years we have modified many aspects of the course to accommodate the increased numbers and to better serve our students.

Conventional lectures have been replaced by student-centered sessions that rely heavily upon CPS clickers. Each student now attends an 80 minute workshop session. A Chemistry Learning Center has been created for walk-in office hours. An army of undergraduate TAs has joined a smaller number of graduate TAs to cover our many workshops and to staff the Learning Center. Examinations have been modified to allow for efficient and uniform hand grading combined with computerized analysis of the results. Personalized web pages are used for communication of examination results to each student. Some of our changes have worked better than others. This presentation will discuss the high-lights. The low-lights are best forgotten.

35. Using a Combined Lecture/Workshop Model to Improve Student Engagement and Self Confidence in Undergraduate Organic Chemistry
Karen E. S. Phillips, Hunter College of the City University of New York, New York, NY

This qualitative study focuses on a combined Lecture/Workshop model for Organic Chemistry instruction. The Workshop is viewed as a site of cultural production and reproduction in which Organic Chemistry is the currency of capital exchange. Specific structures within the Workshop diminish the typical hierarchy associated with science classrooms while increasing student agency. Concepts introduced in lectures are discussed within small interactive sub-groups, with novel, often ambiguous and challenging problems providing the impetus for deep discussion. Students who have already completed the course provide “gentle” guidance during this discussion phase. Self-appointed representatives of each group then explain their solutions to the class, whose members are free to agree or disagree with the explanations given. All students are encouraged to voice their opinions, propose alternatives, and collectively apply their conceptual understanding toward determining whether the proposed solution is accurate and acceptable while continually using the language and syntax specific to the subject. Data gathered from videotape of Workshop activities, student interviews and course evaluations suggest that both components of the Workshops bolster critical thinking skills among students and, together, set the stage for an iterative cycle of increased
engagement and self-confidence in Organic Chemistry. Students report that they are able to apply critical thinking skills developed during this course toward subsequent college work, that they have an easier time on other class exams and on high-stakes standardized tests, and that they have a greater sense of community in college as a result of their involvement in this combined Lecture/Workshop model.

36. How I Increased My Organic Chemistry Class Average 20 Percentile Points
Peter J. Wepplo, Princeton, NJ
Organic chemistry is a notably difficult course. What is the best pedagogy to use? Which textbooks? How can one use POGIL based teaching in a lecture style course without recitation sections? What methods should you use and how do you incorporate them into your class? This is a retrospective look at methods and results.

My teaching started as how I had been taught. Why did student results not match my results? What did I do that students did not?

Organic chemistry has two (or three) major focal points. One is the description and terms associated with chemistry. The second are reaction mechanisms. They present a special challenge to students because they are dynamic. The objective is not what you have, but what it can become. My experience suggests they are the greatest challenge for students and the most important variable responsible for individual scores on the ACS exam. Of many methods, which ones were the most successful?

The percentile ranking on the ACS organic chemistry exams were recorded for all classes and the results of teaching changes will be discussed.

37. Anathons in Developing and Solving Ozonolysis Problems
Ray A. Gross Jr., Prince George's Community College, Largo, MD
Anathons are partial structures found in an analyte, the compound being analyzed. It will be shown how certain anathons can be used to construct hydrocarbons that have structures, which students can determine by an analysis of the ozonolysis products. The compounds afford instructors with a diverse set of structure-determination problems. The compounds have from one to four pi bonds and zero to three rings. Molecular formulas of reaction products, and in some cases, the molecular formula of the reactant are the only data provided to students. Solutions require only a basic knowledge of ozonolysis reactions, but many require students to apply the kind of logic and reasoning that instructors desire to foster in students. Instructors can help students improve their reasoning skills by engaging them in these problems.

38. Student Motivation and Reform in the Organic Laboratory
Gail Horowitz, Yeshiva University, New York, NY
Recent reform efforts in the organic lab have focused primarily on the design of discovery based experiments and project based experiments. This presentation will begin by briefly examining the motivational theories that link these reforms to the enhancement of student motivation. This will be followed by a brief presentation of research findings regarding the intrinsic motivation of students who participated in a project based curriculum, that centered around the adaptation and rescaling of an Organic Syntheses procedure.

David W. Parkin, Adelphi University, Garden City, NY

Chemistry in Context Approach to Teaching Allied Health Chemistry

“Why do I have to learn chemistry, I just want to be a nurse” is arguably the most common question asked by students. A major chasm exists between a chemist’s perception of our courses’ relevance and how allied health students perceive this relevance. I propose we need to introduce biochemical/chemical concepts in the context of medicine and/or physiology. Let’s first focus on the play (physiology), then show students the actors (chemical structures), and how the “actors” work together (chemical reactions or concepts). Finally, we enable our students to see the relationships these chemical/biochemical concepts to the physiological event. Adelphi University’s Physiological Chemistry focuses on the integration of observed physiological events with the underlying biochemical/chemical principle(s). Modules include Prostate Cancer (nature of the atom and periodicity), Chemical Communication (organic chemistry and molecular recognition), and Oxygen and Carbon Dioxide Transport (stoichiometry and Le Chatelier’s Principle). When students make meaningful connections between their inherent interests (physiology) to the chemical/biochemical concepts they should retain these concepts in long term memory instead of short term memory. Meaningful learning underlies the constructive integration of thinking, feeling, and acting, leading to empowerment for commitment and responsibility (Joseph D. Novak). Our hypothesis is meaningful learning has a greater potential to occur if a meaningful learning environment is created. The Chemistry Self-Concept Inventory and CHEMX (chemistry cognitive diagnostic survey) are the diagnostic tools used to evaluate if a meaningful learning environment has been created.

40. Molecules of Life: Exploring Chemical Principles in a Biological Context

Trace Jordan, New York University, New York, NY

We have developed a lecture and laboratory course for non-science majors at NYU that teaches chemical principles through the context of biological molecules. This approach reflects the current trend in scientific research where chemistry and biology meet at the interface of “chemical biology.” Whenever possible, the course uses current issues to engage students with learning chemistry – for example, our section on organic chemistry begins with a consideration of “trans fats.” This presentation will describe the educational goals of the course and the preliminary results of assessment tests of student learning in the areas of three-dimensional visualization and drug development. This project is supported by NSF grant 043014 from the Division of Undergraduate Education.

41. Adding Scientific Process to Chemistry Instruction

Anthony Carpi, John Jay College, New York, NY

Teaching the process of science is critical at the undergraduate level because many students enter college with minimal understanding of the scientific endeavor beyond methodical procedure (Moss et al., 2001; Bell et al., 2003). Unfortunately, the vast majority of students are never taught scientific process; instead, science is presented to them as a system of discipline-specific facts to be memorized. A growing number of studies point to the effectiveness of explicitly teaching the nature and process of science; however textbooks fail to provide any support in this area (Dagher & Boujaoude, 1997). This project was funded in 2006 by the U.S. Department of Education FIPSE program to develop a series of materials targeted at explicitly teaching scientific process. Topics in the series include: Scientific Process and Knowledge, Experimentation, Scientific Theories, Scientific Controversy, Ethics, and more. These materials will be launched and freely available online (http://www.visionlearning.com) where they will be paired with disciplinary science lessons (Atomic Theory, the Periodic Table, Chemical Kinetics, etc.). In this way, they will allow instructors to teach a
stand-alone scientific process course or integrate scientific process directly into disciplinary science courses including general chemistry. This presentation will discuss the materials being developed in more detail and the project's progress to date.

42. Impact of Microcomputer-Based Laboratory Experiences on Content-Related Performance in Science

Fernando Espinoza, SUNY Old Westbury, Old Westbury, NY

The development of scientific literacy, the main goal of the National Science Education Standards can be enhanced through learning environments that incorporate physical experience in the form of direct interaction with natural phenomena, since these have been shown to be more effective in promoting learning than those that don't (Lawson, 1986; Druyan, 1997).

The availability of powerful means of data collection and analysis can transform the traditional role of the laboratory from one of being confirmatory of concepts previously studied and presumably learned, to becoming an exploratory inquiry-based setting. A study of high school students using microcomputer-based chemistry and physical science laboratory activities to predict and observe experimental outcomes provided the means to link process skills, and content retention. Two significantly positive correlations were found: 1) That between the use of two different modes of prediction and the ability to correctly predict an experimental outcome, consistent with previous findings of the performance of high school teachers in the use of the technology in life science and physical science tasks (Espinoza, 2006); 2) That between successful experimental outcomes and a gain in students' performance on content-related tasks.

43. Student Assessment of Engagement in a “Clicker” Classroom

Daniel B. King, Drexel University, Philadelphia, PA

It has been widely reported by faculty that personal response devices (or “clickers”) improve student engagement in the classroom. However, these observations are generally anecdotal, without formal assessment. An attempt was made to quantify this effect. Clickers have been used in a large-enrollment general chemistry class and in upper-level chemistry courses. Student engagement was assessed with several instruments in these classes. A survey was distributed at the start and end of the term in which students reported the percentage of class time they spent at various levels of engagement. Specific questions were added to the end-of-term course evaluations to determine the effectiveness of the clickers. Finally, student usage of the clickers was analyzed over the course of each term. While student feedback about the clickers was positive and exam grades were higher for students who used the clickers on a consistent basis, the student engagement survey generally showed only minimal, if any, increase in engagement in sections where clickers were used.
Clinical Chemistry II and Clinical Chemistry Workshop

Organizer: Clive I. Wynter Nassau Community College, Garden City, NY
Workshop Leader: Jerry DeMenna Sacred Heart, Buck Scientific, Fairfield, CT

Session Overview: This will be a continuation of the morning symposium followed by a workshop session on Clinical Chemistry.

44. Heart Failure: Recent Advances in Diagnosis and Management
Felix Oviasu, Garden City Heart Center, Garden City, NY
This lecture summarizes recent progress in the diagnosis and treatment of Congestive Heart Failure including the use of different imaging modalities.

45. Enriching Patient Population in Oncology Drug Development through Proteomic Studies
Jiwen Chen, Bristol-Myers Squibb, Pennington, NJ
Due to the exceptional biological complexity, heterogeneity and adaptability of human tumors, many investigational drugs in oncology has low response rates in cancer patients. These present a significant hurdle in drug development. One approach of overcoming this problem is to select a subset of patients who are likely to benefit from the therapy. In this study, from an exploratory oncology trial we identified a set of plasma protein makers by label-free protein profiling that differentiated responders from non-responders.

 Plasma samples were collected from patients treated with an investigational drug. Following removal of the top 12 abundant proteins in plasma by affinity depletion, the samples were digested by trypsin. The resulting peptides were analyzed by high resolution LC-MS. Peptides with abundance significantly different between the responder and non-responder groups were sequenced by LC-MS/MS and their corresponding proteins were identified by data base searching

 A set of plasma proteins had expression levels significantly different between the responders and non-responders (p < 0.0001). These markers were in a signaling pathway closely related to the drug target. These results suggested that tumor cells might be unresponsive to the inhibition of the drug target due to the presence of parallel signaling pathways

 This work demonstrated the feasibility of using plasma proteins as biomarkers to select for cancer patients who would likely respond to the investigational drug

46. Oncolytic Herpes Simplex Virus-1 (NV1023) Effectively Treats Anaplastic Thyroid Cancer in An Orthotopic Murine Model
Vincent Reid, South Nassau Communities Hospital, Oceanside, NY and Rickahrd Wong, The Memorial Sloan Kettering Cancer Center, New York, NY

Introduction

Anaplastic Thyroid Cancer (ATC) is one of the most aggressive human malignancies with a median survival of six months and a fatal prognosis. ATC is notoriously resistant to conventional therapy and as such, novel therapies are needed. This study evaluates the efficacy of the recombinant herpes oncolytic virus NV1023 in a murine orthotopic model.

Material and Methods
NV1023 is an attenuated, replication-competent mutant of HSV-1. The ATC cell line DRO90-1 was transfected with constitutively expressed Renilla luciferase and is designated RLucDRO90-1. Nude mice underwent direct intrathyroidal injection with 1e6 RLucDRO90-1 cells. After 13 days, mice were randomized to receive treatment with intratumoral NV1023 or saline. Tumor progression was followed using serial bioluminescence imaging and tumor volumes were measured at autopsy.

Results

RLucDRO90-1 tumors grew rapidly and reliably in the murine thyroid with local tracheal invasion. Bioluminescence imaging allowed for non-invasive tracking of tumor burden. Tumor fluorescence intensity was significantly decreased for animals in the NV1023 treated group. Average fluorescence intensity was 68200 units in the virally treated group and 221800 units in the saline treated group at day 23 of the study (P<0.05). Average tumor volumes were 1229.44 mm³ (± 727.67) and 151.93 mm³ (± 55.15) in the saline and virally treated groups respectively at autopsy (P<0.05).

Conclusions

RLucDRO90-1 is a novel, stably transfected cell line that grows reliably and invasively in an orthotopic murine model of ATC, and allows for non-invasive in vivo monitoring of tumor burden. Intratumoral injection of NV1023 effectively treated ATC in this model.

47. Treatment of Type 2 Diabetes

Kenneth H. Hupart, Nassau University Medical Center, East Meadow, NY

The epidemic of Type 2 Diabetes(DM2) that confronts the population of the US is well documented in scholarly publications and in the popular press. In the US, 7% of the population suffers from this disease. Diabetes prevalence increases with age; 20% of Americans >65yrs are affected. Diabetes disproportionately affects people of color, the poor, and those of low educational attainment. Obesity, lack of aerobic physical activity, and diet also make diabetes more likely to affect individuals. Type 1 Diabetes (formerly Juvenile Diabetes), is an autoimmune disease resulting in the destruction of pancreatic β-cells and absolute insulin deficiency. DM2 (formerly Adult-onset Diabetes), is characterized by a cellular resistance to insulin's effect. Early during the disease course DM2 patients demonstrate elevated circulating insulin concentrations, but with time, an insulin secretory defect develops. DM2 accounts for 90-95% of Diabetic cases. Its prevalence is increasing and now affects adolescents, a previously rare event. Many with DM2 are asymptomatic; perhaps 1/3 patients are unaware that they are affected. Individuals with impaired fasting glucose or impaired glucose tolerance have come to be referred to as Pre-Diabetics; this also affects 7% of the population. Life-style change more effectively prevents progression to overt Diabetes than medication. Diabetes treatment prevents or delays the emergence of complications such as kidney failure, nerve disease and blindness. Important aspects of care target blood glucose, serum cholesterol, blood pressure, and aspirin treatment. Recently there have been new pharmaceutical targets harnessed in the service of controlling blood glucose. Current therapeutic approaches will be reviewed.
Session Overview: HIV/AIDS has many faces. On the research side there are new therapies to be invented. New drugs with new mechanisms are needed to beat the ever present threat of drug resistance. Vaccines and microbicides are still not on the market, and antiretroviral drugs that are on the market in western countries are still waiting to get the green light to be produced and made available in developing countries.

48. Development of a Microbicide to Combat HIV

David Fairhurst, International Partnership for Microbicides, Silver Spring, MD

Activated by the slow pace of progress in developing a vaccine for AIDS, one proposed approach to slow, or reduce the spread of HIV, is to prevent initial infection by the virus through the use of a microbicide. Microbicides are products that could be applied topically to the vagina to reduce transmission of HIV during intercourse. Topical delivery systems (TDS) are many and varied, ranging from ointments to creams/lotions and gels. Each type of TDS was originally designed, and formulated, for a particular application and, thereto, has its own specific advantages and limitations in terms of benefit performance. The first generation products used to test efficacy of anti-HIV microbicides for vaginal administration have been based exclusively on very simple gel formulations comprised of water-soluble polymers. Such formulations imply that the active material is, if not water-soluble, then at least water-dispersible, a fact that is often, demonstrably, not the case. From a practical perspective, these gels have been developed merely as a carrier for the active, with little emphasis on the effect of the formulation in practice, and the acceptability to potential users, i.e. real-life use.

All TDS, however, are multicomponent, heterogeneous compositions that require much iteration to attain the final desired formulation; many factors play a role in determining the outcome. The present paper will outline and review all the relevant factors affecting formulation of a TDS, especially as it applies to the development of a successful microbicide, laying out some basic principles and methods involved.

49. HIV: New Treatments, New Challenges

Sheldon Brown, James J. Peters VAMC, Bronx, NY

The expansion of treatment options for HIV infection over the past two decades has been one of the great accomplishments of contemporary pharmacology, transforming a relentlessly progressive and ultimately fatal disease into a chronic illness with the potential for a near normal life expectancy. Knowledge gained through the development of anti-retroviral drugs has provided the foundation for development of compounds useful for other previously untreatable chronic viral infections. With these successes has come a succession of new and often unanticipated challenges. The management of drug resistance is now a centerpiece of clinical care that has fostered rapid adoption of sophisticated molecular diagnostic tools. Unexpected toxicities have been identified for drugs that were once commonly used and thought to be relatively safe. The range of treatment options is now so large that it is impractical to develop evidenced-based guidance for optimal treatment for all but a few clinical circumstances. The interaction between HIV management and the co-morbidities of an aging population introduces increased complexity to medical decision making. The increased frequency of serious medical conditions that are not traditionally associated with HIV raises new uncertainties about when to begin treatment of HIV. An overview of these issues from the perspective of a practicing clinician will be presented.
50. Investigating An Allosteric Binding Site for a New Class of HIV-1 Protease Inhibitors

Christine L. Shrock¹, Ellen L. Shrock², Melinda M. Layten³ and Carlos Simmerling³, (1)Ward Melville High School, E. Setauket, NY, (2)Long Island School for the Gifted, Huntington Station, NY, (3)Stony Brook University, Stony Brook, NY

HIV-1 protease (HIV-PR) inhibitors are an essential part of current drug treatments to control HIV infections. Currently used drugs of this type are competitive inhibitors, and their effectiveness is reduced by the appearance of resistant strains of HIV. There is thus strong motivation to study potential binding sites for allosteric HIV-PR inhibitors. Here we report results from all-atom simulations, using molecular dynamics, to investigate the effect of small molecules in contact with a certain region (the “elbow” region) on the structure of HIV-PR. We find that these small molecules can have the effect of closing flaps so as to cover the active catalytic site, and hence that the elbow region is a promising binding site for allosteric HIV-PR inhibitors. Our simulations also suggest how the efficiency of allosteric inhibition depends on the specific conformation of the small molecules. Our data provide valuable information for the design of a new class of HIV-PR inhibitors to help control the current AIDS epidemic.

51. Pharmaceutical Production in Africa

Rolande R. Hodel, AIDSfreeAFRICA, Ossining, NY

The speaker recently participated in an expert panel discussion at Yale University entitled: DRUGS, DEVELOPMENT & UNIVERSITIES - “Why are essential medicines still unavailable in poor countries?” The current session will discuss challenges to the successful production of pharmaceuticals in Africa including: the drugs urgently needed in Africa, the process for producing drugs in Africa generally, and the specific challenges involved in the synthesis and production of antiretrovirals. The discussion will be accompanied by pictures from Cameroon that may run counter to your current understanding and expectations about Africa.

As scientists we need to remember that we have choices beyond traditional academic and industry careers. Indeed, in the past several years many scientists have begun to consider the non-profit world as a way to create a more meaningful career. This has been occurring as more people realize that access to potentially life-saving drugs ought to be a human right, like access to food, shelter and education.

Ionic Liquids I: Synthesis and Reactions in Ionic Liquids

Sponsor: CEM Corporation
Organizer: James F. Wishart Brookhaven National Laboratory, Upton, NY
Organizer: Sharon Lall-Ramnarine Queensborough Community College, CUNY, Bayside, NY

Session Overview: Research in ionic liquids (ILs) has exploded in recent years because of their great promise in a broad range of applications in chemistry and chemical technology for process and safety improvement and reduction in overall environmental impact. This three-session symposium features the broad spectrum of ionic liquids research conducted in the Middle Atlantic Region.
52. Manipulating the Properties of Ionic Liquids by Synthetic Design

Sharon Lall-Ramnarine1, Alejandra Castano2, Jasmine Hatcher2, Kijana Kerr1, Xing Li2, Ayisha Munawar1, Ankita Parikh1, Pokay Ma2, Catherine McEntee3 and James F. Wishart4, (1)Queensborough Community College, CUNY, Bayside, NY, (2)Queens College, CUNY, Flushing, NY, (3)Kingsborough Community College, Brooklyn, NY, (4)Brookhaven National Laboratory, Upton, NY

Ionic liquids (ILs) have been described as designer solvents because they can be structurally manipulated to provide desired properties. This work focuses on the preparation of several series of ILs and an investigation of their physical and biological properties. Common cations such as imidazolium, pyridinium and pyrrolidinium with functionalized alkyl substituents and phosphate, bis(triflyl)imide or bis(oxalate)borate anions have been synthesized. Less common cations including 4-dimethylaminopyridine (DMAP), diazabicyclo[2.2.2]octane (DABCO) and diammonium species have also been similarly prepared. The physical properties of several of these ILs such as conductivity, viscosity and thermal profile will be reported. In addition the biological properties of the ILs have been evaluated through collaborative studies and will be briefly discussed. This work was supported in part at BNL by the U. S. DOE Office of Basic Energy Sciences under contract # DE-AC02-98CH10886.

53. Synthesis and Thermochemical Properties of Racemic Dihydroxy Ammonium Salts

Marie Thomas1, Leah Rothman1, Jasmine Hatcher1, Sharon Lall-Ramnarine2 and Robert Engel3, (1)Queens College, CUNY, Flushing, NY, (2)Queensborough Community College, CUNY, Bayside, NY, (3)Queens College of the City University of New York, Flushing, NY

There is increasing interest in quaternary ammonium salts which are liquid at room temperature. These salts referred to as ionic liquids have been studied as catalysts and alternative solvents, used for chemical analyses (e.g., chromatography and electrophoresis), large-scale separations, as media for electrochemical processes and as media for the storage of radioactive waste. The number of applications found for these unique materials continues to grow. Presented in this report is the preparation of racemic ammonium salts containing the 1, 2-dihydroxypropyl unit. Most were solid at room temperature but a few were found to be ionic liquids. The thermochemical properties of these new materials are reported.

54. Radiation-Induced Reactions in Ionic Liquids

James F. Wishart, Brookhaven National Laboratory, Upton, NY

Ionic liquids have many important applications as chemical reaction media and in systems that depend on the transport of charge or redox equivalents. Pulse radiolysis is a powerful technique for measuring fast reaction kinetics, particularly redox processes. We have been using pulse radiolysis techniques to study reactions in ionic liquids. The radiation chemistry of ionic liquids differs from that of conventional liquids in several ways that can be traced back to their unique physical properties. Supported by the U.S. Dept. Of Energy, Basic Energy Sciences, Chemical Sciences Division, under contract DE-AC02-98-CH10886.

55. Ionic Liquids: Vehicle for Pharmaceuticals and Therapeutics

Sanjay V. Malhotra, National Cancer Institute-Frederick; SAIC-Inc., Frederick, MD

Controlled variations of the physiochemical properties of environmentally benign ionic liquids (ILs) influence the process chemistry of nucleosides. This has been seen in our studies with imidazolium-based new ionic liquids, and the IL methodology successfully employed to synthesize a host of nucleoside analogs currently in use as anti viral drugs. Similarly, synthesized coumarin compounds that show anti tumor activity on human cell lines were synthesized using Lewis acid in ionic liquids. Here, milder conditions were effective for synthesis of these compounds as compared to the
conventional methods where strong acid catalysts (e.g. H2SO4, H3PO4, CF3COOH etc.) and high temperatures are required.

In another effort, modification of sodium montmorillonite a cationic clay, has been carried out with pyridinium and imidazolium-based ionic liquids. Our data show an overall increase in interlamellar spacing and improved thermal stability as compared to commercial nano-clays modified with long chain quaternary ammonium salts. This is due to Na+ exchange with cations of the ionic liquids. Utility of the modified montmorillonites has been tested in the preparation of polypropylene nanocomposites. This approach is effective in preparation of biomaterials for the delivery of important therapeutics, illustrated here with representative examples.

Acknowledgment: Funded by NCI Contract N01-CO-12400

**Medicinal Chemistry**

**Sponsor:** ACS Division of Medicinal Chemistry  
**Organizer:** Ralph A. Stephani St John's University, Jamaica, NY  
**Organizer:** Tanaji Talele St. John's University, Queens, NY  
**Organizer:** Vijaya Korlipara St. John's University, Jamaica, NY

56. Protein-Protein Interactions: Drugability, Design Strategies in Lead Identification and Optimization

Hariprasad Vankayalapati, SuperGen Inc., Salt Lake City, UT

Protein-Protein interactions provide a large opportunity space for potential targets due to their unique mode of transforming cellular signaling that leads to important biological functions. It is well documented that the protein-protein interaction surface is too large to be effectively target and disrupt by a small molecule entities. This leads to low potency of the small molecules due to their weak interactions and widely spaced. However a recent developments have clearly demonstrated the drugability of these difficult targets by small molecules with available structural and biochemical information.

Here we present the protein structure and ligand binding information by understanding the buried surface of protein-protein contacts, hot spots, key residues, hydrophobic and polar interactions which are critical for targeting the protein-protein interactions. Also various concepts in lead identification and optimization such as ligand, surface-binding, lipophilic efficiency, predicting metabolism and hepatic stability based on the target class will be presented. Application of design concepts and impact of in-silico approaches will be discussed.

57. Evolution of Selective IGF1R Inhibitors

Kenneth W. Foreman, OSI Pharmaceuticals, Farmingdale, NY

The IGF1 receptor (IGF1R) plays important roles in tumor cell proliferation and survival and its inhibition may be therapeutic in several human cancers. OSI Pharmaceuticals has developed a series of potent imidazo[1,5-a]pyrazines that selectively inhibit IGF1R both in vitro and in vivo. The SAR developed within this series provides some insight into key factors for selectivity, potency, and optimized pharmacokinetics. Structure-based insights bolster these empirical observations. The properties of an advanced lead compound, PQIP, will be discussed in detail. This series of compounds affirms that a strategy targeting IGF1R with small molecule kinase inhibitors can yield novel development candidates to treat human cancer.
58. Discovery of the Multi-Kinase Inhibitor Dasatinib (SPRYCEL®) for the Treatment of Philadelphia Chromosome Positive Leukemias


We have recently identified substituted 2-(aminopyridyl)- and 2-(aminopyrimidinyl)thiazole-5-carboxamides as potent multi-kinase inhibitors with excellent antiproliferative activity against solid tumor and hematological cell lines. Moreover, the orally bioavailable, 2-aminopyrimidinyl derivative dasatinib (SPRYCEL®) retains activity in several clinically relevant imatinib-resistant cell lines and provides complete tumor regressions at multiple dose levels in wild-type and imatinib-resistant in vivo tumor models of chronic myelogenous leukemia (CML). Consistent with these preclinical findings, dasatinib demonstrated significant hematologic and cytogenetic response rates in CML and Ph+ ALL patients with resistance or intolerance to imatinib. Crystallographic analysis of dasatinib bound to the Abl kinase domain reveals that dasatinib binds to the activated form of the kinase. The crystal structure also provides a mechanistic rationale for the ability of dasatinib to overcome all known imatinib-resistant Bcr-Abl mutants, except for the T315I variant. The structure-activity relationship studies, preclinical pharmacology, and structural biology supporting the selection of dasatinib for clinical development will be discussed.

59. Fragment Based Design of p53/MDM2/MDM4 Inhibitors Utilizing Multi Component Reaction (MCR) Chemistry

Barbara Beck¹, Stuti Srivastava¹, Balachandran Raghavan¹, Alexander Doemling¹ and Tad Holak², (1)University of Pittsburgh, Pittsburgh, PA, (2)Max Plank Institute, D-82152 Martinsried, Germany

Fragment-based drug discovery approaches (FDD) make extensive use of structural target information and drug design. Thus they comprise the opposite of chance-based high throughput screening exercises (HTS). A fragment is discovered by screening low molecular weight libraries of molecules in assays yielding structural binding information (NMR, X-ray). Based on the generated hits chemical optimization programs can be started. Fragment-based drug discovery approaches are highly successful and complementary to HTS campaigns.

We herein describe a novel fragment-based approach that is based on the interplay of structural target information, docking and very efficient multicomponent reaction chemistry (MCR). Potential advantages are the following:

- public available structural target data (pdb) can be used - thus there is no need for expensive and/or advanced techniques & instrumentations;
- a very large chemical space based on hundreds of relevant scaffolds is screened – thus the chances of discovery of expandable hits is greatly enhanced;
- due to the efficient chemistry used (MCR), there is a high ratio of success to effort;
- the discovery of multiple target interacting compound classes allows for their parallel optimization, thus greatly enhancing the chance to develop compounds with excellent PKPD properties.

As a validation of our new drug discovery approach we present the parallel discovery of several potent scaffold classes of selective and dual active p53/mdm2/mdm4 antagonists with potential applications in cancer.
60. Potent XIAP Antagonists by a Fragment-Based MCR Approach
Ilaria Monfardini\textsuperscript{1}, Alexander Doemling\textsuperscript{1} and Maurizio Pellecchia\textsuperscript{2}, (1)University of Pittsburgh, Pittsburgh, PA, (2)Burnham Institute for Medical Research, La Jolla, CA

Apoptosis has recently become one of the most intriguing fields explored in cancer therapy. Members of the inhibitor of apoptosis protein family (IAP) are overexpressed in many cancers. IAPs bind the caspase family of apoptotic enzymes, inhibiting their catalytic activity and preventing the programmed cell death. In particular the BIR3 domain of XIAP (human X linked IAP) blocks the active subunit of caspase-9, an initiator caspase of the mitochondria apoptosis pathway. In apoptotic cells the protein Smac/DIABLO has been demonstrated to compete with caspase-9 in binding XIAP through four N-terminal residues Ala-Val-Pro-Ile.

A set of XIAP inhibitors has been designed and synthesized in order to mimic Smac interaction with the BIR3 domain of XIAP.

Multi Component Reaction Chemistry (MCR) was adopted as synthetic strategy: diversified reaction products were obtained starting from the combination of three or four building blocks in a one pot operation. Based on the binding fragment Ala-Val novel potent scaffolds have been discovered also showing cell based activity.

X-ray studies of the synthesized inhibitors with the XIAP binding site compared to the Smac-XIAP complex showed that the H bounds of the Ala-Val portion are retained and can therefore contribute to the selectivity for the target. Instead, the high variability of the heterocyclic moiety leads to new additive interactions with XIAP.

Biological evaluations performed showed promising results, suggesting that a further expansion of the chemical diversity of the heterocyclic moiety may increase the interaction with XIAP.

\textit{Process Chemistry}

Organizer: Rick Sidler Merck & Co.

Session Overview: This session will highlight topics pertaining to the synthesis, optimization, purification and isolation of pharmaceutically interesting compounds or intermediates. Emphasis will be on the development and application of novel and practical solutions to challenges incurred during preparation of these materials.

61. From the Bench to the Plant: Case Studies in the Development and Scale up of Chemical Processes
Akin H. Davulcu, Bristol-Myers Squibb Company, New Brunswick, NJ

This seminar will disclose two recent examples of process research and development efforts at Bristol-Myers Squibb, with an emphasis on the change in philosophy that accompanies the transition from early to late stage process research and development.

Amran Gowani, Merck and Co., Inc., Boulder, CO

Synthetic oligonucleotides are prepared via automated solid phase synthesis techniques on a variety of polymer and controlled-porosity glass (CPG) supports. While automation generally provides
remarkably high yields of synthetic oligonucleotides, subsequent removal of the precious material from the solid support is plagued by degradation and low recovery and requires the use of several potentially hazardous reagents, e.g. concentrated ammonium hydroxide and methylamine. Given these limitations, our goal was to develop an alternative cleavage-deprotection protocol for highly modified synthetic oligonucleotides that is safe and robust. During our studies we have identified several problematic areas such as rapid degradation of specific nucleotides and slow removal of certain protecting groups. To combat this we have implemented a few creative solutions that eliminate these concerns yet allow for rapid throughput of a variety of synthetic oligonucleotide species. These refinements and strategies for this critical process will be presented.

63. A Novel and Efficient Cleavage of Silyl Ethers
Daniel Zewge, Rick Sidler and Raymond Cvetovich, Merck, Rahway, NJ

Abstract: A novel and efficient silyl ether cleavage methodology is described. The new deprotection strategy was demonstrated for the synthesis of a diverse range of oligoribonucleotides.

64. Development of a Scaleable Process for Product Quality Improvement Using Adsorbents
Melodie D. McCain, Jungchul Kim, Jennifer Vance and Thomas Hunter, Schering-Plough, Union, NJ

Adsorbent materials have been widely used in pharmaceutical process development in order remove low-level impurities such as residual metals, colored impurities and organic impurities. Current adsorbent technologies include adsorbent screening kits and adsorbent cartridges.

Two case studies will be presented. The first case will describe the development of a process to remove residual Pd from a pharmaceutical product utilizing adsorbent kit screening. The second case will describe the rapid development of a process to remove blue color from a pharmaceutical intermediate.

65. Recent Advances in the Use of Preparative Chromatography in the Multikilogram Synthesis of Preclinical Pharmaceutical Candidates
Derek Henderson, Merck Research Laboratories, Rahway, NJ

Title: Recent Advances in the use of Preparative Chromatography in the Multikilogram Synthesis of Preclinical Pharmaceutical Candidates

Abstract:
A case study is presented illustrating how preparative chromatography is used in support of preclinical development projects. Delivery of preclinical candidates in multikilogram quantities is expedited through the implementation of flash chromatography, HPLC, and SFC for chiral and achiral intermediates and preclinical candidates.

Examples of approaches to method development, column loading studies and injection techniques in conjunction with separation and synthesis strategies will be presented.

66. Highly Active, Air-Stable Supported and Unsupported Homogeneous Catalysts for Challenging Coupling Reactions in Pharmaceutical Process
Thomas Colacot, Johnson Matthey, West Deptford, NJ

A major challenge in the area of homogeneous relevant to coupling catalysis is the separation of the catalyst/metal from the product. Although Pd/C in the presence or absence of a ligand can be used for coupling of less challenging aryl iodides and bromides, this methodology does not provide any additional advantage over homogeneous systems, as the coupling reaction proceeds via a homogeneous mechanism, evidenced by the three-phase test results from various groups. To solve
some of these issues, Johnson Matthey has taken three different approaches: i) develop highly active homogeneous catalysts so as to minimize the catalyst loading in challenging coupling reactions ii) tune the polyethylene supported FibreCats to be more active and robust iii) use SMOPEX to scavenge any residual metal from the product. This work is focused on the strategy that we employed in developing fully formed Pd(0), Pd(I) or Pd(II) complexes of supported and unsupported monodentate and bidentate ligands, with a view to understand the structure-activity relationship in coupling and thereby understanding the selectivity, activity and robustness of the new catalysts. An example each from the supported and unsupported catalysts is given below. These catalysts have been used for coupling various Ar-Cl compounds such as 3-chlorothiophene, chloromesitylene, 3-chloropyridine, etc., with excellent yield. Several examples of FibreCat gave leaching below 1 PPM with good recyclability. Details of the work will be presented in the talk.

Plenary Lecture I: Ronald Breslow, Columbia University

Organizer: Jack Norton Columbia University, New York, NY

Session Overview: This plenary lecture will discuss SAHA (Vorinostat), an FDA approved anticancer compound with a novel mechanism of action.

67. SAHA (Vorinostat), An FDA Approved Anticancer Compound with a Novel Mechanism of Action

Ronald Breslow, Columbia University, New York, NY

We have started with the observation that DMSO is able to induce erythroleukemia cells to differentiate into normal erythrocytes, and developed this into a group of potent molecules that accomplish a number of important goals in cancer therapy with a wide range of cancer types. 1) The cancer cells cease growth. 2) They can differentiate into normal non-cancerous cells. 3) In some cases they undergo apoptosis, programmed cell death. The compounds do not show significant toxicity, are orally active, and the lead compound has been approved for human use by the U.S. FDA in October 2006, having successfully emerged from clinical trials with flying colors. Ours is the first member of this new class of drugs to be approved, histone deacetylase inhibitors, and it is now being widely studied against many cancers, and other diseases.

The intellectual path that led to the potent compounds will be described, and the evidence on their mode of action and the results of animal and human trials. The importance of only medium strength of binding to the receptor protein in this series will be discussed. The kinetic principles involved may be applicable to many other medicinal series.


**Poster Session I**

**Organizer:** Irina Rutenburg Queensborough Community College, Bayside, NY

**Organizer:** Marie Thomas Queens College, CUNY, Flushing, NY

**68. Catalase-Peroxidase (M. tuberculosis KatG) Forms a Protein-Based Radical during Catalase Turnover**

**Javier Suarez**¹, Shengwei Yu¹, Richard Magliozzo¹ and Kalina Rangelova², (1)Brooklyn College and the Graduate Center of the City University of New York, New York, NY, (2)NIEHS, Research Triangle Park, NC

Heme catalases and peroxidases are ubiquitous enzymes principally responsible for eliminating hydrogen peroxide in aerobic organisms. The catalase reaction mechanism in the dual function enzyme catalase-peroxidase (KatG) found in bacteria and fungi has not been defined in stepwise detail. KatG enzymes contain a unique post-translational modification in the form of a three amino acid adduct (Met255-Tyr229-Trp107) with a specific role in the catalase reaction since mutation of any of the three residues virtually eliminates catalase but not peroxidase activity. During turnover of millimolar hydrogen peroxide at neutral pH, M. tuberculosis KatG forms an EPR silent heme species characteristic of peroxidase Compound III (oxyferrous heme), while at high pH, a low spin ferric species is found. Rapid freeze-quench EPR revealed a narrow doublet signal formed within milliseconds of mixing resting (ferric) KatG with hydrogen peroxide, at both neutral and alkaline pH. This radical persists only while the enzyme dismutates hydrogen peroxide. The mutant enzymes KatG[Tyr229Phe] and KatG[Trp107Phe], which lack the distal side adduct and lack catalase activity as well, do not form this radical. Simulation of the symmetrical narrow doublet EPR signal is consistent with a radical on a modified amino acid according to the observed hyperfine splitting. We propose based on the structural evidence from the EPR spectra that this radical may reside on the MetTyrTrp adduct and describe a mechanism for the catalase reaction involving this unique structural feature. In this mechanism, the protein based radical is involved in the formation and release of dioxygen from the oxyferrous intermediate.

**69. Predictable Transitive RNA Interference Induced by mRNA Hairpins in C. Elegans**

**Jessica Cox** and Matthew Doty, Villa Julie College, Stevenson, MD

The specific silencing of genes through RNA interference by double-stranded RNA is now being studied not only as a means to understand cellular processes, but also as a means of treating patients in the pharmaceutical industry and controlling pests in the agricultural sector. While the protein machinery necessary to cause this phenomenon has been well characterized, it is not always possible to predict the silencing of one specific gene. Using a computer algorithm we developed, we have been able to create maps of gene networks in which such interactions might occur due to sequence homology. One of these networks is now being examined in the nematode Caenorhabditis elegans. Two plasmid constructs have been created. The first targets four genes within the network for silencing through a common hairpin sequence found in each of the genes. The second construct targets just one these genes through sequence homology in an area outside of the hairpin. Both
exhibit impaired movement as compared C. elegans fed the control construct or no construct. This suggests that the pattern of silenced genes in similar between the two groups and that the silencing of the one gene with the second construct might have led to the silencing of the other three genes in manner that we could then begin to predict. We are currently examining RNA levels for all four genes with the C.elegans to determine if this is the case and will begin to examine the RNA levels of other genes within the network as well.

70. Expression and Metal Binding Studies of Tristetrapolin (TTP), a Zinc Finger Protein

Robert DiTargiani1, Sarah L. J. Michel2, Seung Jae Lee3, Sarah Wassink1 and Anab Yusuf4,
(1)University of Maryland, Baltimore, (2)University of Maryland, Baltimore, MD, (3)University of Maryland School of Pharmacy, Baltimore, MD, (4)Villa Julie College, Stevenson, MD

Tristetraprolin (TTP) is a non-classical zinc finger proteins found in man and most other mammals. TTP contains three cysteines and one histidine (Cys3His) that bind to metal ions. During inflammation, TTP regulates the expression of cytokines including tumor necrosis factor a (TNF-a) at mRNA level. In the regulation of cytokines, TTP binds to AU-rich sequence elements (AREs) located on the cytokines' mRNA. Upon binding the TTP/ mRNA complex is degraded by exosomes. It has been established that coordination of zinc ion to the Cys3His sequence of TTP ion is required for TTP to bind with RNA. To evaluate the role of metal ions in TTP function, TTP-2D, a two finger domain was expressed and purified. 0.1 mg of TTP-2D was collected and determined to be over 95% pure by SDS-PAGE and HPLC analysis. Metal binding tests by diTargiani and coworkers provided data that could be fit to yield an upper limit dissociation constant Kd of 3.3 × 10^-6 M for cobalt (II) binding and 6.2 x 10^-11 M for zinc (II).


Stefan B. Schaffer, Zhijun Jiang, Simon S. Buttrick and Derek M. Stein, Brown University, Providence, RI

Biopolymers such as DNA can be analyzed with great precision using nanopores, tiny holes approximately 2-30nm in diameter. Naturally occurring nanopores can be found in the form of membrane-spanning protein channels that allow for the flow of ions across a lipid bilayer. New techniques in micro- and nano-fabrication allow us to drill nanopores through solid-state membranes on silicon chips, which are more robust and versatile than their biological counterparts. Because nanopores are of comparable size to DNA, the “threading” of a single molecule through such an opening has measurable electrical effects. These measurements can provide insight into the characteristic properties of DNA, such as folding conformation and molecular size of the strand in question.

We have designed a fluidic device that fills and bathes the nanopore with an ionic solution. When a voltage is applied across the nanopore, a ~nanoampere current of ions flows through the pore. When negatively charged DNA molecules are injected in our system, they are pushed through the nanopore by an electrophoretic force. The DNA blocks a large portion of the pore and impedes the flow of ions through it, producing a measurable current drop that allows us to electrically detect and analyze individual DNA molecules. We show that our nanopore setup is sensitive to folded DNA conformations but is unable to resolve sequence information along an unfolded molecule. However, if DNA is labeled with sequence-specific MIZF binding proteins, a DNA-protein detection scheme could be used to observe primary sequence features along a DNA double helix.
72. Bacterial Responses to a Combinatorial Environment

Peter Palenchar and Steven Middler, Rutgers University, Camden, Camden, NJ

Bacterial responses to single chemical species/stressors in many cases is well understood. The natural environment though, tends to be combinatorial in nature and multiple different stressors might be present at any given time. Living organisms must be able to sense this combinatorial environment and make "decisions" accordingly. To better understand how bacteria do this on the single cell level, we have tested the effects of three different types of stress induces, hydrogen peroxide, HCl, and EDTA. Each one has been tested for their affect on the growth of E. coli on an individual basis and also all possible combinations. In addition, our analysis gives data about transcriptional/translational control. For this analysis, we have used cells expressing a â-galactosidase gene (lacZ). In the presence of the lacZ gene product and 5-bromo-4-chloro-3-indolyl-beta-D-galactopyranoside (X-gal), the E. coli cells are blue. For this analysis, we have used lacZ being expressed by the normal lac promoter, but also lacZ expressed via other promoters so that different transcriptional responses can be detected.

73. Synthesis and Gp 120 Binding of 1,1-Linked-Disaccharide Mimetics of β-Galactosyl Ceramide (GalCer): Potential Entry Inhibitors of HIV

Stewart Bachan and David R. Mootoo, Hunter College, New York, NY

The interaction between GalCer and gp120 is important for HIV infectivity in CD4 negative as well as CD4 negative cells. Molecules that hinder the interaction between gp120 and GalCer are of interest as potential entry inhibitors of HIV. Novel galactose 1-β→1-α mannose O-disaccharide GalCer analogs, with one or two fatty acid esters on various positions on the mannose residue were designed as mimetics of GalCer, in which the mannose residue serves as a rigid ceramide substitute. The synthesis of these analogs and their interaction with gp120 in a monolayer-binding assay will be presented.

74. Determining the Role of NO / H-Nox in Colwellia Psychrerythraea

Stephanie A. Georgiou and Elizabeth M. Boon, SUNY Stony Brook, Stony Brook, NY

It is of fundamental importance to study and to understand, from a molecular to cellular level, how bacteria respond to their environment. Dissolved gasses (e.g., nitric oxide, NO) are increasingly being recognized as a critical stimuli to organisms. In eukaryotes, the heme sensor protein soluble guanylate cyclase (sGC) is responsible for recognizing and responding to NO. This important enzyme is a member of a broader family of proteins called the Heme-Nitric oxide/Oxygen binding family (H-NOX), which also includes bacterial heme proteins. We have characterized the ligand binding properties of the H-NOX domain from the psychrophile, Colwellia psychrerythraea (Cp) using UV/VIS spectroscopy and found that Cp-H-NOX selectively binds NO with an affinity similar to sGC. In the Cp genome, Cp-H-NOX is located directly upstream from a soluble histidine kinase and a response regulator, prototypical of proteins involved in two component signaling (also known as His-Asp...
phosphorelay signaling). We are investigating the possibility that Cp responds to NO binding to its H-NOX domain through a His-Asp phosphorelay mechanism. Kinetic and spectroscopic data will be presented to support this hypothesis.

75. Engineering Functional Artificial Histone Acetyltransferases

**Man Xia Lee**, Kinjal Mehta, Susheel Kumar Gunasekar, Zhiqiang Liu, Natalya Voloshchuk, Aye Sandar Moe, Phyllis Frankl, Lisa Hellerstein and Jin K. Montclare, Polytechnic University, Brooklyn, NY

In vivo incorporation of non-natural amino acids can be used to improve protein stability. However, there is a trade off; improved stability of the protein may lead to loss in activity. One way to improve function is to employ machine-learning algorithms to identify the variants that improve activity. Our target protein Tetrahymena GCN5 (tGCN5), a member of the Histone Acetyltransferases (HAT) family, acetylates the lysine residues of histones, enabling transcriptional regulation. Experimental data have shown an increase in stability of the protein against protease but loss in activity with the incorporation of para-fluoro-phenylalanine (pFF) into tGCN5 in vivo. Using information from biochemical and structural data, we identified eleven residues to mutate. With the aid of computer guidance, we have designed a set of fluorinated variants and examine the activities.

76. Peptides Inhibitors of F11R/JAM-a Adhesion Molecules

**Cristina C. Clement** and Manfred Philipp, Lehman College, City University of New York (CUNY), Nyc, NY

F11-R receptor was characterized as an adhesion protein, called also aka JAM-A (or JAM-1), which under normal physiological conditions is expressed constitutively on the surface of the platelets and localized within tight junctions of endothelial cells (EC). The utilization of specific F11R/JAM-A peptide antagonists and recombinant proteins supported the role of F11R/JAM-A in the process of platelets adhesion to inflamed endothelial cells and identified plaque formation leading to inflammatory thrombosis and atherosclerosis where the platelets have a critical influence in the progression and development of the cardiovascular disease. Thus, the development of new drugs antagonizing the F11R/JAM-A function could evolve as an effective strategy for the treatment of atherosclerosis, heart attacks and stroke. We present one of the first trials toward development of peptide-based inhibitors of F11R/JAM-A function. Among many trials, the peptide D-Lys-Ser-Val-Ser-D-Arg-Glu-Asp-Thr-Gly-Thr-Thr-Cys-CONH2 proved to be a potent inhibitor of human platelets aggregation in vitro. Further molecular docking experiments showed that this peptide makes favorable hydrophobic and electrostatic interactions within the proposed binding site of JAM-1 (X-Ray structure 1nbq.pdb was used as template).

77. Structure and Stability Analysis of Single-Alanine Mutants of Cartilage Oligomeric Matrix Protein Coiled Coil

**Wendy Hom**¹, Hanna Barra², Susheel Gunasekar¹, Jin Montclare¹ and Jennifer Haghpanah¹,

(1)Polytechnic University, Brooklyn, NY, (2)Polytechnic University, Fresh Meadows, NY

Cartilage oligomeric matrix protein (COMP) is a non-collageneous pentameric glycoprotein of the Thrombospondin family predominantly found in cartilage, tendon, and ligament tissues. It is composed of 5 domains: the N-terminal tail (five stranded coiled-coil (COMPcc) region), the Association Domain, the Type 2 Repeat EGF-like Domain, the Type 3 Repeat Ca²⁺- Binding Domain, and the C-terminal Domain. Structural studies have illustrated that the N-domain of COMP (COMPcc) self-assembles, forming a hydrophobic pore which allows for the binding of small hydrophobic molecules such as Vitamin D₃ and all-trans retinol. To understand which residues in the hydrophobic pore are critical for binding the various small molecules, we performed alanine-scanning mutagenesis. Ten single-alanine mutants in the hydrophobic region of COMPcc have been created via site-directed mutagenesis. Single-alanine mutants were studies and analyzed via circular dichroism (CD) and fluorescence to study the structural integrity and the binding capacity for small molecules.
78. Fluorescence Study of Some Precursors of a Bivalent Src Kinase Inhibitor
Chrystel Dol, Adam Profit and Ruel Z. B. Desamero, York College, Jamaica, NY

Src Kinase is a protein of tyrosine kinases family. This protein is composed of four sites: an SH2 and SH3 domain, an active site and catalytic site. These domains transmit signals from the plasma membrane to other cells. Inhibitors of Src Kinase typically bind the SH2 domain and the active site in a bivalent fashion. Our overall goal is to investigate how this process occurs using spectroscopic measurements. To model some of the plausible interactions that might exist between the protein Src Kinase and its inhibitor, we determined the fluorescence emission and excitation spectra for two amino acids and two peptides. We took the fluorescence spectra of phosphotyrosine and pentafluorophenylalanine in water, methanol, acetonitrile, and chloroform to investigate the effect of polarity, and dimethyl sulfoxide (DMSO) for an aprotic environment. Due to limited solubility problems the peptides where only run in water and DMSO. To help analyze our results, we did some Gaussian 03W calculations to estimate the electronic spectra of each molecule. Comparison of the data collected in water, methanol, acetonitrile, and chloroform, revealed that while the excitation peaks where not significantly shifted, the emission peaks were. In DMSO, the excitation peaks were red shifted while the emission peaks were blue shifted. Our data was analyzed in terms of the sensitivity of these peaks to its environment.

79. Study of in Vitro of Cell Migration
Emily Hughes and Regina Sullivan, Queensborough Community College, Bayside, NY

The Scratch assay is a technique used to analyze breast cancer cell migration in vitro. A monolayer of cells is “scratched” and photographed after the scratch is initially made, and then at regular intervals until the scratch is closed. We will perform a number of scratch assays on the MDA-MB231 cell line on various chemical substrates. The differential rates of cell migration will be assessed, possibly correlating with the rate of cancer cell metastasis in vivo.

80. Characterization of Fluorinated Histone Acetyl Transferase, tGcn5
Natalya Voloshchuk, Anita Yuhua Zhu and Jin Kim Montclare, Polytechnic University, Brooklyn, NY

Incorporation of amino acid analogs expands protein engineering for applications in biotechnology and therapeutics. Fluorinated amino acid analogs have been employed in protein and peptide design to improve conformational stability, self-assembly, and protease resistance. We investigate the effects of residue-specific incorporation of fluorinated phenylalanine analogs, para-fluorophenylalanine (pFF), meta- fluorophenylalanine (mFF), and ortho-fluorophenylalanine (oFF) into a histone acetyl transferase (HAT). The HAT protein tGcn5 is able to activate gene expression by acetylating the lysines of histone tails. Here, we explore how monofluorinated analogs influence overall stability of tGcn5 and its ability to acetylate the target histone peptide.

81. Hormonal Control of Neuron Development
Christina Dewan and Regina Sullivan, Queensborough Community College, Bayside, NY

Androgens have powerful effects on the development of neurons. It has been shown that treating developing Spinal Cord neurons with an anti-androgen alters the number and size of these neurons. In this study the effect of treating another neuronal pool with an anti-androgen will be discussed.

82. Determination of Breast Cancer Cell Migration Rates
Louis Corradino Jr. and Regina Sullivan, Queensborough Community College, Bayside, NY

A scratch assay using breast cancer cells will be performed. Breast cancer cells will be plated, and then scratched with a pipette tip to create a wound in the monolayer. Our goal is to study the effect of different adhesion substrates on the rate of cell migration.
83. Exploiting Non-Natural Amino Acids to Identify Protein Partners of FnTm2
Yan Mei Chan, Peter James Baker and Jin Kim Montclare, Polytechnic University, Brooklyn, NY

FnTm is a novel transmembrane protein found to be up-regulated in the learning system in birds and other mammals. Identifying FnTm protein partners will allow us to clarify the FnTm signaling pathway in the brain. However, identifying protein pairs is often limited because the weak forces by which proteins interact are not sufficient to preserve the protein•macromolecule complex. To circumvent this limitation we are working towards introducing a photocross-linkable non-natural analog of para-azidophenylalanine and photoleucine in a residue-specific manner into FnTm. Here we demonstrate the progress of our efforts to discover the protein•protein interactions involved in learning.

84. Effects of Anti-Androgens on Spinal Cord Motor Nuclei
Sheila Jean-Charles and Regina Sullivan, Queensborough Community College, Bayside, NY

There is vast interest in understanding the differences that are incorporated in the male and female central nervous system (CNS). Within this project rats are used to contrast the spinal motor neurons: bulbocavernosus and levator ani, two penis muscles which are being blocked from producing androgen by flutamide, against the retrodorsal lateral nucleus, which contain motor neurons that innervate the flexor digitorm brevis muscle. Specifically looking at these motor neurons in the CNS will help distinguish differences between the male and female CNS. The methodology that will be used in the experiment is to look at the different morphological conditions that the motor neurons are in, by using computer software Image J. This software will allow measurement and observation of the motor neurons. The results will determine whether the absence of androgen in male rats will show similar or contrasting morphological differences to that of female motor neurons. Thus, a conclusion can be derived that states that the blocking of androgen has a direct or indirect effect of the normal development of male spinal motor neurons.

85. Effects of Varying Levels of Nitrogen, Potassium and Phosphorus on Plant Growth
Sharisse Lewis and Regina Sullivan, Queensborough Community College, Bayside, NY

Plants require an array of chemicals for proper growth. In this experiment, the rapid growth of a Brassica rapa vegetable plant called Wisconsin Fast Plants™ will be utilized in order to investigate the effects of manipulated nutrient levels on plant growth. Each plant will grow with different amounts of nitrogen, potassium and phosphorus in the soil. The degree of growth, the color and appearance of the foliage and the rate of flower production will be measured at maturation. Each plant will then be compared to decide which soil level will yield optimal plant growth.

86. Migration of Rates of Human Breast Cancer Cells
Joseph Mammano and Regina Sullivan, Queensborough Community College, Bayside, NY

Cell migration is the mechanism by which cancerous cells metastasize from primary tumors to invade other organs and tissues. A scratch assay was employed as an in vitro model of this process. A "wound" was created in plated human breast cancer cells and photographs were taken at various intervals to track the rate at which the cells migrated to close the wound. The influence of different adhesion substrate on cancer cell migration will be discussed.

87. Study of Human Breast Cancer Cell Migration
Sakshi Pasricha-Katyal and Regina Sullivan, Queensborough Community College, Bayside, NY

Cell migration is the mechanism by which cancerous cells metastasize from primary tumors to invade other organs and tissues. A scratch assay was employed as an in vitro model of this process.
A "wound" was created in plated human breast cancer cells and photographs were taken at various intervals to track the rate at which the cells migrated to close the wound. The influence of different adhesion substrate on cancer cell migration will be discussed.

88. The Anti-Androgen, Flutamide Causes Organizational Changes in Spinal Cord Motor Nuclei
Marie-Pierre Payen and Regina Sullivan, Queensborough Community College, Bayside, NY
Androgens plays an important role in initiation and maintenance of the masculinization process in vertebrates. Levator ani and the bulbocavernoase muscles seem to exhibit multiple structural changes related to androgen level in male and female. Research done by Grisham et al. treated the spinal motor neurons that innervate those muscles in the penis with Flutamide (an antiandrogen). The results showed a demasculinization of those neurons in males. This project extends these findings by looking at a second motoneuron pool present in the retrodorsal lateral nucleus of male and female rat's fetus. We used the tools in NIH ImageJ software to measure the size variation in neurons.

89. Human Breast Cancer Cell Migration
Nicole Perrotta and Regina Sullivan, Queensborough Community College, Bayside, NY
Metastasis is the spread of disease from one organ or part to another non-adjacent organ or part. Studying cell migration, a step in metastasis, may be a key element in discovering novel therapeutic strategies for controlling invasive tumor cells. In our research, we will use in vitro scratch assay to measure the rate of cell migration of human breast cancer cells. We will investigate the effects that various substrates have on the migration of these cells, including collagen and fibronectin.

90. The Alu Insert and Human Diversity
Brooke Rodriguez and Regina Sullivan, Queensborough Community College, Bayside, NY
The ALU insertion is proliferated throughout the biodiversity of the natural world with an assertive approximation of one million copies in the primate genomes alone (M.Batzer, et.al). ALU Repeats and Human Genomic Diversity, Nature Publishing Group. 2002) and an even more astounding display in the human genome. The repetitive sequence has been preserved throughout genomic narration and is acknowledged as a "Jump" or "Junk" gene, which is appropriate to its mobility and non-coding disposition. The objective of the study was to evaluate hair samples obtained from the college students and their friends/family and analyzed by means of PCR and electrophoresis. The Hardy Weinberg population genetics was then used to determine the over all frequency of the ALU gene within the college student population (including their friends/families). Through this study a broader understanding of human diversity as just one of many parts in the continuance of the natural world's epic tale.

91. Studies of Cell Migration
Darryl Williams and Regina Sullivan, Queensborough Community College, Bayside, NY
The movement of cancer cells will be explored. The goal of this study is to perform several scratch assays using breast cancer cells, which have been placed in several different mediums to observe the cells migration. Using this data we can attempt to correlate in vitro cell migration to metastasis in the human body.

92. Comparing the Effects of Anti-Androgens on Two Groups of Nuclei
Liang Xiang and Regina Sullivan, Queensborough Community College, Bayside, NY
The blockage of androgen receptors during a male organism's development can change the characteristics of neurons. More specifically, treating neurons in the spinal cord with Flutamide, an
anti-androgen in male subjects de-masculinizes their neurons (Grisham et al.) This study examines the effects of an anti-androgen on a second motorneuron pool present in the retrodorsal lateral nucleus and the role it plays in an organism’s sexual development.

93. The Alu Genotype
Yun Zhao and Regina Sullivan, Queensborough Community College, Bayside, NY
In contrast to prokaryotic genomes, eukaryotic DNA (including humans) contains large portion of noncoding sequences. The Alu sequences are present in human noncoding sequences. Our hypothesis is that the presence of Alu sequences varies among ethnicities. Polymerase chain reaction will be used to determine Alu genotypes of individuals from different ethnic groups.

94. Synthesis and Study of Nano-Adsorbents
Philip Botelho, Christopher Rodriguez and Girija Subramaniam, Penn State University, Hazleton, PA
Composite metal oxide samples were synthesized using all natural ingredients by a special slow combustion process. The samples thus prepared have very good adsorbing capacity for both liquids and vapor and gases. The adsorption seems to be a function of the natural ingredients as well as the mode of synthesis. The samples synthesized via the special slow process have unique properties as opposed to those made by normal combustion.

A detailed investigation to decode the origin of these unique properties has been undertaken by study of its composition, adsorption isotherm, particle size by various instrumental techniques including Scanning Electron Microscopy. The results will be discussed in our presentation.

95. Mechanism Based Inhibitors of Adenylyl Cyclase: Insight into Binding and Reactivity in the Active Site
Morris Krauss, Scientist Emeritus, National Institute for Standards and Technology, Rockville, MD 20850, Rockville, MD
Active site structures of mechanism-based inhibitors of mammalian adenylyl cyclase are calculated from templates based on theoretical structures of the native reaction path bound in the active site. Adenine specificity is maintained for all calculated analogues along the reaction path. Reaction was initiated by autocatalytic activation of the 3’OH of the ribose by the desolvated &Alpha phosphate. Stabilization of the developing charge on the 3’O primarily by MgA in the intermediate and transition state then lowers the activation energy. This mechanism is explored in reactant analogue inhibitor structures for the deoxy 3’OH, the deoxy 2’OH group, the P&Alpha thiophosphate, and adenosine 5’ phosphonate. The calculated structures for all reactive analogues find the 3’OH hydrogen-bonded to the &Alpha phosphate in position for the abstraction of the 3’H. In order to follow reactive behavior, binding of the concomitant intermediate analogue in the active site for some of these examples is also calculated.

One set of product analogues is based on an experimentally observed class of potent inhibitors consisting of adenine bound to hydroxamic acid through various flexible linkers. The dissociation of the proton from the hydroxamate to produce a potent metal binder within the active site suggests analogous groups such as a sulfonamide can reach the enzyme as a neutral molecule but bind ionically as a product analogue within the active site.

96. Discovery of Substituted Dipiperidine Acids and Alcohols as CC Chemokine Receptor-2 Antagonists
Mingde Xia, Cuifen Hou, Duane DeMong, Scott Pollack, Meng Pan, James Brackley, Chrissy Gerchak, Monica Singer, Ravi Malaviya, Michele Matheis, Gil Olini, Druie Cavender and Michael Wachter, Johnson & Johnson Pharmaceutical Research and Development, L.L.C., Cranbury, NJ
Monocyte chemoattractant protein-1 (MCP-1) and its receptor CC-chemokine receptor-2 (CCR2) have been implicated in inflammatory disease pathologies such as rheumatoid arthritis, multiple sclerosis, Crohn's Disease, uveitis, diabetes and diabetic complications, allergic rhinitis, Chronic Obstructive Pulmonary Disease (COPD) and allergic asthma. There remains a need for small molecule CCR2 antagonists for preventing, treating or ameliorating a CCR2-mediated inflammatory syndrome, disorder or disease resulting from MCP-1 induced monocyte and lymphocyte migration to a site of inflammation. We have discovered a series of substituted dipiperidine acids and alcohols as selective CCR2 antagonists. Exploratory SAR studies led to the remarkably potent CCR2 antagonists displaying excellent binding affinity and functional antagonism with values in the nanomolar or picomolar range. Some of compounds showed excellent efficacy in adjuvant-induced arthritis model, collagen-induced arthritis model, and allergic asthma model. The detail SAR, in vitro and in vivo activities will be discussed.

97. Biodiesel Synthesis and Characterization in a General Chemistry Laboratory

Rebecca L. Sanders, The Pennsylvania State University, University Park, PA

Increasing gas prices and concerns about global warning have resurrected interests in alternative fuels. An experiment entitled Biodiesel Synthesis and Characterization has been tailored to tie the topic of alternative fuels with the themes typically covered in the general chemistry laboratory at the Pennsylvania State University. Students ran a transesterification reaction where methyl esters were synthesized by reacting vegetable oil with methanol in the presence of a base catalyst. While the reaction was running, students worked in pairs to characterize two premade biodiesel samples by measuring their viscosities and densities. They applied their knowledge about appropriate fuel specifications to the collected data to identify which sample had the best fuel quality. Finally, the students used thin layer chromatography to determine if their reactions had gone to completion. Students were questioned on a range of topics including limiting reactants, catalysts, and separations. 28 students successfully completed this lab within a four hour lab period in the fall of 2007. When surveyed, they reported that they liked this experiment more than most other experiments they performed and also stated that they felt this topic was relevant to current chemical issues.

In the spring of 2008, this experiment was implemented into a second semester environmentally focused general chemistry lab. The experiment was modified to allow students to change one component of their reactions and to predict about how the change would influence the success of the reaction.

98. Teaching Scientific Writing to Second-Language Students

Mark Kobrak, Brooklyn College and The Graduate Center of the City University of New York, Brooklyn, NY

Learning the conventions of scientific writing is a challenge for any student, but students non-native speakers of English are at a significant disadvantage. The conventions of basic collegiate writing are often violated when discussing technical questions, and the extended vocabulary necessary for scientific presentations is an additional challenge. We review the existing literature on the teaching of writing to non-native speakers, and discuss strategies for providing support to these students.

99. Pokeweed Antiviral Protein: Understanding Its Role in Plant Related Forensics

Jeannine DeGrazia¹, Kana Noro¹ and Diana E. Friedland², (1)John Jay College of Criminal Justice and the Graduate Center of the City University of New York, New York, NY, (2)John Jay College of Criminal Justice and the Graduate Center of the City University of New York, New York, NY

Ribosome inactivating proteins (RIPs) depurinate ribosomal RNA (rRNA) disrupting the synthesis of proteins. This causes cell death imparting the toxicity that RIPs possess. One very specific RIP of interest is ricin; used as a biological weapon, it can have a direct impact on agriculture, the
economy, and human life. Owing to the devastating impact that ricin can have, its function, structure, and biochemical nature are of interest to many different scientific disciplines such as biochemistry, medicine, and the forensic science community. However, ricin is a hazardous protein to work with because it affects eukaryotic rRNA. Pokeweed antiviral protein (PAP), on the other hand, behaves very similarly to ricin but cannot directly access the eukaryotic cell as ricin can, making it safer for study while serving as an important model. PAP is a single-chain RIP purified from the leaves of Phytolacca Americana and has been found to depurinate the conserved á-sarcin/ricin loop of the large ribosomal subunit in plant viruses. It has also been found that PAP depurinates uncapped mRNA indicating a specific site on the mRNA that PAP can bind to and possibly use as a mechanism to interfere with protein synthesis. Certain structural elements of uncapped mRNA may be of key interest in elucidating this process. We use Tobacco Etch Virus (TEV) mRNA as a model for these studies. Differing constructs of the mRNA containing specific pseudoknots, stems, and loops of the non-translating region in the TEV uncapped mRNA are analyzed for their effects on equilibrium binding with PAP.

100. Novel and Rapid HPLC Method for the Quantitation of Guaifenesin: Application to Pharmacokinetic Studies

Sangeeta Chavanpatil¹, Ramesh Reddy Putheti², K.G Akamanchi³, and R N Okigbo⁴, (1)Department of Pharmacy, University of Mumbai, India, Institute of Chemical Technology, India, (2) Actavis Pharmaceuticals, Research scientist, Analytical Research and Development, 10065 Red Run Blvd, Owingsmills, MD 21030, (3)Department of Pharmacy, Institute of Chemical Technology, University of Mumbai, India, ID 21030, India, (4)Department of Botany, Nnamdi Azikiwe University, Awka, PMB 5025, Anambra State, Nigeria

A novel, sensitive, simple, rapid and economical method for the determination of the Guaifenesin in API and finished dosage formulations was validated using HPLC. Guaifenesin is a classical drug extensively used as an expectorant in symptomatic management of coughs, associated with the ability to loosen and thin sputum. Guaifenesin was dissolved in methanol and chromatographed on a c18 spherisorb (250cmX 4.5 mm, 5μm). Detection was performed on a JascoUV-975 detector with the mobile phase ratio of water:methano:acetonitrile(70:20:10 v/v/v respectively). Detection was absorptimetric at 276nm. The method was linear in the concentration range of 10-35μg/ml (r²=0.9995). The intra and inter-day precision was within ±2%. The assay accuracy was within 2%. The method was successfully employed in a pharmacokinetic study after an oral administration of a formulation, containing 1000 mg guaifenesin.

101. Functional Significance of Protein Kinase Cα And Hsp90 Interaction in a Yeast Model

Tae Young¹, Sheila JeanCharles¹, Corinne A. Michels², Susan A. Rotenberg³ and Nidhi Gadura¹, (1)Queensborough Community College, CUNY, Bayside, NY, (2)Queens College, CUNY, Flushing, NY, (3)Queens College, Flushing, NY

Hsp90 is a molecular chaperone essential to the folding, activation and maturation of small number of distinct client proteins. It is involved in regulating cell growth and differentiation. Levels of Hsp90 increase in cancer cells, therefore, it is of critical importance to cancer-related phenotypes. Hsp90 client proteins bind to the multi-component Hsp90 chaperone complex. Results from Rotenberg Laboratory show that Hsp90 and PKCα co-immunoprecipitate, suggesting a functional relationship between Hsp90 and PKCα. We will use Saccharomyces as a model system to explore the possibility that PKCα is an Hsp90 client. Bovine PKCα will be expressed in Saccharomyces strains carrying defects in the Hsp90/Hsp70 chaperone machinery and its impact on PKCα catalytic function will be determined. The proposed work will look at the expression levels of 3HA-tagged PKCα in wild-type as well as various Hsp90 mutants. We will also test to see if bovine PKCα co-immunoprecipitates with Hsp90 and Hsp70 complex. PKCα will be partially purified by immunoprecipitation and its kinase activity monitored by an in vitro assay using a known PKCα substrate, MARCKS protein.
102. Synthesis of the Guaifenesin Impurities and Their Spectral Properties  
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Anambra State, Nigeria  

Guaifenesin is a [(R, S-3-92-methoxyphenoxy) propane-1,2-diol] is a classical drug extensively used  
as an expectorant in symptomatic management of coughs, associated with the ability to loosen and  
thin sputum and bronchial secretions and cease expectoration. It combined with bronchodilators;  
decongestant, antihistaminics or opiate antitussives in numerous commercial liquids cough  
preparations. The objective of the present study is to synthesize the four impurities formed during  
the synthesis of guaifenesin, to establish the spectral properties of four impurities. It was observed  
that during the synthesis of guaifenesin many impurities were found. Apart from 1.5% of (2-  
methoxyphenoxy)-1,3-propanediol (guaifenesin â-isomer), and 0.03% of guaicol, and other four  
impurities were detected by LC-MS data. These impurities were never synthesized and no structure  
elucidation was done to establish the LC-MS data. As an effort an attempt was made to synthesize  
these impurities and their structures were elucidated by spectral properties i.e., MASS, H NMR and  
IR. Thus, the purity profile of guaifenesin is successfully established.

103. Environmental Microbiological Monitoring and Source of Contamination in the  
Pharmaceutical Industry—a Case Study  
Ramesh Reddy Putheti1, R N Okigbo2, Madhusoodan Sai Advanapu3, and Radha Leburu4,  
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Madras, India (4)Department of Biotechnology, S.V University, India  

An environmental monitoring study has been conducted in the clean room areas and controlled areas  
of a pharmaceutical formulation facility in Hyderabad India by using settle plate, surface testing, air  
sampling and personnel monitoring to isolate and identify the microbial contamination in the area  
and their source of entry. Environmental samples were collected for the five consecutive days from  
the clean rooms and controlled areas. The isolated microorganism was identified as Staphylococcus  
epidermidis, Staphylococcus xylosus, Staphylococcus haemolyticus, Micrococcus lylae, Micrococcus  
luteus and Kocuria rosea using API Identification system. Among the isolates identified from the  
clean room and controlled area are of human origin and it is clear that the major source of  
contamination is personnel in clean room and controlled area. Based on the identification of the  
isolates it was concluded that most of the contamination to the clean room and controlled area are  
passes through the personnel.

104. One-Pot Friedländer Quinoline Synthesis: Scope and Limitations  
Ti Wang, An-Hu Li, Mridula Kadalbajoo, Andrew Kleinberg, Kristen M. Mulvihill, Dan Sherman, Kam  
W. Siu, Arno G. Steinig, Doug Werner and Mark J. Mulvihill, OSI Pharmaceuticals Inc., Farmingdale,  
NY  

Quinolines are a class of important heterocycles that are traditionally known as antimalarial agents  
and more recently as key pharmacophores in protein kinase inhibitors for cancer treatments. Such  
beneficial biological activities make quinolines attractive targets for both synthetic and medicinal  
chemists. Among a variety of methods for constructing the quinoline ring, the Friedländer synthesis  
has proven to be one of the most powerful and versatile tools (a review: Cheng, C.-C.; Yan, S.-J.  
61), we reported a highly effective and practical one-pot Friedländer quinoline synthesis utilizing

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inexpensive reagents, i.e., iron, HCl, and KOH. In this process, o-nitroarylcarbaldehydes were reduced to o-aminoarylcarbaldehydes with iron in the presence of catalytic amount of HCl (aq) and subsequently condensed in situ with respective aldehydes or ketones to form mono- or di-substituted quinolines in good to excellent yields (27-99%). This novel procedure worked well with a wide variety of (het)aryl o-nitro carboxaldehydes and carbonyl compounds, tolerating a wide range of functionalities. In this report, we disclose the full results from our investigation, including the scope and limitations of our one-pot Friedländer synthesis protocol.

105. pH-Response of PMAA Hydrogel Multilayer Capsules Crosslinked with Adipic Acid Dihydrazide

Svetlana Pavlukhina, Veronika Kozlovskaya and Svetlana A. Sukhishvili, Stevens Institute of Technology, Hoboken, NJ

Hydrogel hollow capsules were produced by chemical cross-linking of hydrogen-bonded poly(methacrylic acid) (PMAA)/polyvinylpyrrolidone layers deposited onto silica core followed by core dissolution. Chemical crosslinks of ethylenediamine (EDA) or adipic acid dihydrazide (AADH) within the capsule wall were introduced using carbodiimide (EDC) chemistry. Reversible capsule swelling can be controlled through variation of cross-linking agent. Unlike EDA- crosslinked capsules which are highly swellable at acidic and basic pH due to excess positive and negative charge in the capsule wall and have minimum size at pH 5.5, AADH-crosslinked capsules did not show swelling at low pH. Zeta-potential measurements of PMAA capsules crosslinked with AADH indicate existence of negative or no surface charge. Swelling degree of PMAA capsules crosslinked with the AADH crosslinker for the same time was higher than that for EDA-stabilized PMAA capsules. We found that pH-dependent swelling of PMAA hydrogel capsules crosslinked with AADH is significantly prolonged in time which can be used for sustained release applications.

106. Chemical Shift Modulation by Peptide Bond Distortion

Adrienne F. Alimasa, Lee Zhang and Ronald L. Koder, The City College of New York, New York, NY

High resolution crystal structures have established the distortion of the peptide bond's planarity. We are cross-correlating high resolution (less than 1Å) structures from the RSCB Protein Data Bank (PDB) and the Biological Magnetic Resonance Bank (BMRB). The dependence of backbone atom chemical shifts on peptide backbone dihedral angles /g301 and /g442 has been described by others. It is possible that the out-of-plane peptide bond torsion angle (/g468) exerts further influence on these chemical shifts. Thus this work may improve the accuracy of chemical shift-based protein structure determination.

107. A Demonstration of Both the Regio- and Stereochemical Outcome of Alkene Hydration

Thomas Lobasso, Christa Iwanoski, Shahrokh Saba and Donald D. Clarke, Fordham University, Bronx, NY

Our students hydrate 1-hexene to make 2-hexanol, illustrating Markovnikov’s rule. Though it isn’t apparent from their data (bp and 1H/13C NMR spectra), we tell them the main product is a racemic mixture of (R)- and (S)-2-hexanol. We describe here an experiment for students to prove this by reacting their alcohol with a chiral auxiliary. Mosher's acid chloride is often used for this in industry but is too expensive for a large class. An affordable chiral reagent is the chloride of (1R)-(−)-10-camphorsulfonic acid (CSA). Few alkyl esters of CSA are described in the literature and these are made using metal alkoxides. We deemed that unsuitable for our students. A procedure was developed where the reactants are mixed with triethylamine in CH2Cl2 to produce the desired CSA esters of (R)-2-hexanol [1] and (S)-2-hexanol [2]. These differed by 0.11 ppm at C-2 of the hexyl group in the 13C NMR spectrum. Authentic (R)-2-hexanol was converted to 1 and used to identify the diastereomers. The C-2 chemical shift of 1 was less than that of 2. Calculations, using Gaussian,
predicted this result correctly. The rearranged product 3-hexanol is formed also and it can be shown to be a racemate by making its CSA ester. Supported in part by a Faculty Research Grant from the Fordham University Research Council.

108. Learning from An Orange Beard
Brahmadeo Dewprashad and Latfa Hadir, Borough of Manhattan Community College, New York City, NY

This presentation describes an engaging and colorful demonstration that was inspired by the observation of a beard that was dyed orange. The compound 2-hydroxy-1, 4-napthoquinone is the chemical which gives Henna, a natural dye, its characteristic color. The compound is yellow under acidic conditions, but orange under basic conditions. The demonstration uses an invisible ink of a dilute basic solution to write a message on a filter paper. On spraying the developing solution of 2-hydroxy-1, 4-napthoquinone in ethanol, the message is highlighted in orange whilst the background appears yellow. On then spraying a dilute acidic solution to the paper, the message disappears. The demonstration can be quickly, easily and safely prepared for use in a classroom or laboratory. The presentation will describe how the demonstration can be used, not only to attract students' attention, but to make concrete the concepts of resonance stabilization, keto-enol tautomerization and relative acidities.

109. Reactions of Hexachloroacetone with Aliphatic Diamines: Syntheses of Bis(trichloroacetamide) Derivatives
Yoomi Kim and Jun H. Shin, Queensborough Community College, Bayside, NY

The reactions of hexachloroacetone (HCA) with aliphatic diamines gave bis(trichloroacetamide) as white solids at room temperature in high yield. The amide compounds have been characterized by FT-NMR and FT-IR. The molecular structure of N,N'-ethylenebis(trichloroacetamide) has been also determined by X-ray diffraction confirming that the ethylene group is bridging two trichloroacetamido units.

\[
2 \text{Cl}_3\text{C} \equiv \text{C} - \text{Cl}_3 + \text{H}_2\text{NCH}_2\text{CH}_2\text{NH}_2 \rightarrow \text{Cl}_3\text{C} \equiv \text{C} - \text{NHCH}_2\text{CH}_2\text{NH} \equiv \text{C} - \text{Cl}_3 + 2 \text{CHCl}_3
\]

110. Reactions of Hexachloroacetone with Aromatic Diamines: Syntheses of N,N'-Phenylenbis(trichloroacetamide)
Emily Hughes and Jun H. Shin, Queensborough Community College, Bayside, NY

N,N'-phenylenebis(trichloroacetamide) was obtained by the reaction of hexachloroacetone (HCA) and phenylenediamines (meta and para) after refluxing overnight in chloroform. The products were characterized by FT-NMR and FT-IR. Also the intermediate, N-p-aminophenyltrichloroacetamide, was isolated in benzene and spectroscopically characterized.

\[
\text{Cl}_3\text{C} \equiv \text{C} - \text{Cl}_3 + \text{H}_2\text{N}-\text{NH}_2 \rightarrow \text{Cl}_3\text{C} \equiv \text{C} - \text{NH}\text{-Ph} - \text{NH}_2 + \text{CHCl}_3
\]

\[
\text{Cl}_3\text{C} \equiv \text{C} - \text{NH}\text{-Ph} - \text{NH} \equiv \text{C} - \text{Cl}_3 + \text{CHCl}_3 \rightarrow \text{HCA}
\]
111. Determination of Refractive Index of Methanol Solutions Using a Laser Pointer: Relation to Density and Concentrations

Jeffrey Park, Crystal Park and Jun H. Shin, Queensborough Community College, Bayside, NY

Refractive index is one of well-known analytical technique to identify a liquid compound, and it was successfully measured using a laser pointer and a chromatography column with high accuracy. We expanded the system to binary organic liquid mixtures and found that there was a good relationship between the refractive index and various types of concentration such as %volume, %mass, molarity and density. This system could be used not only for the qualitative analysis, but also for the quantitative analysis.

112. Determination of Refractive Index Using a Laser Pointer: Non-Ideal Behavior of Aqueous Solution

Crystal Park and Jun H. Shin, Queensborough Community College, Bayside, NY

A good linear relationship between the concentrations of binary organic liquid mixtures and their refractive index was observed, however, we found that there was a non-ideal behavior of refractive index on aqueous solutions. In many occasions, the refractive index of the mixtures was higher than that of pure organic liquid used. The deviations were greater as the refractive index difference (ΔRI) between water and the other liquid were smaller, however, an ideal behavior was observed for the aqueous solution of ethylene glycol which had the largest ΔRI among the solutions investigated.

113. Aflatoxin Exposure: Does It Account for Higher Incidence of Liver Cancer

Joanna Magda and Angelo Raymond Rossi, York College - City University of New York, Jamaica, NY

This work describes those methods used for the extraction of mycotoxins, including aflatoxins, from a variety of foods. The aflatoxin is known to be a potent carcinogen, primarily affecting the liver. The principles involved in extraction of the toxin from food samples leads to questions such what is the origin of the toxin, how does it end up in our food, and most importantly, how dangerous is it to our health. This research presents a number of compelling arguments and studies related to aflatoxin exposure.

114. Growth Mechanism of Highly Luminescent ZnO Nanoparticles

Alexandra Turner and Temer S. Ahmadi, Villanova University, Villanova, PA

Colloidal ZnO nanoparticles have been studied extensively in the past three decades. Luminescense of these quantum dots is dominated by both excitonic and a broad visible emission associated with the anion/cation deficiencies of the lattice. In this work, we present synthesis and characterization of highly blue-emitting ZnO colloidal nanoparticles and their thin films supported by UV-visible, fluorescence, Raman, and FTIR spectroscopies as well as TEM and Powder XRD. A mechanism for the growth of the colloidal particles, in particular the role of temperature, is also presented.

115. Extraction Methods Used for Fresh Produce (E302 Methods)

Angelo Damanti¹, Yelena Karaseva¹ and Angelo Rossi², (1)U. S. Food and Drug Administration, Jamaica, NY, (2)York College - City University of New York, Jamaica, NY

The Pesticide Analytical Manual (PAM) is published by the Food and Drug Administration (FDA) as a repository of the analytical methods used by FDA laboratories in examining food commodities for pesticide residues and chemical contaminants for regulatory purposes. The multiresidue method that is presented in detail is PAM Vol I 302 E1. Most nonionic pesticide residues are extracted from nonfatty foods (like fresh fruit and vegetables) by blending with acetone or water/acetone mixture. Residues are transferred from aqueous acetone to methylene chloride / petroleum ether partitioning. Salt is added to aqueous layer after the first partitioning to aid transfer. Methylene chloride is
removed by evaporation and concentration steps in the presence of petroleum ether. Final extract is in acetone. Extract is amenable to analytical testing by many determinative steps including gas chromatography, liquid chromatography and mass spectrometry.

116. Utilization of HPLC-CAD (Charged Aerosol Detection) for Assessing Impurity Profiles in Synthetic Pulmonary Surfactant SURFAXIN® Versus the Current Marketed Animal-Derived Product Surfactant

Michelle A. De Crosta and Victoria Scott, Discovery Laboratories, Inc, Warrington, PA

Purpose

A new method has been developed utilizing Carona Charged Aerosol (CAD-PLUS) detection, whereby molecules with and without chromophores can be assessed and tracked in both synthetic and animal-derived lung surfactants via charged nebulization of the sample with nitrogen flow, capable of assessing four actives and related impurities in Lucinactant (SURFAXIN®; Discovery Laboratories, Inc., Warrington PA), a precision-engineered synthetic lung surfactant.

Method

Analytics utilizing HPLC-CAD (Charged Aerosol Detection) has been developed to assess product impurity profiles in various pulmonary surfactant formulations, both synthetic and animal-derived.

Results

Employ of HPLC-CAD analysis provides a means for impurity profiling and analytic assessment, with concomitant laboratory efficacy benefits, of a new synthetic pulmonary surfactant (Surfaxin®) versus currently marketed animal-derived surfactants. This analytical platform allows for all lipid-related impurities to be tracked and targeted with respect to their active parent compounds. One method of analysis was able to be developed using CAD detection, whereas prior several methods had to be employed, as some compounds lacked chromophores. Increased specificity and sensitivity was achieved using HPLC-CAD. Mass Spectrometry was conducted to support compound identification and method specificity.

Conclusion

The application of HPLC-CAD analytics allowed for the development of one method capable of monitoring four actives (R2 ≥ 0.99) and six known impurities (R2 ≥ 0.98) within SURFAXIN® drug product. Use of this new method also provides a means of assessing and comparing impurity profiles between synthetic surfactant drug product versus that exhibited by current marketed animal-derived surfactant drug product.

117. From SAMs to Drugs: Design and Development of SLx 2101, a Novel PDE5 Inhibitor for the Treatment of Cardiovascular Diseases

Farah Dhun, Brian Kirk, Dominick Casalena, Elsa Paradise, Andrew Saati, James Ellis, John Ferkany, Enoch Kim, Stewart Campbell, Michael Grogan, Paul Sweetnam and Bridget Cole, Surface Logix, Inc, Brighton, MA

Phosphodiesterase-5 inhibitors are therapeutically beneficial for the treatment of conditions where endothelial dysfunction plays a role in the underlying pathology. Although FDA approved PDE5 inhibitors demonstrate modest efficacy for the treatment of cardiovascular ailments such as PAH, these pharmaceutical agents are typically administered TID and may be associated with adverse events. Surface Logix has developed a novel PDE-5 inhibitor, SLx-2101, using the Pharmacomer™ Technology Platform to drive small molecule drug design. This proprietary technology, based upon
research pioneered by Professor George Whitesides, uses self-assembled monolayers (SAMs) to model small molecule-protein interactions and interfacial properties that determine PK and PD parameters. Utilization of the Pharmacomer™ Platform allowed Surface Logix to specifically modify both the tissue distribution and the half life of a well-known short acting PDE pharmacaphore to deliver a drug that preferentially circulates into cardiovascular tissue to induce dose-responsive reduction of systolic blood pressure and heart rate in spontaneously hypertensive rats.

118. How Does the U.S. FDA Test for Pesticides in Produce?
Yelena Karaseva¹, Angelo Damanti¹ and Angelo Rossi², (1)U. S. Food and Drug Administration, Jamaica, NY, (2)York College - City University of New York, Jamaica, NY

Pesticides are substances which protect plants against molds, fungi, and insects; therefore decreasing the percent of crop loss for harvest and potential illness. Most pesticides are produced by plants naturally to ward off their predators. The amount of man-made pesticides applied and their residue allowed to remain on products at market are regulated and inspected by the U.S. Department of Agriculture, the Environmental Protection Agency and the Food and Drug Administration. The Food and Drug Administration (FDA) has three main objectives in respect to pesticides: 1) to sample and analyze fresh and processed domestic and imported foods for pesticide residues and industrial chemicals; 2) to initiate enforcement action for shipments found to contain illegal residues; 3) to generate information on the incidence and levels of pesticide residues in domestic and imported foods. Sample analysis is performed according to official pesticide methods that published in the FDA Pesticide Analytical Manual (PAM) and other analytical methods published in scientific journals.

119. Distribution of Periodontal Pathogens in the Third Molar Region of Adult Asian Indian Patients
Darryl Williams, Dr. Raji Subramaniam and Dr. Patricia Schneider, Queensborough Community College, Bayside, NY

Adult periodontal disease is associated with anaerobic gram-negative bacteria, in particular Prophyromonas gingivalis, Treponema denticola, and Tannerella forsythensis. Recent studies have linked the onset of periodontal disease in young adults with wisdom teeth or third molars. Wisdom teeth are difficult to clean due to their location and are prone to periodontal infection which can spread to other teeth. This study investigated the distribution of the three pathogens in wisdom teeth and in anterior teeth of Asian Indian patients at a private dental clinic. The BANA (N-benzoyl-DL-arginine-2-napthyamine) enzyme assay was performed on subgingival plaque samples taken during routine scaling. DNA was extracted from paper points used by the dentist to collect samples of subgingival fluid. The polymerase chain reaction (PCR) detected specific pathogens based on the amplification of signature sequences of the small subunit16S rRNA genes. We examined the relationship between bacterial distribution, BANA score, demographic factors (age and gender) and clinical parameters (pocket depth, dental history and bleeding on probing).

120. Effect of Microstructure on Enzymatic Degradation of Polycaprolactone
Gabriela Sekosan and Nadarajah Vasanthan, Long Island University, Brooklyn, NY

Polycaprolactone films (PCL) with different degree of crystallinity were prepared by solvent casting and the effect of microstructure on enzymatic degradation by a lipase type enzyme was studied in vitro. The extent of degradation of PCL films was examined by weight loss, differential scanning calorimetry (DSC), FTIR spectroscopy and optical microscopy. Weight loss during enzymatic degradation of PCL films having different crystallinity as a function of time suggested that that the degradation depends on crystallinity and morphology of starting PCL films. PCL film with lower crystallinity (24%) degrades in a way of layer-by-layer. Enzymatic degradation of low crystallinity PCL film usually starts from the amorphous region where the degradation rate is much higher than
that in the crystalline region while degradation of PCL film with higher crystallinity (45%) occurs in the crystalline region as well in the amorphous region. Effect of degradation on crystallinity, melting temperature and conformational changes if any were investigated using FTIR and DSC. These results will be discussed.

121. Experimental Design and Inquiry: Exploring the Chemistry of Dental Health Care Products

Ann E. Shinnar and Marc Nemetsky, Lander College for Men, Touro College, New York, NY

To expand our undergraduate laboratory curriculum, we are developing experimental sessions that encourage students to cultivate their own experimental inquiry and involve them in experimental design. Towards the end of a 2-semester general chemistry sequence, one laboratory session is designated for exploring chemical reactions involved in denture cleansers. The goals of this session are (1) to stimulate students to observe chemical systems and to formulate their own questions about these systems, (2) to give students an opportunity to propose their own simple experiments that focus on testable parameters, and (3) to introduce students to chemistry of oxidation-reduction reactions used in dental health care products. Initially, students are provided only with denture cleanser tablets such as Efferdent, a beaker of water, and a timer. After making initial observations, students are asked to generate a list of questions and to propose how they would study parameters such as pH, temperature, rates, concentration, etc. using simple materials and equipment available in the laboratory. Proposals for identifying the gases released and the components that change color usually necessitate the use of textbook and internet sources. Such activities introduce undergraduates to concepts in experimental design, which they might implement in additional laboratory sessions. Furthermore, the choice of commercially available denture cleansers provides an opportunity to review the oxidation-reduction reactions of peroxide compounds and their important role as bleaching compounds and anti-bacterial agents. These exercises give students segue to experimental design in research and to the chemistry of everyday health care products.

122. Synthesis and Catalytic Properties of Novel Chiral Polyamines

Mindy Levine, Craig Kenesky, Shengping Zheng and Ronald Breslow, Columbia University, New York, NY

Chiral polyamines can be utilized for a variety of potential applications, ranging from asymmetric catalysis to nonviral gene delivery systems for DNA and RNA. They can also be utilized to solubilize carbon nanotubes. Thus, methods for the straightforward synthesis of chiral polyamines are needed. We present herein two synthetic strategies for accessing chiral polyamines. One strategy leads to polyethyleneglycol – chiral polyamine block copolymers, and the other leads to well-defined oligoamines from the reduction of chiral polypeptides. The potential of these chiral amines to catalyze two organic reactions with a high degree of chiral induction is also explored.

123. Plant Phenols - Polymer Interactions: Effect on Tyrosinase and Elastase Activities

Michael Koganov and Artyom Duev, Integrated Botanical Technologies, LLC, Ossining, NY

Inhibition of tyrosinase and elastase is required to control skin pigmentation and inflammation. Only a few plant phenols provide a balanced inhibition of both enzymes (Koganov & Duev, MARM 2007). Optimization of topical products requires further investigation of interactions among selected phenols and components of delivery system because certain polymers capable of modulating the activity of enzymes associated with skin inflammation (Koganov, US 20050175579). Twenty phenols with common structure: C15 (C6–C3–C6) flavone nucleus including two benzene rings (A & B) linked through O-containing pyran or pyrone ring (C) were investigated. Conjugated n bonds in A and B rings and n bond between C2 and C3 play an important role in tyrosinase and elastase inhibition. Presence of 6-O-α-L-rhamnosyl-D-glucose at C3 decreased the activity of phenol. Presence of 4-
hydroxyphenyl or 3,4,5-trihydroxy-benzoil at C3 and of 3,4-dihydroxyphenyl at C2 significantly increased enzyme inhibitory activities. Hydroxylation in positions B3', B5', C3 also increased inhibitory activities. Selected acrylic polymers potentiate elastase inhibition of certain phenols. However, these polymers were inactive against tyrosinase and didn't affect tyrosinase inhibition activity of phenols. Enzymes inhibition in systems containing most active polymers and phenols (Rosmarinic Acid – RMA and Epigallocatechin Gallate – EGCG) were analyzed. RMA’s elastase inhibitory activity includes electrostatic interactions. Tyrosinase inhibition by RMA is relatively insensitive to electrolyte concentration. EGCG’s inhibitory effect of both enzymes includes hydrophobic interactions. When applied together, RMA competes with EGCG for tyrosinase and elastase inhibition. Development of novel skin whitening/lightening and anti-inflammatory ingredients and optimization of delivery systems will be discussed.

124. Stabilization and Continuous Processing Techniques for Manufacturing Phenol/Formaldehyde Resins Used in Making Photoresists

M. Dalil Rahman, AZ Electronic Materials USA Corp., Somerville, NJ and Stanley F. Wanat, Union County College, Cranford, NJ

Phenol/Formaldehyde resins are a main component of the photosensitive coatings used to make circuits in computer chip preparation. Since the resins are formed in reversible acid catalyzed reactions, they are prone to unwanted mixtures of various molecular weight fractions. This paper outlines various techniques (steam distillation, base neutralization etc.) to stabilize the molecular weight distribution of the resins and prevent reverse reactions from occurring. Performance characteristics of the resins were further optimized by selectively fractionating the resins and this paper will compare the various fractionation methods used to make the best resins used for making micro-circuits.

125. Taking the “Nip” out of Catnip: An Undergraduate Experiment Involving Isolation and Identification of Nepetalactone Diastereomers from Commercial Samples of Nepeta Cataria L.

James A. Ciaccio, Rabeka Alam and Christina D'agrosa, Fordham University, Bronx, NY

Student interest is often stimulated by naturally occurring compounds that possess biological activity. One example known for many years, but not often described in introductory organic textbooks, is nepetalactone: a monoterpene-derived fused bicyclic enol lactone. Recognized mostly as feline stimulants, the two major diastereomers of nepetalactone found in N. cataria also possess the ability to repel some insect species and their potential as biological control agents have recently been investigated. To independently establish the essential oil composition of N. cataria our students steam distilled the organic volatiles from seven brands of commercial catnip to obtain 20-40 mg of viscous oil from 10 g of dried plant material. Analysis by GC-MS and $^1$H/$^{13}$C NMR spectroscopy, in comparison with reported spectral data, revealed that five samples contained either the cis-fused lactone (1) or the trans-fused lactone (2) as the predominant steam-volatile product, along with 1-8% of the other diastereomer. A sixth sample contained a mixture of 1, 2 (with a 1:2 ratio of 90:10) and significant amounts of several other substances. A seventh, spurious sample contained predominantly menthol with no detectable amounts of nepetalactone. Lactones 1 and 2
are separable by TLC and visualized using standard methods; thus, even without access to spectral
data each student can analyze their own sample, and by co-spotting their sample along with those
of other students they readily establish that most commercial sources of catnip contain one of two
possible compounds (1 or 2) as the single, predominant steam-volatile product.

126. Metabolic Profiling of the Coral Pathogen Vibrio Coralliilyticus

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The coral pathogen Vibrio coralliilyticus has been implicated in bleaching events for the coral
Pocillopora damicornis. As part of a larger effort to understand the temperature-dependent
pathogenicity that has been observed with V. coralliilyticus, its metabolic profile was analyzed using
Nuclear Magnetic Resonance (NMR)-based metabolomics. V. coralliilyticus was cultured at 24°C,
where it displays no toxicity, and 27°C, a temperature at which it triggers coral bleaching.
Metabolites were extracted from cell cultures whose cellular processes had been quenched with
liquid N₂ using a 2:1 hot methanol:water solution. The spectral data was binned and analyzed using
Principal Component Analysis (PCA) and Partial Least Squares Analysis (PLS). Class separation was
observed between cultures grown at different temperatures. Analysis is on-going to determine what
specific metabolic changes occur and how these changes may be linked to virulence.

127. A Study of the Ideal Conditions Required for the Uptake of Lawsone from
Henna (Lawsonia Inermis) as a Greener Approach to Dyeing

Samuel Ganta and Kishore K. Bagga, Holy Family University, Philadelphia, PA

The primary purpose of this investigation was to further the understanding of using Henna as a
dyestuff. A dyestuff is a colored substance which can be used for staining or coloring other
materials. The dyestuff found in henna is lawsone which is an orange pigment present in the leaves
of the plant. The research involved the dyeing of: jute, silk, nylon, wool, linen, and a blend of nylon:
polyamide (50:50). Each material was investigated individually under specified conditions to
determine the most ideal set of conditions required for the material to adsorb lawsone. Uptake
studies of lawsone were quantified based on percent change in absorbance of the aqueous henna
solution. The parameters investigated were: temperature, duration and concentration. The studies
indicate that under comparable conditions, nylon: polyamide (50:50) along with wool had the
highest uptake of lawsone of the materials investigated. This study about dyeing with henna will
provide more insights on its possible use as a natural agent and, promote its use as a substitute for
synthetic dyes as a more environmental friendly, greener approach to dyeing.

128. Absolute Configuration Determination of a Biologically Active Diol

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In the following the absolute configuration of 17,20αβ-dihydroxy-4-pregnen-3-one, a fish
pheromone, is investigated by means of different techniques.
129. Quinones, Monoradicals and Diradicals from 3- and 4-Mercaptocatechol, and 3,4-Bismercaptocatechol: A Computational Study of a Plausibly Biomimetic Reaction

Alvaro Castillo¹, Joel F. Liebman² and Alexander Greer¹, (1)City University of New York, Brooklyn College, Brooklyn, NY, (2)University of Maryland, Baltimore County, Baltimore, MD

Little attention has been focused on radical and diradical formations from compounds that contain both phenol and thiol groups. Computational studies were conducted on radicals and diradicals from mercapto- and bismercaptocatechols to provide insight into their relative stability. The loss of a hydrogen atom from mercapto- or bismercaptocatechol produces S- and O-centered radicals of similar energy. The loss of two hydrogen atoms from 3,4-bismercaptocatechol is an example where a number of quinone and diradical structures become possible. However, the energetics are consistent with a 4-membered ring disulfide (dithiete) playing an important role in the two electron oxidation reaction of 3,4-bismercaptocatechol.

130. Structures and Energies of Models for Reduced Symmetrically and Anti-Symmetrically Methylated Arginine Side Chains

Edward M. Barbieri and Margaret Mandziuk, Manhattan College, Riverdale, NY

The roles of proteins that have methylated arginines have been identified in many cases, and include RNA processing, signal transduction, DNA repair, cardiovascular disease and cancer. The specific interactions caused by methylation itself, however, are not fully established.

We have been investigating whether one electron reduction of the cationic side chain may play a role in methylation. Our models in calculations were N-methylated triaminomethyl radicals. Here we present and compare the structures and energies of models for reduced, symmetrically and anti-symmetrically dimethylated arginine side chains. The calculations were performed with the B3LYP density functional, using cc-pVTZ and aug-cc-pVTZ basis sets.

131. The Incorporation of Fluorinated Phenylalanine Analogs into Histone Acetyltransferase

Anita Y. Zhu, Polytechnic University, Brooklyn, NY

Biochemical approaches of expanding the genetic code dramatically increase the methodologies available to manipulating protein structure and function. The introduction of fluorinated amino acids into proteins has been used to design proteins with improved thermal stability and increased resistance to denaturants. Histone acetyltransferases (HATs) represent a group of proteins that acetylate the lysine residues on histone tails using acetyl coenzyme A. The molecular basis for HAT specificity was conducted on Tetrahymena Gcn5 (tGcn5) in complex with its substrates by Poux and Marmostein. Our goal is to explore the effects fluorinated amino acids have on the stability and function of HAT tGcn5. In this study, we have biosynthetically replaced phenylalanines in tGcn5 with a series of fluorinated analogs: p-fluorophenylalanine (pFF), o-fluorophenylalanine (oFF), and m-fluorophenylalanine (mFF). We demonstrate high levels of substitution and investigate its effects on protease degradation and activity for the target H3p19 substrate.

132. Biological Activity of a Water-Insoluble Benzopentasulfane Compound

Adaickapillai Mahendran¹, David Aebisher¹, Konstantin Astafurov¹, Rafael Ovalle¹, Akira Kawamura², Ernest Boamah², Jill Bargonetti² and Alexander Greer¹, (1)City University of New York, Brooklyn College, Brooklyn, NY, (2)City University of New York, Hunter College, New York, NY

Benzopentasulfane (o-C₆H₄S₅) possesses biological activity, but has poor water solubility. o-C₆H₄S₅ is sparingly soluble even in DMSO (2.03 mg/mL), which has led to difficulties in evaluating the
bioactivity. In DMSO, o-C₆H₄S₅ displays IC₅₀ 100 ng/mL activity against mammalian Leukemia (Jurkat) cells, 1-10 mg/mL activity against Saccharomyces cerevisiae (X2180), and 0.1 μg/ml (10 μM) cytotoxicity to DLD-1 cancer cells absent of the p53 protein.

133. Lysine-Triggered β-Lactam Ring Formation of Deoxyguanidinoproclavaminic Acid Which Involves a Rebound of the Phosphate Ion Leaving Group: A Combined DFT and Mutational Analysis

Mary Raber¹, Michael Freeman¹, Alexander Greer² and Craig A. Townsend¹, (1)Johns Hopkins University, Baltimore, MD, (2)City University of New York, Brooklyn College, Brooklyn, NY

An experimental and computational study implicate lysine443 in the activation of N²-(2-carboxyethyl)-arginine (CEA) to facilitate the formation of the β-lactam deoxyguanidinoproclavaminic acid (DGPC). The importance of lysine443 as an acid catalyst is demonstrated by its mutation to arginine (60-fold reduction on kcat). A low energy pathway to β-lactam formation was computed by density functional theory. We show that the energetics are consistent with a facile proton-transfer from lysine to the carbonyl oxygen of CEA, which triggers a nucleophilic attack by the adjacent amine. DFT predicts β-lactam formation may proceed without the lysine acid catalyst; however, the reaction is highly endothermic.

134. Asymmetric Transfer Hydrogenation of Allylic Alcohols with Homogeneous Chiral Ruthenium Catalysts

Marie G. Beauchamps and John R. Sowa Jr., Seton Hall University, South Orange, NJ

Asymmetric transfer hydrogenation of allylic alcohols with ruthenium complexes is a novel reaction. We have been able to convert geraniol to citronellol with an in situ catalytic system [RuCODCl₂]n and chiral bidentate ligands in 95% yield and 90% ee. The mechanism of this reaction has been investigated with deuterated IPA. We have evidence that the allylic alcohol isomerizes to the enol, which subsequently undergoes hydrogenation. The results of the isomerization reactions, the deuterated experiments, and the use of a known catalyst {Diacetato[(S)-(-)-2,2'-bis(di-p-tolylphosphino)-1,1'-binaphthyl]ruthenium(II)} will be presented.

135. Nucleotide Reversible Terminators for Pyrosequencing

Jian Wu, Columbia University, New York, NY

Pyrosequencing is a method used to sequence DNA by detecting the pyrophosphate (PPI) group that is generated when a nucleotide is incorporated into the growing DNA strand in the polymerase reaction. However, this method has an inherent difficulty in accurately deciphering homopolymeric regions of DNA templates. We report here the development of a method to solve this problem by using nucleotide reversible terminators. These nucleotide analogues are modified with a reversible chemical moiety capping the 3'-OH group to temporarily terminate the polymerase reaction. In this way, only one nucleotide is incorporated into the growing DNA strand even in homopolymeric regions. After detecting the PPI for sequence determination, the 3'-OH of the primer extension product is regenerated through different deprotection methods. Using a library of chemical moieties
allyl, 2-nitrobenzyl and azidomethyl) as the reversible groups to cap the 3'-OH of the four nucleotides, we have synthesized three sets of 3'-O-modified nucleotides, as reversible terminators for pyrosequencing. The capping moiety on the 3'-OH of the DNA extension product is efficiently removed after PPI detection by either a chemical method or photolysis. To sequence DNA, templates containing homopolymeric regions are immobilized on Sepharose beads, and then extension–signal detection–deprotection cycles are conducted by using the nucleotide reversible terminators on the DNA beads to unambiguously decipher the sequence of DNA templates. Our results establish that this reversible-terminator-pyrosequencing approach can be potentially developed into a new methodology to accurately determine DNA sequences.

136. You Are What You Eat!

Peter L. Bastos, Hunter College, New York, NY

The world health organization (WHO) made a study a number of years ago and estimated that out of the over six billion people on this planet, approximately 300 million are overweight. Numerically this statistic works out to roughly 5% of the world's population. This in itself is not alarming, what is surprising, however, is that two thirds of this overweight population resides in the United States! This implies that nearly 70% of the population of this country has some weight issues. The question of being overweight will be looked upon as an energy balance between the average human's energy needs (i.e., roughly 1,500 to 2,000 daily Caloric intake), to the actual Caloric intake. A virtual fast food menu will be presented in order to illustrate that one's daily Caloric needs are satisfied in roughly one meal in these establishments. Since three meals a day is the norm for most people then the excess food consumption, to an extent, is metabolically converted into lipids. Once the cumulative effects of this daily regiment is taken into consideration then a better understanding of the obesity concern of this country could be addressed.

137. Synthesis and Application of Water-Soluble Nanocapsules

Xuejun Liu and Ralf Warmuth, Rutgers, The State University of New Jersey, Piscataway, NJ

Molecular container compounds are hollow, spherical molecules with inner cavities which can accommodate guest molecules.[1] They have demonstrated great potential in applications such as catalysis, reaction control and separation technology. Recently, we have developed highly efficient one-pot procedures for the synthesis of nanometer-sized covalent molecular capsules.[2] Here, we report the synthesis of a water-soluble octahedral nanocapsule. Binding studies in water demonstrate that this capsule encapsulates multiple negatively charged organic molecules. Electrostatic and hydrophobic interactions act cooperatively during the complex formation.


138. Morphine as a Mimic of the Backbone of Opioid Peptides

Zhijun Wu, ABC Resources, Plainsboro, NJ

"Despite of the recent advances in the structural investigation of complex molecules, the comprehension of the 3D features responsible for the interaction between opioid peptides and micro-opioid receptors still remains an elusive task. This has to be attributed to the intrinsic nature of opioid peptides, which can assume a number of different conformations of similar energy..." -Gentilucci, L. and A. Tolomelli (2004). Recently, we had an interesting observation: morphine, the well-known natural opioid receptor ligand, appears to closely mimic the backbone of opioid peptides (See the picture below). In this presentation, the related supportive materials
will be discussed. Hopefully, this observation can serve as a novel clue for the active conformation of opioid peptides.

139. Characterization of Pokeweed Antiviral Protein's Interaction with Eukaryotic Initiation Factors and a Sarcin/ricin Loop Oligoribonucleotide

Diana E. Friedland¹, Dixie J. Goss², Jeannine DeGrazia¹ and Amy E. Baldwin³, (1)John Jay College of Criminal Justice and the Graduate Center of the City University of New York, New York, NY, (2)Hunter College CUNY, New York, NY, (3)Pace University, New York, NY

Ribosome-inactivating proteins (RIPs) are naturally occurring cytotoxic N-glycosidase agents and are found in numerous plant, fungi, and bacterial species. They inhibit protein synthesis by depurinating A4324 on the conserved sarcin/ricin loop (SRL) of the 28S rRNA. Pokeweed Antiviral Protein (PAP) is a type I RIP that has also long been recognized as an important antiviral agent. It is also able to inhibit infection without loss of host cell translation.

We report in vitro fluorescence spectroscopic studies of PAP-eIFiso4G binding revealing a binary interaction with a Kd of approximately 100 nM. This interaction enhances PAP's binding to the cap analog m7GTP 3.6-fold. Our measurements place PAP's affinity for cap between that of the wheat germ cap binding proteins eIFiso4E and eIFiso4F. ATP and GTP compete with cap for PAP binding; both nucleotides and the cap analog show little salt dependence in binding, suggesting that the interactions are specific for these nucleotides. The biological significance of the cap binding remains unclear, however this may serve as a means to target RNA or, since ATP binds to the same site, this may be a protective mechanism for host cell capped RNA. The interaction with eIFiso4G suggests that additional proteins may aid PAP in accessing particular RNA and distinguish structural elements of the RNA. These results support a model where PAP's interaction with initiation factors may play a regulatory role in its enzymatic activity. PAP's binding to the SRL oligonucleotide sequence was measured; it is weaker than for cap analog and is described.

140. Detection of rRNA Depurination by Pokeweed Antiviral Protein: Fluorescence Detection of Adenine Release

Nicole DeLuca¹, Ana Sanchez¹, Eugenia Pontacq¹, Jacqueline Chaparro¹ and Diana E. Friedland², (1)John Jay College of Criminal Justice, New York, NY, (2)John Jay College of Criminal Justice and the Graduate Center of the City University of New York, New York, NY

Many plants, fungi, and bacterial species have cytotoxic agents called Ribosome Inactivating Proteins (RIPs). Due to the fact that the RIPs have a broad spectrum of antiviral activity, they have become an intricate part of making advancements in the study of antiviral agents. One such protein, Pokeweed Antiviral Protein (PAP), is a type I RIP which inhibits protein synthesis by depurinating the conserved Sarcin/ricin loop (SRL) of the large ribosomal RNA (rRNA). Our lab used 16S+23S and 18S+28S rRNA for protocol refinement and in order to confirm that our PAP from locally harvested plants is depurinating rRNA. Our modified protocol converts the free adenine into the fluorescent etheno-adenine derivative using chloroacetaldehyde. We then monitor the emission intensity using
steady-state fluorescence spectroscopy. Here we report our PAP purification protocol, our modified fluorescence protocol for detection of adenine release, and depurination studies using an SRL oligoribonucleotide with three known depurination sites. This oligo can also be transcribed as a capped variant. This data will be correlated with binding data performed in our lab to explore the relationship between mRNA structure and depurination by PAP. In analyzing this relationship, it can lead to improving the application of RIPs to anti-pathogenic studies (plant and mammalian) as well as bioterrorism toxins.

141. Sub-Cloning of Protein Kinase C-α3HA in a Yeast Plasmid

Shih Wei Chiang, Sakshi Pasricha-Katyal and Nidhi Gadura, Queensborough Community College, CUNY, Bayside, NY

Hsp90 is a molecular chaperone essential to the folding, activation and maturation of small number of distinct client proteins. We hypothesize that PKCa is a possible client protein of Hsp90; we base this hypothesis according to the results from Rotenberg laboratory showing that Hsp90 and PKCa co-immunoprecipitate. A sub-cloning project was done as part of this bigger project. We subcloned bovine PKCa-3HA gene into a yeast plasmid. In order to accomplish my project, I digested a mammalian plasmid pCMV4 PKCa with EcoRI & XhoI restriction enzymes. Then I cleaned the DNA fragments from a gel. This was followed by a Ligation reaction with Vector and Insert fragments. The recombinant DNA was transformed with E.coli DH5α competent cells. We selected on the LB & Amp plates. Finally we confirmed our recombinant plasmid that has bovine PKCa-3HA gene in the new yeast plasmid by a) EcoRI & XhoI digestion and running gel b) PCR amplification of PKCa gene-3HA in the new plasmid and finally c) sequencing the gene. This gene will be expressed in different yeast strains and the amount of protein and its activity will be measured.

142. Analysis of Mycotoxins Using HPLC

Frandaluz Cuevas¹, Paris Svoronos¹ and Barry Mopper², (1)Queensborough Community College, Bayside, NY, (2)Food and Drug Administration, Jamaica, NY

Molds are fungi that produce mycotoxins, some of which are capable of damaging the immune and nervous systems while others are known carcinogens. At the Food and Drug Administration (FDA) in Jamaica, NY the levels of mycotoxins are tested in dry foods as well as in chemotherapeutics in aquaculture. The four mycotoxins tested are deoxynivalenol and ochratoxin (found in wheat and maize), patulin (encountered in fruits and vegetables including apple juice and apple cider) and aflatoxin (found in nuts, figs and some spices). Mycotoxins are examined and analyzed using the spot testing method. The chemotherapeutic agents tested for are fluoroquinolone antibacterials that include ciprofloxacin, enrofloxacin, sarafloxacin, and difloxacin. The determination of these four fluoroquinolones is achieved using HPLC.

143. NMR Studies on the Conformational Exchange in 1-Benzazepines

Ngai Hin Lo¹, Sasan Karimi¹, Keith Ramig², and Gopal Subramaniam³, (1)Queensborough Community College, Bayside, NY (2)Baruch College - CUNY, New York, NY (3) City University of New York, Queens College, Flushing, NY

Benzazepines are a pharmacologically important group of compounds used in the treatment of HIV and many other illnesses. A facile synthesis of 3H-1-benzazepine was reported by one of us recently. Energy minimization by MM2 force field shows that the molecule adopts a conformation where the C3 is out of the plane of the heterocyclic ring system along with one of the two phenyl rings attached to the C2 and C4-positions. At room temperature, the NMR spectrum of 1-benzazepine shows only one resonance at 3.4 ppm for the methylene protons at C3, suggesting that the molecule equilibrates rapidly between two conformations (C3 above or below the plane). At -65 °C, the exchange is slow and two separate resonances are observed at 4.5 and 2.2 ppm. The low temperature experiment is explored to assign the proton and carbon NMR spectra of 1-benzazepine.
derivatives. We will also describe calculations to measure the activation barrier for the conformational equilibrium.

144. Synthesis of Biologically Active 1-Benzazepines
Michelle J. Cho\textsuperscript{1}, Gopal Subramaniam\textsuperscript{2}, Keith Ramig\textsuperscript{3}, and Sasan Karimi\textsuperscript{1}, (1)Queensborough Community College - CUNY, Bayside, NY (2) City University of New York, Queens College, Flushing, NY, (3) Baruch College - CUNY, New York, NY

Benzazepines are a pharmacologically important class of heterocycles. The biological activity of this class of heterocycles gave us the impetus to investigate a generalized approach towards the synthesis of little known 3H-1-benzazepines. To test the generality of the approach, new derivatives of 1-benzazepines containing substituted aryl groups at positions 2 and 4 were synthesized. The orientation of the aryl groups at positions 2 and 4 with respect to the plane of 1-benzazepine ring moiety were examined using various NMR experiments.

145. The Oxidized LDL/HDL Ratio Test Is An Automated Immunoassay for Identifying Patients with Coronary Artery Disease
Tod Schild, Anne McGarrett, Sanford Moos, Marta Moos, Patricia R. Romano and Harold M. Bates, Shiel Medical Laboratory, Brooklyn, NY

Low-density lipoprotein cholesterol (LDL-C) levels in plasma/serum are currently used by physicians to identify patients at risk for developing coronary artery disease (CAD) and for the diagnosis and therapeutic management of lipid disorders, particularly hyperlipidemias and dyslipidemias. LDL-C is one of the major risk factors for CAD, and several studies have demonstrated the benefits to patients who lower their LDL-C levels by therapy with statin drugs. It is important to note that not all patients with CAD are identified by LDL-C testing. We will demonstrate that our oxidized LDL/HDL ratio test (the ratio of atherogeneity/anti-atherogeneity) identifies about 50% more patients with clinical evidence of CAD than the LDL-C test. Oxidized LDL is the atherogenic form of LDL-C and is found in atherosclerotic plaques, but not in healthy arteries. We will compare the results of our automated oxidized LDL/HDL ratio test in (1) patients in the general New York patient population; in (2) presumably healthy, elderly Swedish patients without CAD; and (3) in Swedish patients with acute coronary syndrome. We will demonstrate by receiver-operating-characteristic curve (ROC curve) analysis and odds ratios that the oxidized LDL/HDL ratio test has greater diagnostic accuracy in discriminating between healthy control subjects and CAD patients when compared with other currently available lipid/lipoprotein biomarkers. The oxidized LDL/HDL ratio test could become the replacement for the time-honored LDL-C test.

146. Synthesis of Novel Macrocyclic Compounds in the Development of New Chemical Entities for Drug Discovery Research
David P. Brown and Thomas Wong, St. John University, Jamaica, NY

Macromolecules have been the targets of the synthetic efforts of investigators, largely because of their widespread applications related to their medicinal, insecticidal and/or phytotoxic properties.
Accordingly, we endeavored to synthesize a new series of macrocyclic systems as possible candidates in the development of New Chemical Entities for Drug Discovery Research. Thus, stable macrolactones and macrolactams have been synthesized from substituted phenylalkanoic acid systems in modest yields, employing the Ring Closing Metathesis strategy in the macrocyclization steps.

147. The Synthesis of Potential Transdermal Pain Killers
Constance N. Bezankeng, Susan Caspa, Oyedotun Oyewole and Nadene Houser-Archield*, Prince George's Community College, New Carrollton, MD

The orally administered carboxylic acid analgesics salicylic acid, aspirin, ibuprofen, naproxen and ketoprofen are known to cause stomach bleeding. Endeavoring to synthesize fat soluble derivatives of these analgesics for potential transdermal administration, we have esterified them with the primary alcohol derivatives of the major fatty acids in human fat; namely, oleyl alcohol (a derivative of oleic acid aka (Z)-octadec-9-enoic acid, 46% of human fat) and cetyl alcohol (aka 1-hexadecanol, a derivative of palmitic acid, aka hexadecanoic acid, 25% of human fat). We have also attempted to di-esterify these analgesics with the water soluble diol, polyethylene glycol—molar mass 8000 (PEG 8000); these results are currently inconclusive. PEG 8000 is soluble in some fats. Derivatives of this polymer are used as orally ingested laxatives and in skin creams/lotions. Thus far, we have studied the structures of these compounds by thin layer chromatography, and infrared spectroscopy. Attempted methods, successful methods, and characterization of structure will be discussed.

148. Novel Organosilane Chemistry for Approaches to Bioactive Ether Targets
Stephen Philip Fearnley, The City University of New York - York College, Jamaica, NY and Pedro J. Lory, Lamar University, Beaumont, TX

We have recently developed a general methodology for the construction of cis-fused bicyclic ether arrays. Our overall approach involves the intramolecular attack of a proximally tethered vinylsilane at an oxocarbenium moiety, generated in situ from the corresponding cyclic acetal under appropriate Lewis acid catalysis. This has allowed direct access to a variety of richly-functionalized cis-fused architectures, many of which are pertinent to specific bioactive natural products. One such example is the styryl lactones – a class of plant metabolites with wide-ranging cytotoxic properties. A concise synthesis of deoxyaltholactone analogs will be presented.

149. Synthesis of Nantenine: AN Antagonist of the Designer Drug “Ecstasy”
Onica Le Gendre, The City University of New York, New York, NY and Wayne Harding, Hunter College, New York, NY

MDMA (3,4-methylenedioxy-N-methylamphetamine) known on the street as “Ecstasy”, “Adam”, “XTC”, “hug”, “beans”, and “love drug”, is an illegal class A synthetic drug structurally similar to methamphetamine or “crystal meth” that acts as a stimulant and psychedelic. Consumption of “Ecstasy” by humans can lead to severe adverse effects including development of hyperthermia,
hallucinations, organ failure and in extreme cases, death. Cognitive impairment has also been reported in "Ecstasy" users and there is evidence that the drug has addictive properties.

Nantenine is a naturally occurring aporphine alkaloid isolated from the Japanese fruit of Nandina domestica. Nantenine has been shown to block and/or reverse behavioral and physiological effects of MDMA in mice. A large body of literature evidence indicates that behavioral and physiological effects of MDMA are mediated by the 5-HT2A receptor and (+) nantenine has been shown to antagonize this receptor. In order to further evaluate the anti-MDMA effects of nantenine in animal models, a good supply of the compound is required and thus a high-yielding synthetic route to the compound is desirable. Additionally, synthesis of nantenine will allow for the preparation of structural analogs which will be useful for evaluating structure-activity relationships at the 5-HT2A receptor.

We have synthesized nantenine in 0.1 %yield using a PIFA-mediated oxidative cyclization as a key step. We will present findings on the synthesis of nantenine as well as our attempts at optimizing the synthetic route.

150. An NMR Demonstration of Nonequivalent Methylene Hydrogens
Donald D. Clarke and Shahrokh Saba, Fordham University, Bronx, NY

While enantiotopic hydrogens of a methylene group are isochronous in an achiral environment, this is no longer true in a chiral one. In an unrelated study of the diastereomers derived from the R and S enantiomers of 2- and 3-hexanol, we prepared the 1-(R)-10-camphorsulfonate ester of 1-hexanol. While all of the methylene hydrogens of 2- and 3-hexanol are diastereotopic due to the nearby asymmetric center, the methylene hydrogens at C-1 of 1-hexanol are enantiotopic; however, in the sulfonate ester they are diastereotopic and hence anisochronous with appreciably different chemical shifts. This signal shows 10 distinct lines. A simpler example of this phenomenon is provided by the ethyl ester of 1-(R)-10-camphorsulfonic acid (CSA). Instead of the usual quartet these protons now show 12 lines. This seems to be a useful pedagogic example to present to our students. Because of the difference in chemical shifts of the methylene hydrogens we can measure both the vicinal and the geminal coupling constants. Supported in part by a Faculty Research Grant from the Fordham University Research Council.

151. Synthesis of Substituted Benzofuran-2-Carboxylic Acid Ethyl Ester
Luisa Martinez Troncoso and Dr. Kenneth Yamaguchi, New Jersey City University, Jersey City, NJ

In this experiment, the synthesis of a series of substituted benzofuran-2-carboxylic acid ethyl esters will be described under microwave-assisted conditions. Microwave-assisted organic synthesis allows not only for the improvement of reaction yields but also decreases reaction time. Microwave assisted organic synthesis help shorten the synthesis and isolation of the product and in turn, reduces environmental hazards.

A variety of substituted salicylaldehyde and Î±-halogenated ethyl acetate esters (X) were combined using a phase-transfer agent, different microwavable solvents, and bases. The synthetic conditions for this base-catalyzed cyclocondensation reaction will be discussed.

The scope of the reaction is being worked under several different modifications of the protocol in hopes of increasing reaction yields. The desired product for this synthesis is a heterocycle compound; heterocycles are an important class of organic compounds because of their biological activity and industrial importance.
152. The Transition Between the Closed and Semi-Open Form of Apo HIV-1 Protease through the Rearrangement of Hydrophobic Cores

Fangyu Ding and Carlos Simmerling, Stony Brook University, Stony Brook, NY

Anti-viral treatment has made a dramatic increase in the survival of AIDS patients; however, the success of conventional long-treatment therapies has been limited due to the emergence of drug-resistant mutants of HIV-1. Therefore, complete understanding of the structure and molecular dynamics associated with the conformational changes of HIV-1 protease is crucial in rational design of more effective treatment regimes. The flap regions of the protease, which exhibit much higher flexibility than other regions in apo HIV-1 protease, are believed to control the access to the active site; therefore a prime target of anti-AIDS drugs. In this work, one microsecond, unrestrained, all-atom molecular dynamics simulations with an explicit solvent model were performed on a wild type HIV-1 protease using the Amberff99SB force field. The flaps showed complex dynamics and various flap conformations (closed, semi-open, open and curled) during the simulations. Significantly, we observed not only multiple conversions among different states of the flaps, but also well reproduced the two major crystallographic forms of HIV-protease with flap Root-mean-square deviations (RMSD) less than 2Å from two crystal structures. The global dynamics obtained from these explicit solvent MD simulations agree very well with those from X-ray and NMR observations and our previous implicit solvent simulations. Our simulations gain insights into the flap conformational changes that are associated with the function of this enzyme. We propose that the rearrangement of intra- and inter- monomer hydrophobic clusters triggers the transition of the flap conformations.

153. Phototoxicity of 2-Substituted Quinoline Analogs

J. Cobar, E Milner, D Goodine, T Heady, W McCallmont and G Dow, Walter Reed Army Institute of Research, Silver Spring, MD

The active ingredient in Cinchona bark has been used for more than 3 centuries to treat malaria. The identification of the 2-hydroxy derivative, carbostyril, as a major urinary metabolite of cinchonine led to the synthesis of compounds designed to block the metabolic attack and thus increase effectiveness. A phenyl substituent at the 2-position increased antimalarial activity and many 2-phenyl-4-quinolinemethanols were synthesized and tested in vivo. Analogs of this type were originally abandoned in clinical trials as a result of a long-lasting phototoxic reaction. The phototoxicity associated with this type of analog may be related to the extended n-electron system involving the quinoline and phenyl substituent. This system results in a general delocalization of the electrons across all of the adjacent n-orbitals, which increases stability and thereby lowers the overall energy of the molecule. In order to disrupt the delocalization of the n-electrons, a methylene spacer was introduced between the quinoline and phenyl substituent. In addition, the increase in rotational freedom about the benzylic carbon inhibits the molecule from adopting a planar conformation. The effect of such substitutions on antimalarial activity and phototoxicity will be reported.

154. Synthesis, Anticonvulsant Activity and Neurotoxicity of New N-1',N-3'-Disubstituted, 2'H,3H,5'H-Spiro-(2-benzofuran-1,4'-imidazolidine)-2',3,5'-Triones

Pallavi Gutta, Hardik J Patel, István Lengyel and Ralph A. Stephani, St John's University, Jamaica, NY

Previously we reported the anticonvulsant activity of an initial series of N-1',N'-3' disubstituted-spiro-phthalidyl hydantoins that were prepared by reaction of the corresponding N-1',N'-3'-disubstituted ureas with ninhydrin, followed by treatment with aqueous sodium periodate oxidation. The new class of spirohydantoins exhibited anticonvulsant activities in both the maximal electro shock (MES) and pentylene tetrozole (PTZ) tests. While N-1'-aryl substituted hydantoins showed appreciable anticonvulsant activities in PTZ assay, they exhibited less in the MES test. With increase in chain length there is increase protection against PTZ induced convulsions. In the rotarod test,
compounds bearing straight alkyl chain at the para position of N-1'-aryl group were less neurotoxic than the branched groups like t-butyl at the para position. Also change in position of the substituent from para to ortho does not greatly affect the anticonvulsant activity. Results of these latest tests will be discussed in terms of ED50's and structure activity relationships for its anticonvulsant activity.

**155. Layer-by-Layer Surface Engineering Approach for in Vivo Targeting Delivery of siRNA**

Oleh Taratula¹, Paul Kirckpatrick¹, Ronak Savla¹, Ipsit Pandya¹, Tamara Minko²,³ and Huixin He¹,³, (1)Department of Chemistry, Rutgers University, Newark, NJ, (2)The Ernest Mario School of Pharmacy, Rutgers, the State University of New Jersey, Piscataway, NJ, (3)Cancer Institute of New Jersey, 195 Little Albany Street, New Brunswick, NJ 08903

The main obstacle in siRNA therapy is RNA delivering to the cytoplasm where it can guide sequence-specific mRNA degradation. Attempts to develop effective nonviral vectors for in vivo delivery of nucleic acids through a systemic route are hampered by difficulties of combining of high extracellular stability with ready availability of the nucleic acids following entry into cells. Extracellular stability is essential as the delivery system should be capable of withstanding the aggressive biological environment en-route to the target site, while availability of the nucleic acids is to permit efficient therapeutic effects within the cells. Other challenges with non-viral gene delivery include limitation in target-cell specificity. Here we demonstrate that the caging of siRNA-PPI nanoparticles with a dithiol containing crosslinkers provides lateral stabilization, preventing unfavorable dissociation of the nanoparticles before entering the cytoplasm of target cells through the interaction with negatively charged biomacromolecules in the entity. Further PEGylation of the caged nanoparticles stabilize them against aggregation induced by salts and proteins existed in the serum. Due to the reductive environment in the cytoplasm, the disulfide bonds could be reduced, the lateral crosslinks are removed and the siRNA is released for expression. Furthermore, PEG coating can effectively eliminate nonspecific delivery, increasing targeting delivery efficiency after a specific targeting groups attached to its distal ends.

**156. Development of 5HT2A Antagonists Based on the Aporphine Alkaloid Nantenine**

Stevan Pecic and Wayne Harding, Hunter College, New York City, NY

MDMA (3,4-methylenedioxy-N-methylamphetamine), most commonly known by the street names Ecstasy, E, X, or XTC is a semi-synthethic derivate of the phenethylamine family. MDMA acts directly on a number of receptors, including á1-adrenergic and 5-HT2A receptors. Use of “Ecstasy” is accompanied by several adverse physiological effects including the development of hyperthermia, organ failure and death in extreme cases. Cognitive impairment has also been reported in “Ecstasy” users and there is evidence that the drug has addictive properties. Nantenine (1) is an aporphine alkaloid isolated from the Japanese fruit of Nandina domestica. Nantenine shares structural similarities to MDMA and is an antagonist at serotonin 5-HT2A and adrenergic á1 receptors. Up to the present time, very little structure-activity relationship (SAR) studies have been performed on nantenine in relation to its antagonist activity at these receptors. It is the goal of this project to synthesize analogs of nantenine and to explore the functional group and spatial characteristics of the molecule which are required for antagonist activity at 5HT2a receptors. The analogs will also be evaluated for their ability to block the discriminative stimulus effects of MDMA in mice. These combined efforts will allow for the development of potent 5HT2a antagonists based on the nantenine core structure through iterative synthesis and in vitro screening and will also identify molecules with potent in vivo MDMA antagonist activity. Our efforts towards synthesis of nantenine analogs to date will be presented.

*(See Figure on Next Page)*
157. Bioassay-Guided Isolation of African Ethnobotanical Anthelmintics

**Carrie Waterman**, University of the Sciences in Philadelphia, Philadelphia, PA

Currently one third of the World's population is infected with soil transmitted helminthes (STH) and schistosomiasis. The burdens of these diseases are serious, including limited physical and mental ability as well as exacerbating malnourishment. Since intestinal worms are endemic to Africa, new anthelmintic compounds should be found in the plants used by traditional healers for treating worm infections. The use of C. elegans as a model organism in our bioassay-guided fractionation successfully demonstrates which plant extracts, subsequent fractions, and isolated compounds have significant nematocidal activity. Our research is investigating 21 plant species used for intestinal medicine in Sub-Saharan Africa. Our newly developed anthelmintic bio-assay utilizes tetrazolium salts (MTT) to statistically determine worm mortality, a method superior to current assays based solely on worm movement observations. Extracts from six of the 21 plant species have thus shown significant nematocidal activity. Our chromatographic separations have identified isolates from one extract showing increased activity. LCMS and NMR are currently being used to isolate and characterize the active constituent, suspected to be an ellagic acid derivative. Chemical characterization of isolates can be used to improve the safety and efficacy of traditional treatments and will allow for the development of novel anthelmintic drugs to treat infections in humans, livestock and crops.

158. Design and Synthesis of De Novo Paclitaxel Mimics Based on REDOR-Taxol Structure

**Liang Sun**, Department of Chemistry, State University of New York at Stony Brook, Stony Brook, NY and **Iwao Ojima**, Department of Chemistry and Institute of Chemical Biology and Drug Discovery, State University of New York at Stony Brook, Stony Brook, NY

Paclitaxel (Taxol®) currently serves as one of the most important drugs in cancer chemotherapy. The complex baccatin core could be mimicked by a structurally simpler scaffold that retains its essential features based on the binding conformation of paclitaxel in microtubule. We designed novel baccatin-free paclitaxel mimic 3 that can take the “REDOR-Taxol” structure at the binding site in beta-tubulin. Fused 5-6-6 and 5-7-6 tricyclic ring systems 2 have been synthesized from hydroxyproline derivative 1. Molecular modeling studies, synthesis and biological evaluation of these novel paclitaxel mimics will be presented.
159. Synthesis and SAR Study on Novel Benzimidazoles for Antituberculosis Drug Discovery, Targeting FtsZ

Kunal Kumar¹, Ilaria Zanardi², Béla Ruzsicska², Richard A. Slayden³ and Iwao Ojima², (1)State University of New York, stony Brook, Stony Brook, NY, (2)Institute of Chemical Biology and Drug Discovery, State University of New York, Stony Brook, NY, (3)Colorado State University,, Fort Collins, CO

FtsZ, a tubulin homologue, is a ubiquitous bacterial cytoskeletal protein. In the presence of GTP, FtsZ polymerizes to form a highly dynamic helical Z-ring at the mid cell eventually leading to septation. Inhibition of FtsZ results in the absence of septation contributing to arrested bacterial growth. Therefore, we hypothesized that FtsZ-inhibitors can be developed into antibacterial agents possessing novel mechanism of action. Accordingly, we designed and synthesized a library of novel trisubstituted-benzimidazoles through rational and systematic design. A number of these compounds exhibited < 6 ìg/mL MIC99 activity in the preliminary screening against Mtb H37RV strain. Polymerization assay confirmed that these compounds inhibited Mtb-FtsZ in dose dependent manner. Synthesis, biological evaluation and SAR of novel benzimidazoles will be presented.

160. Synthesis and Evaluation of Tumor-Targeting Folate-Taxoid Conjugates

Manisha Das and Iwao Ojima, State University of New York at Stony Brook, Stony Brook, NY

Folic acid has been chosen as the tumor-targeting molecule (TTM) in our ongoing studies on tumor-targeting drug delivery systems. Folate receptors are overexpressed on many types of cancer cells making these receptors an attractive target for delivery of cancer drugs. We have designed a folate-taxoid conjugate to target these tumor cells specifically. SB-T-1214, a highly potent second-generation taxoid was chosen as the cytotoxic drug. This drug was conjugated to folic acid through a novel disulfide linker developed in our laboratory and a PEG-spacer. Upon internalization into the tumor cell the potent taxoid will be released from the conjugate by the action of glutathione present in the tumor cell. The synthesis and study on the internalization using the fluorescence-labeled conjugate will be presented.
161. Design, Synthesis and Biological Evaluation of Novel Tumor-Targeting Conjugates

Edison S. Zuniga¹, Xianrui Zhao¹, Shuyi Chen¹, Jin Chen¹, Jingyi Chen² and Iwao Ojima³, (1)State University of New York at Stony Brook, Stony Brook, NY, (2)Brookhaven National Laboratory, Upton, NY, (3)Department of Chemistry and ICB&DD, State University of New York at Stony Brook, Stony Brook, NY

Novel biotin-taxoid conjugates have been evaluated for their efficacy in tumor-targeting drug delivery using confocal fluorescence microscopy. Recently, it has been shown that vitamin receptors, including biotin receptors, are overexpressed in various tumors. Thus, the biotin receptor is an excellent biomarker for tumor-targeting drug delivery via receptor-mediated endocytosis. A novel disulfide linker was designed and used for conjugating biotin and a taxoid, which would release the active taxoid inside tumor cells by the action of intracellular glutathione. Three conjugates were designed and prepared for process verification, i.e., biotin-conjugate internalization, disulfide bond cleavage, and active taxoid release, respectively. At each stage, a fluorescent or fluorogenic moiety was employed to visualize the progress. The design and synthesis of these biotin-taxoid-conjugates, as well as the cell-based evaluation of their tumor-targeting efficacy against L1210FR leukemia cell line, will be presented.

162. Design, Synthesis and Biological Evaluation of a Novel Tumor-Targeting Drug Delivery System Based on Functionalized SWNT

Edison S. Zuniga¹, Shuyi Chen¹, Jingyi Chen², Xianrui Zhao¹, Stanislaus S. Wong³ and Iwao Ojima⁴, (1)State University of New York at Stony Brook, Stony Brook, NY, (2)State University of New York at Stony Brook and Materials Science Department, Brookhaven National Laboratory, Stony Brook, NY, (3)State University of New York at Stony Brook, Upton, NY, (4)Department of Chemistry and ICB&DD, State University of New York at Stony Brook, Stony Brook, NY

A SWNT-based biotin-taxoid conjugate, in which biotin was introduced as the tumor-targeting moiety, was designed and synthesized for evaluation of its efficacy in tumor-targeting drug delivery. The conjugate consists of a novel self-immolative disulfide-linker which releases the taxoid inside tumor cells by the action of intracellular glutathione. It has been reported that biotin receptors are overexpressed in various cancer cell lines, including leukemia cells. Thus, biotin is a viable tumor-targeting moiety. The cellular uptake of a fluorescence-labeled conjugate and the drug release were investigated by confocal fluorescence microscopy using L1210FR leukemia cell line. The successful real-time observation of the receptor-mediated endocytosis and the intracellular drug release of the fluorescence-labeled biotin-SWNT-taxoid conjugate will be presented.
163. Coulomb's Law and Trends in Sizes of Atoms and Ions
Parinbam (RAJ) K. Thamburaj, Ohio University-Zanesville, Zanesville, OH

Coulomb's law is a complex but a very useful relationship encountered in introductory general chemistry. In its mathematical form it may be expressed as,

\[ F = \frac{k\cdot Q^+ \cdot Q^-}{R^2} \]

where \( F \) is force of attraction between two oppositely charged species (\( Qs \)), \( k \) is a proportionality constant and \( R \) is the distance between the charged particles.

The sizes of atoms and ions are dependent on the force of attraction between the valence electrons and the nucleus. None of the popular textbooks presents an explanation of trends in sizes based on Coulomb's law. A life experience that parallels the law and a simple application Coulomb's law to explain trends in sizes among members of periodic groups and rows will be presented.

Polymer I (Materials Synthesis)
Sponsor: Center for Engineered Polymeric Materials
Organizer: Moni Chauhan CUNY-Queensborough Community College
Presider: Nan-Loh Yang CUNY-College of Staten Island, Staten Island, NY

164. Nanostructured Functional Materials Via ATRP with Ppm Amounts COPPER
Krzysztof Matyjaszewski, Carnegie Mellon University, Pittsburgh, PA

Copper-based ATRP (atom transfer radical polymerization) catalytic systems with polydentate nitrogen ligands such as bpy and aliphatic polyamines is among most efficient controlled/living radical polymerization systems (CRP).\(^1,2\) New ATRP initiating systems allow to decrease level of Cu-catalyst to a few ppm with preserved control.\(^3\) ATRP of (meth)acrylates, styrenes, acrylamides, acrylonitrile and other vinyl monomers provides polymers with low polydispersities and molecular weights in a range 200\(>M_n>20,000,000\). Polymers can be formed quantitatively in bulk, in solution and in emulsions. Block, graft, star, hyperbranched, gradient and periodic copolymers as well as molecular brushes have been prepared.\(^2\) The (co)polymers made by ATRP have many potential applications as components of coatings, elastomers, adhesives, surfactants, dispersants, lubricants, additives, but also as specialty materials in biomedical and electronic areas and will affect the
market of ~$20 billion/year. Examples of design, synthesis, characterization and applications of nanostructured multicomponent polymeric materials enabled by various CRPs will be presented.

Chemistry

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Mechanisms:
- catalyst structure
- ligand design
- model kinetics
- polymerization
- modeling

Processes:
- catalyst optimization
- catalyst recycling
- monomer range
- functional initiators
- reaction media
- reaction conditions


165. Atom Transfer Radical Polymerization Initiated from Surfaces of Ordered Mesoporous Silicas

Michal Kruk¹, Bruno Dufour², Liang Cao¹, Ewa B. Celer³, Tomasz Kowalewski², Mietek Jaroniec³ and Krzysztof Matyjaszewski², (1)College of Staten Island and Graduate Center, City University of New York, Staten Island, NY, (2)Carnegie Mellon University, Pittsburgh, PA, (3)Kent State University, Kent, OH

Ordered mesoporous silicas with cylindrical pores of diameter ~10 and ~15 nm (SBA-15) and spherical pores of ~15 nm (FDU-1) were synthesized and atom transfer radical polymerization (ATRP) of acrylonitrile, 2-(dimethylamino)ethyl methacrylate, styrene and methyl methacrylate initiated from their surfaces was studied. The surface-initiated ATRP allowed us to introduce a controlled amount of uniform polymer chains in nanopores of diameter as low as 10 nm. In some cases, the polydispersity index of the polymer graft was only about 1.1, which is very low for a polymer obtained through surface-initiated polymerization. In cases of the surface-initiated ATRP in cylindrical and spherical mesopores of diameter ~15 nm, it was possible to introduce a significant loading of polymer without making the mesopores inaccessible. The surface-initiated ATRP in nanopores can be optimized to achieve very good control over the uniformity of the polymer graft. This work demonstrates new opportunities in the synthesis of well-defined nanostructured/nanoporous silica/polymer hybrids.
166. Synthesis and Assembly of Nanoparticles for Chemical and Biological Applications

Chuan-Jian Zhong, State University of New York at Binghamton, Binghamton, NY

A key to the exploitation of nanoparticle-structured materials for chemical and biological applications is the ability to synthesize and assemble the nanoscale building blocks controllable desired size, shape, composition and spatial properties. We have been investigating molecularly engineered and mediated synthesis and assemblies of nanoparticles as a general bottom-up pathway towards this ability. This presentation focuses on the discussion of recent findings of the synthesis and assembly of gold, alloy and magnetic core@shell nanoparticles. The size, shape, composition, and spatial properties of the nanoparticles and their assemblies are controllable by a combination of molecular/polymeric mediators or templates in solutions. The electronic, optical and magnetic properties of the nanoparticles and assemblies are fine-tunable by manipulating the composition of the nanoparticles, the structure of the mediator, and the interparticle molecular interactions. Recent results from the study of these nanostructured materials for chemical and biological applications will also be discussed.

167. Mother NATURE as a Source of NEW Materials: EVERYTHING Old IS NEW Again

James A. Moore, Rensselaer Polytechnic Institute, Troy, NY

In July, 1969 we began a preparing monomers from cellulose. Polymers were prepared by the standard methods of acid-catalyzed polyesterification and interfacial polycondensation of diacid chlorides. The polymers were characterized using Infrared, and NMR Spectroscopy. Molecular weights were assessed by viscosity and gpc.

Cellulose can be hydrolysed to glucose which can be oxidized to glucaric acid. Elimination of water and cyclization yields 2,5-furan dicarboxylic acid (2,5-FDA). We have mostly used interfacial polycondensation of the acid chlorides of the various isomers of FDA (2,5; 2,4; 2,4; 3,4) as a route to polyesters and polyamides. Polymers with intrinsic viscosities in the range of 0.1 – 0.7 dl/g could be prepared. Nonactin, a macrocyclic tetraester acts by binding potassium ions and disrupting synaptic signal transmission. A casual examination of this molecule led us to try to generate a helical polymeric analog? We tested the general idea by making reduced derivatives of 2,5-FDA We also made polymers derived from the lactone and the analogous lactam from tetrahydro-2-hydroxymethyl-5 furoic acid and they exhibit varying degrees of ion binding ability.

The major hydrolytic degradation product of cellulose is levulinic acid which can be condensed with phenol to yield a bis-phenol called diphenolic acid which can be protected as a t-butyl ester. The ester allowed us to prepare a variety of homo- and copolycarbonates in which, after selective removal of the t-butyl group, the carboxyl group can be used as a site for further modification.

168. Nano-Structures of Polyurea Synthesized in Ionic Liquids

Chien-Yueh Huang, NJIT and Center for Engineered Polymeric Materials, College of Staten Island, CUNY, Staten Island, NY and Mu-Ping Nieh, Canadian Neutron Beam Center, National Research Council, Chalk River, ON, Canada

Recent reports on special nano-size structures inorganic compounds synthesized in room temperature ionic liquids (ILs) such as ZnO, TiO2, and silica, have attracted attentions to the molecular interactions and alignments mediated by the ILs during the synthetic reactions. In this work, we present exotic nano-porous structures observed in polyurea synthesized by interfacial polymerization between n-hexane (with 2,4-toluene diisocyanate, TDI) and a series of 1-alkyl-3-methylimidazolium tetrafluoroborates and 1-alkyl-3-methylimidazolium hexafluorophosphates (with ethylene diamine or 1,4 diaminobutane). Depending on the ionic liquids and diamines, polymer fibrils of sizes around 50 nm forming porous structures with pore size ~ 300 nm were observed.
under SEM. Other morphologies including volcano, coral reef, or sphere (~100 nm) were also observed. SAXS results depict the porous structures with characteristic lengths around 30~40 nm. FTIR shows the same characteristics as those synthesized without ILs, indicative of insignificant/ or no changes in the chemical structures of the products.

We also present a novel process employing a uniform electric field to control the morphology of polymer synthesized at the interface between an organic liquid and an immiscible IL. SEM and SANS data showed the morphology and microstructure of polymer varied with the intensity and the angle of the external field, which induced excess ions, changed the molecular orientations and thermal fluctuations at the interface, and affected the coarsening and aggregation of the polymeric precipitates. From a general perspective, this work imparted a new concept that may be applicable to non-charge transfer liquid-ionic liquid processes enhanced by external electric fields.

169. Nitroxide-Mediated Copolymerization of Acrylic Acid Derivatives with Styrene

Milan Maric and Benoit Lessard, McGill University, Montreal, QC, Canada

Controlled free radical polymerization chemistry has increased the ease by which polymers with well-defined microstructures are made compared to traditional "living" methods such as ionic polymerization. For example, acrylic acid can be directly polymerized by controlled radical methods without being in its protected form such as tert-butyl acrylate. Styrene/tert-butyl acrylate (S/t-BuA) as well as styrene/acrylic acid (S/AA) mixtures were copolymerized using nitroxide-mediated polymerization at 115-120°C using an alkoxamine unimolecular initiator, 2-[N-tert-butyl-2,2-(dimethylpropyl)aminoxy] propionic acid (BlocBuilder^−), along with additional N-tert-butyl-N-[1-diethylphosphono-(2,2-dimethylpropyl)] nitroxide as a free nitroxide (SG1) to observe the effect of additional SG1 on polymerization kinetics and copolymer composition. Adding 4.5 mol% SG1/BlocBuilder greatly improved the control of random S/t-BuA copolymerization with much lower polydispersities (1.14-1.22) and a linear increase in number average molecular weight M_n with conversion up to 50%. In contrast without additional SG1, M_n versus conversion was only linear up to ~20%. In both cases, the copolymers were sufficiently "living" to re-initiate styrene polymerization to cleanly extend the chains with narrow and monomodal molecular weight distributions. S/AA copolymerizations required higher levels of free nitroxide (9 mol% SG1/BlocBuilder) compared to S/t-BuA copolymerizations to compensate for SG1 degradation by attack from the acrylic acid monomer and to avoid excessive exotherms. Molecular weight distributions were broader for S/AA compared to S/t-BuA random copolymerizations (polydispersities ~ 1.3-1.4 at 9 mol% SG1/BlocBuilder) and chain extensions of S/AA copolymers with styrene resulted in copolymers with broader molecular weight distributions (polydispersities >1.5) compared to their chain-extended S/t-BuA counterparts.

170. Preparation and Characterization Nanoneedles of Polythiophene, Polyaniline and Polypyrrole from An Interfacial Polymerization

Kai Su\(^1\), Nurxat Nuraje\(^2\), Lingzhi Zhang\(^3\), I-Wei Chu\(^4\), Hiroshi Matsui\(^2\) and Nan-Loh Yang\(^5\), (1)Ciba Specialty Chemicals, Tarrytown, NY, (2)CUNY, Hunter College, New York, NY, (3)College of Staten Island, Staten Island, NY, (4)CUNY, College of Staten Island, Staten Island, NY, (5)CUNY-College of Staten Island, Staten Island, NY

Single crystalline nanoneedles of three families of most studied conductive organic polymers - polythiophene, polyaniline and polypyrrole - were synthesized for the first time using an interfacial polymerization process that takes place with simultaneous crystallization. As the crystal growth is concurrent with polymerization, more ordered crystal packing can be expected. Most of the bulk conducting-polymer systems studied previously contains regions that are inhomogeneous. Single nanocrystals of conducting polymers have not been reported, although needle-shaped bulk crystals of the quarterphenyl cation radical salt have previously been studied. The investigation of processes in a nanodomain of a single crystal is critical in ascertaining the inherent electronic properties of polymer nanoelements.
The organic conductive nanoneedles were characterized using TEM, HRTEM, electron diffraction, EDS, and EPR to establish their crystal structure and composition. Scanning tunneling microscopy/spectroscopy (STM/STS) investigation was conducted to examine their electronic conduction behaviors, leading to the discovery a field-induced conductance switching with response times on or faster than the millisecond level. The switch voltages are in the range of 3 to 4 volts, consistent with the trend of the band gap of the polymers.

**Analysis of Biomolecules**

**Sponsor:** Novartis Pharmaceutical Corporation and ACS Division of Analytical Chemistry  
**Organizer:** Rosario LoBrutto Novartis Pharmaceutical Corporation  
**Organizer:** Richard Thompson Novartis Pharmaceutical Corporation

**Session Overview:** Advances in proteomics and genomics have led to a greater emphasis on the analysis and characterization of biomolecules such as phosphopeptides, monoclonal antibodies, proteins, and SiRNAs. There are many analytical technologies available for the determination of the chemical purity, aggregation, physical characteristics, and conformational state of biomolecules as well as studying how the folding/stability of these biomolecules impact biological function. This symposium will discuss the current state of application of these technologies and strategies for analysis of biomolecules from both an academic and pharmaceutical perspective.

**171. Analytical Ultracentrifugation Analysis in the Biopharmaceutical Drug Development Process**  
**Steven A. Berkowitz,** Biogen Idec, Cambridge, MA

The development and use of the analytical ultracentrifuge for studying the solution behavior of biomacromolecules goes back to the early pioneering efforts of Svedberg and his coworkers in the 1920s and 1930s. From this early period of time up until the 1970s analytical ultracentrifugation (AUC) played an important role in formulating our knowledge of the biophysical properties of biopolymers. Hence our early basic understanding of biomacromolecular structure and molecular biology is significantly indebted to this important analytical instrument. Nevertheless, with the development of size-exclusion chromatography, SDS-PAGE, and soft ionization mass spectroscopy techniques, along with major shifts in research in the biological and biomedical sciences during the following decades the role of AUC diminished to the point where it virtually disappeared as a form of macromolecular analysis. However, developments in electronics and computer technology (which has brought low cost computer power to the scientist's desktop) along with the renewed interests in understanding protein-protein interactions, and the realization of the need to have alternate analytical techniques to characterize the homogeneity and aggregation present in biopharmaceuticals has lead to the modernization and renewed interest in the analytical ultracentrifuge. Hence the subject of this presentation will focus on how AUC can be integrated into today's biopharmaceutical development process to help accelerate the successful discovery and development of new biopharmaceutical drug products.

**172. Application of Light Scattering for Analysis of Protein-Protein Interaction and Aggregation**  
**Ewa Folta-Stogniew,** Yale University, New Haven, CT

Static and dynamic laser light scattering are discussed as tools for studying protein-protein interactions, protein oligomerization, and aggregation. Dynamic light scattering (DLS) is very well
suited for detection of small quantities of aggregates in protein samples because DLS can easily analyze samples with broad distribution of sizes. No fractionation is used and sample is analyzed in batch mode without any chromatographic separation. DLS detector can also be used as an “on-line” detector coupled with a fractionation step.

Static light scattering (SLS) is best utilized for measurement of molar masses as an “on-line” detector coupled with size exclusion chromatography (SEC), refractive index (RI) and ultraviolet (UV) detection. Since static light scattering provides only the weight-average molar mass, Mw, of the species in solution, the SEC separation plays an integral role in the overall analysis, albeit, the elution from SEC does not need to correlate with the molar masses of the species being studied. SEC/LS allows determination of molar mass of unmodified proteins with a precision of ±5% in a single experiment that uses <100 μg of protein; for DLS “on-line” measurement, ~400μg is needed. Monitoring the elution from SEC by three detectors, UV, LS and RI, provides an excellent tool for detection of sample heterogeneity. Potential loss of protein on the SEC column, sample dilution, and restriction on elution solvent are major limitations of SEC/LS analysis. SEC/LS is suitable for analysis of glycoproteins, proteins modified by polyethylene glycol as well as membrane proteins solubilized in non-ionic detergents.


Birendra N. Pramanik, Schering-Plough Research Institute, Kenilworth, NJ

Our earlier work has demonstrated that enzymatic cleavages of proteins (including tightly folded macromolecules) into smaller peptide fragments can be achieved in minutes under microwave irradiation, in contrast to hours needed by conventional methods. This novel approach has significantly accelerated the peptide mass mapping process by using mass spectrometric (MS) methods. The present work describes assessment of conformational changes in proteins upon microwave irradiation by hydrogen/deuterium (H/D) exchange experiments, followed by electrospray ionization (ESI) MS analysis. The MS data indicates that the level of deuterium exchange in proteins under microwave irradiation condition (vs. without microwave) is increased by more than 50%. However, no noticeable difference in the charge state distributions of the protein was detected in the ESI-MS. Protein-inhibitor interaction studies by H/D exchange method will also be discussed.

174. Phosphopeptide Analysis by Directly Coupling 2D Pec/tlc with MALDI-TOFMS

Ira S. Krull, Northeastern University, Boston, MA

A new strategy is presented for the separation of complex peptide mixtures using 2D planar electochromatography (PEC) and thin-layer chromatography (TLC). Phosphorylated peptides migrate more slowly in the first dimension based upon their anionic phosphate residues, and certain predominantly acidic phosphopeptides even migrate in the opposite direction, relative to the bulk of the peptides. Phosphopeptides are further distinguished based upon hydrophilicity in the second dimension. This separation mechanism, which then permits a restricted region of the plate to be interrogated for the presence of phosphopeptides by MS. Analysis of phosphopeptides directly from the plates using matrix-assisted laser desorption/ionization time-of-flight MS (MALDI-TOF MS) and tandem MS enabled peptide sequencing and identification. The nature of the original protein can then be discerned once all the peptide fragments have been fully characterized and identified. These somewhat newer analytical approaches represent a new and novel route for investigating peptidomic and proteomic, as well as other "omic" type samples.
175. Ultrasonic Storage Modulus as a Novel Parameter for Analyzing Protein-Protein Interactions in High Protein Concentration Solutions

Devendra Kalonia, University of Connecticut, Storrs, CT

Abstract: Current market trends for high dose therapeutic proteins require concentrated liquid formulations for the patient convenience, in home subcutaneous administration, to cut manufacturing costs and to improve product marketability. Protein-protein interactions in these solutions need to be characterized to prepare these solutions with desired viscosity and stability during storage. An ultrasonic shear rheometer based on impedance analysis of piezoelectric quartz crystals was developed for rheological analysis and viscosity measurement of liquids at small sample volumes. Rheological analysis and biophysical characterization conducted on a model monoclonal antibody, IgG2, between pH 4.0 to 9.0 and ionic strengths between 4 mM and 300 mM demonstrated the significant role of protein-protein interactions in governing the solution behavior of protein in concentrated solutions. Results indicated that solution G’ could serve as a parameter for assessing protein-protein interactions in high protein concentration solutions. Its validity for this purpose was confirmed by static and dynamic light scattering measurements under relatively dilute solutions. The measured second virial coefficient (B22) and interaction parameter (kd) were found to be consistent with the solution G’ measurements.

176. Unraveling the Mystery of the Analysis of the Aggregation Behavior of a Non-Covalently Self-Associating Peptide

Raymond S. McGill, Joseph Valente, Jennifer S Pickett, Vipan Taneja and Rosario LoBrutto, Novartis Pharmaceuticals, East Hanover, NJ

During the development of a therapeutic peptide or protein drug product one of the main aspects that the manufacturer has to evaluate is aggregation, especially when the protein is highly concentrated. Typically this assessment is focused on the evaluation of irreversible (i.e., covalent) aggregates. However, the characterization of reversible aggregates is also important since an increase of long lived reversible aggregates in IV formulations may lead to immugoenicity issues, affect PK/PD, and change bioactivity (due to change in secondary structure upon aggregation). The characterization of the aggregation behavior of a reversibly self-associating peptide is presented and the analytical challenges faced are discussed. The use of light scattering (dynamic/static), CD, native page, SEC (disruptive and nondisruptive conditions), and sedimentation velocity AUC were all used to ascertain the nature of the aggregates and the behavior of the peptide in solution at increasing concentrations.

177. The Impact of Conformational Fluctuations on the Analysis and Design of Protein Pharmaceuticals

Vincent J. Hilser, University of Texas Medical Branch, Galveston, TX

Proteins differ from small molecule pharmaceuticals not just in their chemical complexity, but in the breadth of their conformational repertoire. In fact, in recent years it has become clear that the static representation afforded by the high-resolution structure is generally insufficient to explain the impact of mutations or changes in solution conditions on the activity or the physico-chemical properties of proteins. Here, we describe how isothermal titration calorimetry (ITC) can be used to in conjunction with other techniques to characterize conformational fluctuations proteins, and that this characterization can lead to a predictive model of physico-chemical behavior.
Antimicrobials

Sponsor: Ciba Corporation
Organizer: Ted Deisenroth Ciba Specialty Chemicals Corporation, Tarrytown, NY

Session Overview: The antimicrobial symposium will cover new technologies that are effective against bacteria, fungi and viruses. Today there is an ever growing concern of pathogenic organisms developing resistance to antibiotics. This is now evident in the current awareness and concern of the general public to MRSA. New antimicrobial technologies are required to be effective against resistance strains of organisms. Infection is not the only concern of these organisms. Both fungi and bacteria attack coatings and materials affecting not only their appearance, but also durability. Technologies will be presented that could have potential application in medicinal, medical and industrial applications.

178. Antimicrobial Substituted Bis-Alkylaminopyrimidines and Their Uses
Todd Elder¹, Ted Deisenroth¹, Sophie Marquais-Bienewald², Werner Hoelzl², Andrea Pruess² and Fadi Khawam¹, (1)Ciba Specialty Chemicals, Tarrytown, NY, (2)Ciba Specialty Chemicals, Grenzach, Germany

Microbial contamination of surfaces continues to be a significant problem in not only the medical field but also in the home. Of particular concern is the growth of mold and mildew. Mold/mildew is not just an unsightly problem, but it can also trigger health issues, such as allergies and asthma. Our labs have been investigating substituted bis-alkylaminopyrimidines as a source of novel antimicrobial agents. A number of substituted aminopyridines have been prepared in order to optimize the surprising broad spectrum activity against bacteria and fungi. Given the diverse chemical structures of these analogs, the synthesis of a number of analogs will be described. The antimicrobial activity of these analogs will be detailed along with various application testing which demonstrates their utility as potential antimicrobial agents.

179. Metal_Loaded Chitosan Nanoparticles with Antibacterial Activities
Sudeep Banjade, Thong Vo, Gerhard Haas and Mihaela Leonida, Fairleigh Dickinson University, Metropolitan Campus, Teaneck, NJ

Chitosan (CS) is a derivative of chitin and is a biocompatible polysaccharide that is composed of 2-amino-2-deoxy-α-D-glucan monomers. Due to its capacity to form interactions with polyanions, CS has been widely used in various studies to prepare chitosan nanoparticles (CNP) for potential applications as delivery systems for therapeutic agents. However, research done on antibacterial potencies of CNP and CNP loaded with metal ions has been limited. In the present study CNP, CNP loaded with copper ions (Cu-CNP), and CNP loaded with silver ions (Ag-CNP) were prepared and studied. Three different grades (molar mass) of CS were used to prepare CNP and CNP enhanced with metal ions. Copper sulfate was used as source of Cu2+ and silver nitrate was used as source of Ag+. The nanoparticles were characterized by scanning electron microscopy (SEM) and the metal content was determined by electrodeposition (for Cu2+) and titration (for Ag+). The antibacterial properties of CNP and metal enhanced-CNP were tested against Gram negative and Gram positive bacteria. CNP showed increased antibacterial activity compared to CS and positive coaction with the metal cations.
180. Novel Penems Bearing a Bicyclic or Tricyclic Heterocycle on Methylidene Linkage as Broad Spectrum B-Lactamase Inhibitors and Their Mechanism of Inactivation

Aranapakam M. Venkatesan, Takao Abe, Hideki Ushiroguchi, Atul Agarwal, Itsuka Yamamura, Osvaldo Dos Santos, Yansong Gu, Fuk-Wah Sum, Zhong Li, Lijing Chen, Yang I. Lin, Gulnaz Khafizova, Peter J. Petersen, Youjun Yang, Patricia Bradford, David M Shlaes and Tarek S Mansour, Wyeth Research, Pearl River, NY

Inhibitors of bacterial b-lactamases in combination with other antibiotics have been used extensively in the clinical setting to overcome resistance due to b-lactamase production. Clinically used antibiotic/inhibitor combinations cover class-A producing pathogens, but have very little effect on class-C and ESBL producing organisms. However, methylidene penem inhibitors have shown promising broad-spectrum activity. In the present work, based on modeling studies, novel methylidene penems 3, having bicyclic and tricyclic heteroaryl moieties were designed and synthesized by a novel route. The structure activity relationship and mechanism of action of this class of compounds will be discussed.

181. Antimicrobial Pharmaceuticals without Resistance

Robert Engel1, Cathy Xiong1, Karin Melkonian2, JaimeLee Rizzo3 and Mary Cloninger4, (1)Queens College of the City University of New York, Flushing, NY, (2)C.W. Post College of Long Island University, Greenville, NY, (3)Pace University, (4)Montana State University, Bozeman, MT

The problem of development of bacterial resistance to antibiotics is a most serious one. Bacteria rapidly develop alternative modes for survival in spite of antibiotics chemically interrupting some critical chemical process. We have accomplished the goal of developing macro-surfaces that kill bacteria on contact by detergent action on the cell wall. The current effort relates to the application of this approach to the generation of pharmaceuticals that embody the same approach to antimicrobial action. Dendrimers and hyperbranched polymers have been developed to serve as scaffolding on which cationic detergents are attached. These serve as micro-surfaces that are soluble in aqueous media and can be used in solution. The attachment functionalities of the scaffolding are also subject to hydrolytic action such that the agent does not exist indefinitely in the host organism being treated.

182. Small Talk: Molecules That Control Quorum Sensing in Vibrio Cholerae

Martin F. Semmelhack1, Megan E. Pomianek1, William E. Brow1, Shawn R. Campagna1, Douglas A. Higgins1 and Bonnie L. Bassler2, (1)Princeton University, Princeton, NJ, (2)Howard Hughes Medical Institute, Chevy Chase, MD

*Vibrio cholerae*, the causative agent of the human disease cholera, uses cell-to-cell communication to control pathogenicity and biofilm formation. This process, known as quorum sensing, relies on the secretion and detection of signaling molecules called autoinducers. At low cell density *V. cholerae* activates the expression of virulence factors and forms biofilms. At high cell density the accumulation of two quorum-sensing autoinducers represses these traits. These two autoinducers, cholerae autoinducer-1 (CAI-1) and autoinducer-2 (AI-2), function synergistically to control gene
regulation, although CAI-1 is the stronger of the two signals. *V. cholerae* AI-2 is a furanosyl borate diester, which was identified and fully characterized in *Vibrio harveyi*. CAI-1 is (S)-3-hydroxytridecan-4-one, a new type of bacterial signal. The structure elucidation, synthesis, mechanism of action, and structure-activity relations for both AI-2 and CAI-1 will be discussed. CAI-1 represses production of the canonical virulence factor TCP (toxin co-regulated pilus) which suggests that CAI-1 could be used as a therapy to prevent cholera infection and, furthermore, that strategies to manipulate bacterial quorum sensing hold promise in the clinical arena.

183. Ceragenins: Small Molecule Mimics of Antimicrobial Peptides

Paul B. Savage, Yanshu Feng and Jake Pollard, Brigham Young University, Provo, UT

Ceragenins are cholic acid-based antimicrobial agents that mimic the amphiphilic morphology of antimicrobial peptides. Antimicrobial peptides selectively disrupt bacterial membranes and are one of Nature's primary solutions for controlling the growth of bacteria in organisms ranging from mammals to insects. The ubiquity of antimicrobial peptides argues that targeting bacterial membranes may be an effective, long-term approach for controlling bacterial growth. As mimics of antimicrobial peptides, ceragenins display potent bactericidal activity against a broad range of bacteria including Gram-negative and positive organisms. Drug-resistant bacteria, including methicillin-, and vancomycin-resistant *Staphylococcus aureus*, are highly susceptible to ceragenins. As part of their mechanism of action, ceragenins bind to bacterial membrane components and cause membrane depolarization and permeabilization. Due to their relatively small size and affinity for bacterial membranes, ceragenins are active against established bacterial biofilms. As polycations, ceragenins can be sequestered by anionic polymers, and controlled release of ceragenins from thin films on medical devices can be achieved using water-insoluble anionic polymers. Thin films containing ceragenins prevent bacterial biofilm formation on surfaces even in the presence of large inocula of bacteria. Ceragenins are well tolerated by cells types that are normally exposed endogenous antimicrobial peptides. Furthermore, they are relatively easy to synthesize and are much more stable than antimicrobial peptides, that is, they are not substrates for proteases. Consequently, the ceragenins appear well suited for replacing or augmenting the antibacterial activities of antimicrobial peptides.

184. Antisense Approaches for Antibiotic Discovery, Discovery of Platensimycin and Platencin

Sheo Singh, Merck Research Laboratories, Rahway, NJ

FabH and FabF are essential enzymes in type II fatty acid synthesis and are promising targets for antibacterial drug discovery and development. A new approach using a xylose inducible plasmid to express antisense RNA (AS-RNA) in *Staphylococcus aureus* has been recently described. In order to identify FabF/Fab target specific cell permeable inhibitors from natural products, we developed an agar-diffusion two-plate differential sensitivity assay. Because both the fabH and fabF genes share the same operon, the increase in fabF AS-RNA levels decreases the expression of FabH and FabF proteins, making the cells more sensitive to FabF and/or FabH inhibitors. Using this assay, we screened over 250,000 natural product extracts followed by confirmation in biochemical assays, giving a hit rate of 0.1%. We discovered all known FabH and FabF inhibitors that included cerulenin, thiolactomycin, thiotetromycin and Tu3010 from natural product extracts for the first time using a mechanism based screening approach. We discovered a number of novel natural products as FabF inhibitors including platensimycin and platencin. The details of discovery process, structures, biological activities, in vivo efficacy, mechanism of action and inhibitor bound X-ray crystal structure will be discussed.
185. REP3123: A New Agent for CDAD?
Joseph Guiles, Xicheng Sun, Sarah Strong, Ian Critchley, Thale Jarvis and Nebojsa Janjic, Replidyne Inc., Louisville, CO

Diaryldiamines are a new class of antibacterial agents that inhibit methionyl t-RNA synthetase (MetRS). These inhibitors prevent protein synthesis and arrest the growth of bacteria cells. The diaryldiamines are particularly potent agents against a wide spectrum of Gram+ organisms. This presentation will focus on our discovery of a new diaryldiamine, REP3123, with particularly potent activity against Clostridium difficile. This anaerobe if present in the lower GI leads to a particularly debilitating clinical condition labeled Clostridium difficile associated disease (CDAD).

186. Understanding Host-Pathogen Interactions: Mycobacteria within Macrophage Cells
John T. Groves, Princeton University, Princeton, NJ

A promising avenue to the control of tuberculosis is limiting iron acquisition by the pathogen. Mycobacterium tuberculosis produces non-ribosomal peptide mycobactins during periods of iron limitation. Full virulence has been shown to require production of these siderophores. Like its deadlier cousin M. tuberculosis, Mycobacterium paratuberculosis is known to survive assault from the immune system by living within macrophage lysosomes. We have shown that mycobactin J, produced by mycobacterium paratuberculosis, localized to lipid droplets upon metal binding within macrophages. We have also shown that mycobactin J causes large disruptions to cellular metabolism, including decreased protein production and changes in several major metabolic pathways. This lecture will describe our current efforts to understand the roles of siderophores in pathogenesis and host response.

187. Structured Water Facilitates Ligand Binding in M. Tuberculosis Catalase-Peroxidase
Richard S. Magliozzo, Brooklyn College and the Graduate Center of the City University of New York, New York, NY

Catalase-peroxidase (KatG) is a key enzyme in M. tuberculosis because it is the sole catalase in this pathogen, and because it is responsible for activation of the oldest, most potent anti-TB agent, isoniazid (INH). Peroxidative activation of INH by KatG leads to an intermediate that acylates nicotinamide adenine dinucleotide cofactor, forming a potent inhibitor of a mycolic acid biosynthetic enzyme known as InhA and causing cell wall damage. Activation is deficient in the Ser315Thr KatG mutant associated with INH resistance worldwide. The early phase of catalytic turnover in KatG and three Ser315 mutants was probed using peroxide and the peroxide surrogate, HCN. Equilibrium and kinetics methods along with EPR measurements were used to characterize ligand binding. kON and kOFF rates were evaluated and ligand binding to five or six coordinate heme iron species in the resting enzymes could be separately probed using cyanide. While peroxidases generally contain five coordinate heme iron in their resting state, in KatG, the six-coordinate heme sub-population, which contains a distal water molecule associated with heme iron, was found to be the preferred species in the ligand binding process. According to its three-dimensional crystal structure, the Ser315Thr KatG mutant lacks structured water in the active site and in a substrate access channel, and manifests
slow ligand binding. The results suggest that the reaction mechanism in catalase-peroxidases should include a specific role for water molecules in the active site required for substrate (peroxide) access and deprotonation allowing coordination of HOO- to heme iron for initiation of turnover.

188. Fluorescent Probes for Intracellular Manganese(II)

James W. Canary¹, Francesca Gruppi¹, Jian Liang¹, Maksim Royzen¹ and Zhaohua Dai², (1)New York University, New York, NY, (2)Pace University, New York, NY

Manganese is a widespread element, essential for human health. However, over-exposure to manganese can be harmful, especially to the nervous system. Optical assays for Mn(II) are therefore of interest as environmental tools as well as for biological studies. We have developed a supramolecular displacement assay for Mn(II) involving a chelating dye, a colorless chelator, and a reporter ion. This assay reveals the presence of Mn(II) with a visible color change. As a result of a unique combination of properties, Mn(II) has been employed as a tool to study calcium channels and brain function. For studies of Mn(II) transport in tissues, fluorescent assays are of great utility. Previous fluorescent probes for Mn(II) have involved fluorophores that are quenched as a result of interaction between the fluorophore and unpaired electrons in the metal. A similar displacement assay involving two chelating fluorophores and a reporter ion provides an “on-fluorescence” signal. The method was shown to give ratiometric fluorescence in solution and in cells. Ongoing work is aimed at optimizing Mn(II) selectivity properties of the chelating fluorophores among other challenges.

189. Toxicity of Lead: Quantum-Mechanical Exploration of Lead Poisoned Zinc Fingers

Andrzej Jarzecki, Brooklyn College, City University of New York, Brooklyn, NY

We report a quantum-mechanical study aimed at elucidating connections between lead coordination and toxicity. In agreement with experimental data, lead binds to cysteine-rich sites and introduces new coordination preferences that do not stabilize the proper form of zinc-binding domains. Electronic structure calculations and orbital analysis reveal that the classical role of stereochemically active lone-pair orbital might be simplistic. The optimal ligand arrangement is modulated by s-p orbital mixing and stabilization of lone-pair orbital, which is differently influenced by S- and N-donor atoms. Computed structural parameters agree with crystallographic data. Computed UV spectra identifies characteristic bands for lead poisoned peptides at 260 and 330 nm, assigned as ligand-to-metal charge-transfer bands. Comparison of computed spectra with model peptides suggests 4- and 3-coordinated lead domains coexisting in the poisoned protein environment.

We conclude that sensitive structural and dynamic probes such as resonance Raman (RR) spectroscopy guided by calculations could become an essential tool for understanding lead poisoning mechanisms. Simulations of RR spectra of cysteine-rich lead domains indicate that a specific structure and coordination mode of lead might be detectable by RR spectroscopy. We predict that when the excitation wavelength is in resonance with UV lead bands, the enhancement of vibrational modes is found for Pb-S stretching and bending modes and also for characteristic C-S stretching and CH2 bending modes of cysteine. More importantly, computed RR intensities for lead domains show unique patterns and might be successfully applied to identify and/or monitor structure and coordination of lead in poisoned proteins.

190. Deciphering Natural Heme Proteins Using De Novo Design

Brian R. Gibney, Amit R. Reddi, Koon C. Ching, Sean D. Moran, Margaret M. Elvekrog and Jaclyn I. Catalano, Columbia University, New York, NY

Our approach to the study of metalloproteins is to engineer and fabricate peptide structures that incorporate metal cofactors toward the goal of generating molecular maquettes, protein-based
synthetic analogues. Herein, we have analyzed all structurally characterized natural heme proteins to guide our design of synthetic heme protein maquettes for the investigation of the fundamental design principles of natural heme proteins involved in electron transfer reactions (the cytochromes) and dioxygen transport (the globins). Using heme protein maquettes, we have delineated the environmental factors which alter the heme reduction potential, a fundamental chemical property of natural cytochromes. By evaluating the coordination equilibria of ferric and ferrous heme to natural and synthetic protein scaffolds, we are providing fresh insight into the absolute (de)stabilization of these states by the protein environment The axial ligand σ-donor ability, porphyrin type, local electrostatic environment and heme burial all contribute to the modulation of the heme reduction potential over a 500 mV range. These dissociation constant and electrochemical data are used to discriminate between proton-coupled electron transfer (PCET) mechanisms in designed proteins. In addition, these data are used to develop a simple method for converting the reduction potential of any heme protein into the ratio of the ferric and ferrous heme dissociation constants as well as the difference in free energy of protein folding in the two oxidation states. These results will be discussed in light of current proposals on the necessity of the various porphyrin structures observed in biology.

Frontiers in Nanoscience and Nanotechnology - I
Sponsor: Momentive Performance Materials
Organizer: Bhanu P. S. Chauhan William Paterson University
Organizer: Kenrick Lewis Momentive Performance Materials, Tarrytown, NY
Presider: Bhanu P. S. Chauhan William Paterson University, Wayne, NJ
Presider: Kenrick Lewis Momentive Performance Materials, Tarrytown, NY

Session Overview: The presentaiions will cover all fundamental aspects of nanoscience

191. Complex Particles and Patterned Substrates: Opportunities in Life Sciences and Material Science
Joseph M. DeSimone, University of North Carolina at Chapel Hill, Chapel Hill, NC

This lecture will focus on opportunities for complex particles and patterned substrates for applications in the life science and in material science areas using a novel fabrication method called PRINT (Particle Replication In Non-wetting Templates). PRINT takes advantage of the unique properties of elastomeric molds comprised of a low surface energy perfluoropolyether network, allowing the production of monodisperse, shape-specific nanoparticles and particle arrays from an extensive range of organic and inorganic liquid precursors.

Life Science: We are taking a pharmaco-engineering systems approach to develop the next generation of delivery systems with programmable, multi-functional capability. PRINT allows for the precise control over particle size, shape, composition, cargo, modulus and surface properties. Extensive in vitro and in vivo studies have begun focused on fundamental cellular uptake and intra-cellular trafficking of particles; in vivo biodistribution; and in vivo tissue and cellular targeting.

Material Science: Opportunities for PRINT in advanced material science applications include the development a novel robotic system whose dimensions and physical properties have the ability to adapt and reversibly change from solid- to liquid-like. We envision a system that can be structurally rigid but, on command, “dissolves” into a state that is highly malleable. The basic science behind this approach relies on the fact that granular materials undergo dramatic changes in rigidity at the so-called jamming transition. In addition to particle jamming, the discussion will focus on the details
for roll-to-roll processing, application of PRINT in patterned arrays and films for use in structural composites, electrets and photovoltaics.

192. Distance and Orientation Effects at Chomophore/Semiconductor Interfaces

Elena Galoppini, Rutgers-Newark, Newark, NJ

Highly ordered semiconductor films morphologies such as nanowires, nanotubes and other examples grown from ZnO, TiO2, and other metal oxides has attracted much attention for the development of solar cells, optoelectronic devices, and sensors. The control and characterization of the binding mode, dye orientation, distance, aggregation phenomena, and in general of all aspects of the contact between a bound molecule and the semiconductor, are critically important to the understanding of electronic processes and for any kind of application. We will describe the synthesis and study of porphyrin model compounds and other organic dyes to study binding and electronic processes on ZnO, TiO2 and ZrO2 nanoparticles films as well as more ordered morphologies.

193. An Approach to Modeling Interlocked Macromolecular Complexes: Application to Binding Site Preference in a Molecular Abacus

Karl Sohlberg and Joseph P. Angelo, Drexel University, Philadelphia, PA

One of the roadblocks to the rapid penetration of nanotechnology into new areas of commercialization is the dearth of existing design engineering tools that are applicable to nano-scale mechanical systems. While it is well known that nanosystems are governed by the laws of quantum mechanics, one needs more than the Schrödinger equation for design engineering of nanosystems; one needs thoroughly vetted procedures that incorporate correct quantum mechanics. We seek to develop theoretical techniques for the design of mechanical molecular devices based on interlocked macromolecular complexes. A [3]rotaxane is such a complex that contains a long dumbbell-shaped molecule, (called the shaft) that threads two ring molecules. The three components are therefore chemically independent yet mechanically linked. If the shaft contains three or more potential binding sites for the rings, multiple co-conformations are possible, a molecular topological equivalent to an
abacus. We address the question, how does strength of ring-binding to the shaft vary with respect to position on the shaft? Previous studies have found that a shaft with three binding sites exhibits strongest ring binding at the center site. Here a five-binding-site shaft is studied. We employ a novel method to partition the total energy of the system into contributions from inter-component binding and intra-component strain. The method uses the output of quantum mechanical electronic structure calculations to determine fitting parameters in a set of coupled equations. The solutions of the equations yield the energy partitioning. It is found that co-conformational preference is a compromise of ring strain and inter-component binding.

194. Characterization Methods for Nanoparticle Properties for Biosystems
Alamgir Karim, National Institute of Standards and Technology, Gaithersburg, MD

We are developing reference test methods in collaboration with NIOSH, FDA and NCI for quantifying the physical, chemical and biological properties of nanoparticles (used for therapeutics, diagnosis and imaging) in synthetic and natural biofluidic environments such as lung fluid. X-ray, light scattering, MALDI, and XPS are the key measurement tools being developed for the complex task of solution characterization of nanoparticles in biofluids where nanoparticles can interact with macromolecules like proteins and lipids. To measure nanoparticle interactions in a biomimetic environment of oil and water, we have developed a platform known as Fossilized Liquid Assembly. We are also developing quantitative measures of cellular uptake of nanoparticles and methods to assess the cytotoxicity pathways that ultimately destroy cellular mechanisms. Nanoparticles being investigated include Quantum Dots, Gold, TiO2, SWCNT and Iron Oxide. NIST Gold nanoparticle Reference Material (RM) are currently available and SWCNT is being developed in this NIST wide effort.

195. Synthesis of SBA-15 Silica with Very Large Mesopores
Liang Cao¹, Tiffany Man² and Michal Kruk¹, (1)College of Staten Island and Graduate Center, City University of New York, Staten Island, NY, (2)College of Staten Island, City University of New York, Staten Island, NY

The low-temperature synthesis of large-pore SBA-15 silicas with 2-D hexagonal structure using EO20PO70EO20 triblock copolymer template and a variety of micelle expanders was explored. The micelle expanders studied included hexane, pentane, cyclohexane, 1,3,5-trimethylbenzene and 1,3,5-triisopropylbenzene. The selection of an appropriate micelle expander, the adjustment of initial synthesis temperature and other synthesis conditions allowed us to obtain well-ordered SBA-15 (with three or more peaks on small-angle X-ray scattering, SAXS, pattern) with d(100) interplanar spacings tunable in the range from 11 to 21 nm and with pore diameters up to about 20 nm. These materials exhibited narrow pore size distributions (PSDs) and large pore volumes (above 1 cm³ g⁻¹). The capillary condensation pressure of nitrogen at 77 K was observed at a relative pressure as high as 0.92 for some of these samples, which to the best of our knowledge, is the highest capillary condensation pressure reported for good-quality SBA-15 silicas whose cylindrical mesopores were not merged with one another to any significant extent. The pore diameter of silicas with uniform mesopores were adjusted to much larger values (on the order of 30 nm), as seen from the occurrence of capillary condensation at relative pressures of up to 0.96, but PSDs of these materials were much broader, the mesopore volumes were somewhat lower and there was no evidence of 2-D hexagonal ordering. For some of these samples, peaks corresponding to interplanar spacing values of up to 24 nm were observed.

196. The Advantages of Nanoparticulate MRI Contrast Agents, a Review
Marc Walters, New York University, New York, NY

Chelating moieties can be incorporated in micelles or attached to the surface of metal nanoparticles through sulfur linkages via physi- and chemisorption. Methods are well developed for producing
nanoparticles that are highly monodisperse, which is important to ensure a uniform response when the agent is administered to an organism. The resulting constructs consisting of derivatized micelles and metal particles have been characterized by solution NMR and show great potential as imaging agents for magnetic resonance imaging (MRI).

197. Silylation of Single-Walled Carbon Nanotubes
Tirandai Hemraj-Benny, SUNY@Old Westbury, Old Westbury, NY and Stanislaus S. Wong, State University of New York at New York at Stony Brook, Stony Brook, NY

Carbon nanotubes are widely known at a fundamental research point of view for their unique structural, electronic and mechanical properties in many fields, including biological, electronics and materials. However, before they can reach their full potential in practical and affordable applications, issues such as purity, solubility and homogeneity of nanotube type need to be resolved. Specifically, to solve issues of solubility and homogeneity, silylation of relatively pure as-prepared single-walled carbon nanotubes was carried out, which provided for increased solubility and reactive selectivity towards semiconducting tubes of specific diameter range. The fundamental point to note is that coatings of dielectric materials can be placed onto SWNT ends and sidewalls through a well-defined, relatively mild molecular reaction, which is structurally non-destructive to the nanotube itself. In addition, this coating has facilitated an increased solubility and stability of the trimethoxysilane – SWNTs adduct in DMF. Techniques such as SEM, TEM, AFM, NMR, IR, UV-Vis, XPS and Raman were used in analyzing nanotube samples.

Green Chemistry
Sponsor: The Green Chemistry Institute Pharmaceutical Roundtable
Organizer: John Leazer Merck & Co., Rahway, NJ

198. Copper-Catalyzed Air Oxidation of Cyclopentadienes to Cyclopentadienones
Brian S. Hickory and Paul A. Deck, Virginia Tech, Blacksburg, VA

Cyclopentadienes bearing combinations of perfluoroary and tert-butyl substituents are oxidized to the corresponding cyclopentadienones in 60-95% yields with copper(II) bromide pyridine complex and sodium acetate in ethyl acetate solution. Application to the synthesis of monomers for Stille-type Diels-Alder polyphenylenes will be discussed.

199. Green Chemistry and Green Workflows at Merck
Roy Helmy, John Leazer, Tim Rhodes, Wes Schafer, David Tellers, Steve Weissman and Jia Zang, Merck & Co., Inc., Rahway, NJ

From both a financial and environmental perspective, green chemistry has impacted the way chemists perform discovery and development. Towards that end, examples will be given highlighting green process development within Merck. In addition, we have begun analyzing our workflows with
the goal of reducing solvent and consumable usage. These workflows include catalyst screening, sample preparation and analysis, and crystallization studies. These efforts, which rely heavily on automation, will be described.

200. Catalytic Borylation/Cross-Coupling Protocols That Avoid the Preparation of Haloaromatics

Robert E. Maleczka Jr., Ghayoor A. Chotana, Venkata A. Kallepalli, Daniel Holmes, A. Monica Norberg, Luis A. Sanchez, Feng Shi and Milton R. Smith, III, Michigan State University, East Lansing, MI

Organoboron species are useful building blocks for pharmaceuticals, materials, and other valuable compounds. Such molecules serve as starting materials for a wide array of synthetic transformations. In particular, the Suzuki-Miyuara coupling of boronic acids or esters with alkenyl or aryl halides and their triflates is a well-established, mild, and versatile method for constructing C–C bonds. The aryl boronic acids and esters used in these reactions are usually prepared from the corresponding aryl halide. Such a reliance on halogenated starting materials was first eased in 1999 by the invention of a thermal, catalytic arene C–H activation/borylation reaction. Shortly thereafter we entered into a collaboration that has led to the development of novel organic transformations utilizing Ir-catalyzed borylations. These reactions are high yielding, functional group tolerant (alkyl, halo-, carboxy, alkoxy-, and protected amino), efficient, and uniquely regioselective. In brief, catalytic C–H activation/borylations allow for the direct construction of aryl boronic esters from hydrocarbon feed stocks in a single step, avoiding aryl halides. Just as significantly, the reactions are inherently clean as they can often be run without solvent and occur with H2 as the only stoichiometric byproduct. Lastly, once the boronic esters are formed they can be cross-coupled without isolation. Recent advances and applications of this chemistry will be presented.

201. Development of An Enzymatic Process for Lipitor

Michael P. Burns1, David W. Bauer2, Simon Davidson3, Alastair Denholm3, Aoife Fahy3, Cathal Healy3, John O'Shaughnessy3, Éanna O'Maitiú3, Floriana Stomeo3, Gillian Whittaker3 and John W. Wong1, (1)Pfizer, Groton, CT, (2)Pfizer, Kalamazoo, MI, (3)Pfizer, Cork, Ireland

A process for the biocatalytic reduction of (R)-tert-butyl 6-cyano-5-hydroxy-3-oxohexanoate was developed and implemented at commercial scale. The resulting (3R,5R)-tert-butyl 6-cyano-3,5-dihydroxyhexanoate is a key intermediate in the synthesis of atorvastatin (Lipitor). The benefits of the biocatalytic process include elimination of hazardous and toxic reagents, elimination of cryogenic reaction conditions and multiple distillations, reduction of organic solvent waste, and improved product purity and quality.

202. Supercritical Fluid Chromatography (SFC) as a Green Chromatography Technique for Support in Rapid Development of Pharmaceutical Candidates

Jimmy DaSilva, Henry Shiuhang Yip, Vinod Hegde PhD and Alex Zaks PhD, Schering-Plough Research Institute, Union, NJ

This talk will demonstrate the capabilities of the Supercritical Fluid Chromatography (SFC) and how it can be utilized as a "Green" chromatographic tool for rapid separations. SFC has several advantages over HPLC in terms resolution, loading and use of hazardous solvents. SFC uses supercritical carbon dioxide fluid as one of the main solvent for chromatography. This is a faster and "Greener" chromatographic technique that can be used to rapidly purify pharmaceutical products. The process is environmentally friendly and minimizes use of large amounts of organic solvents. SFC increases productivity by reducing separation times on an average of 20 times. Moreover, it reduces the total amount of solvent usage by 80-95% as a result of shorter run times and the use of CO2 instead of the typical hydrocarbon in the mobile phase. The CO2 needed is acquired from
environment and often recycled in large scale processes. Scale up in the case of SFC is more linear than HPLC.

We have used SFC to investigate the chromatographic resolution of various intermediates of drug candidates. Samples are initially screened using analytical SFC followed by method development and loading studies on a preparative SFC. We have utilized SFC to support the purification of several intermediates at different stages in development.

SFC also has a high potential for the resolution of chiral molecules compared to HPLC. Several examples will be provided to show its potential for the purification of racemic, diastereomeric and chiral compounds with a direct comparison to HPLC.

203. An Efficient Asymmetric Synthesis of the Tricyclic Indole Prostaglandin D2 Receptor Antagonist Laropiprant

Peter Maligres, Merck & Co., Inc, Rahway, NJ

An asymmetric synthesis was developed for the production of a prostaglandin D2 receptor antagonist for the treatment of allergic rhinitis. The stereogenic center was set using asymmetric hydrogenation, and the core of the structure was constructed via Fischer Indole methodology using a benzyl aryl hydrazine derived from a regioselective hydrazine alkylation. Several other synthetic approaches to the tricyclic indole system are also presented.

204. Ionic Liquids in Extreme Cold: Proposed 100 Meter Lunar Liquid Mirror Telescope

Gregory A. Konesky, SGK Nanostructures, Inc., Hampton Bays, NY

In order to study the oldest and most distant objects in the universe, a 100 meter diameter Liquid Mirror Telescope has been proposed for deployment on the Moon. High redshift places the spectral region of interest of these objects in the 1 to 10 μm wavelength region. This requires that the optics be kept very cold, typically at or below 130 K, which precludes the use of the traditional liquid Mercury mirror. The ionic liquid 1-ethyl-3-methylimidazolium ethyl sulfate has been coated with Silver by Physical Vapor Deposition (PVD) under high vacuum, and shows good reflectivity properties
while remaining liquid down to 175 K. An approximately 10 nm thick Chromium diffusion-stop layer previously deposited before the Silver further improves reflectivity. Both the Silver and the Chromium exist as a colloidal dispersion in the ionic liquid, rather than as a continuous solid layer.

Details of the process of depositing reflective layers on an ionic liquid by PVD are discussed, and consideration is given to the potential scale-up process for in-situ coating of a 100 meter ionic liquid mirror telescope on the Moon.

**205. Electroplating and Electropolish Using Ionic Liquids**

*Gregory A. Konesky*, SGK Nanostructures, Inc., Hampton Bays, NY

Electroplating and electropolish typically employ large volumes of hazardous and toxic materials. Ionic liquids provide a “green” and environmentally-friendly alternative to both processes, generally improve a number of process parameters, and can permit processes that are difficult or impossible in aqueous approaches.

When ionic liquids replace aqueous chemistries for electroplating, energy efficiency of the plating process typically increases from 20% to 90%; hydrogen gas production is significantly reduced. The non-volatile nature of ionic liquids reduces the need for air pollution controls. Electroplating Chromium using ionic liquids is especially advantageous in that hexavalent Chromium, which is highly toxic and carcinogenic, can be replaced by the trivalent form, which is much less toxic. While most metals that can be electroplated from aqueous solution can also be electroplated from ionic liquids, two examples are presented where the reverse is not true. The results are presented of electroplating Aluminum and Molybdenum using an ionic liquid composed of Urea and Choline Chloride.

Electropolishing is a complimentary process to electroplating in that microprojections (peaks) on a metal surface are preferentially electrochemically etched, while microdepressions (valleys) are minimally etched. This produces a surface that is mirror-like and smooth on an atomic scale. Ionic liquids composed of choline chloride and propylene glycol have been used to replace the toxic and hazardous electropolish baths using concentrated sulfuric and phosphoric acids. Greater electrical current efficiency, reduced Hydrogen production, reduced generation of acid mists, and room temperature operation are additional benefits. Results of ionic liquid electropolishing of Stainless Steel are presented.

**206. Induced Amphotropic and Thermotropic Ionic Liquid Crystallinity in Phosphonium Halides: “Lubrication” by Hydroxyl Groups**

*Kefeng Ma*¹, B. S. Somashekhar², G. a. Nagana Gowda³, C. L. Khetrapal² and Richard G. Weiss¹, (1)Georgetown University, Washington, DC, (2)Sanjay Gandhi Post Graduate Institute of Medical Sciences, Lucknow, India, (3)Purdue University, West Lafayette, IN

The influence of covalently attaching hydroxymethylene to the methyl groups of methyl-tri-n-alkylphosphonium halides ($[\text{H(CH}_2\text{)}_n]\text{P}^+\text{CH}_3\text{ X}^-$, where $n = 10$, 14 or 18, and $\text{X}^- = \text{Cl}^-$ or $\text{Br}^-$), $[\text{H(CH}_2\text{)}_n]\text{P}^+(\text{CH}_2)_2\text{OH X}^-$, or adding methanol as a solute to the $[\text{H(CH}_2\text{)}_n]\text{P}^+\text{CH}_3\text{ X}^-$ salts on their solid, liquid-crystalline (smectic A₂), and isotropic phases has been investigated using a variety of experimental techniques, which include optical microscopy, thermogravimetry, differential scanning calorimetry, X-ray diffraction, and $^2\text{H}$-NMR spectroscopies. These structural and compositional changes are found to induce liquid crystallinity in some cases and to enhance the temperature range and lower the onset temperature of the liquid crystalline phases in some others. The results are interpreted in terms of the lengths of the three n-alkyl chains attached to the phosphorus cation, the nature of the halide anion, the influence of H-bonding interactions at the head group regions of the layered phases, and other solvent-solute interactions. The fact that at least 1 molar equivalent of methanol must be added to effect complete conversion of a solid methyl-
tri-n-alkylphosphonium salt to a liquid crystal demonstrates a direct and strong association between individual methanol molecules and the phosphonium salts.

We thank the National Science Foundation for financial support.

207. Exploring the Potential of Amphotropic Liquid Crystals as Orienting Media for NMR Spectroscopy

Astghik A. Shahkhatuni¹,², Kefeng Ma² and Richard G. Weiss², (1)Molecule Structure Research Center, National Academy of Sciences, Yerevan 0014, Armenia, (2)Georgetown University, Washington, DC

Amphotropic liquid crystals (ALC) are possible aligning media for 3D structure determinations of various molecules by NMR spectroscopy because they can be oriented within strong magnetic fields and, thereby, orient the solute molecules being investigated. Here, we report the results of a systematic investigation of liquid-crystalline methyl-tri-n-alkylphosphonium salts (PmA, where m =10, 14, and 18 is the number of carbon atoms in the long alkyl chains and A an anion such as Cl⁻, Br⁻, NO₃⁻, PF₆⁻, BF₄⁻, or (CF₃SO₂)₂N⁻. The phase diagrams, transition temperatures, and liquid-crystalline properties of the thermotropic liquid-crystalline phases of the neat compounds, as well as the lyotropic phases formed in the presence of various concentrations of organic liquids such as methanol, butanol, hexanol, decanol, and DMSO have been investigated by NMR spectroscopy and polarizing optical microscopy. The concentration of liquid is critical to obtaining pure lyotropic liquid-crystalline phases. Changing the type and concentration of the liquid, the anion structure, and the length of alkyl chains permit the mesophase temperature ranges and the degrees of orientation in magnetic fields to be varied over a wide range. In turn, the degrees of orientations of selected solutes were also varied in this way. Aspects of the liquid crystalline phases and some preliminary results demonstrating the ability of the PmA to yield structural parameters from residual dipolar couplings will be presented.

We thank the US National Science Foundation for its support of this research and the Fulbright Foundation for a Visiting Researcher Fellowship to A. A. S.

208. Enzyme Electrodes Using Lactate Dehydrogenase Modified with Ionic Liquids

Sujan Shrestha, Amol Kafle and Mihaela Leonida, Fairleigh Dickinson University, Metropolitan Campus, Teaneck, NJ

Lactate dehydrogenase (LDH) was reversibly denatured using 1-ethyl-3-methylimidazolium tetrafluoroborate (IL), in the presence and absence (respectively) of water. LDH was reversibly denatured and “wired” at the same time with flavin adenine dinucleotide (FAD), an intrinsic group of the enzyme. The modified enzymes, after renaturation, were assayed and the activities compared with that of the starting LDH. In a second assay, they were evaluated for potential use in enzyme electrodes. Immobilization of the IL-modified LDH was done using different methods and the results are discussed comparatively. The performance of the “wired” LDH is also compared to that of the enzyme using as mediator FAD in solution. The electrodes were evaluated also for catalytic effect, linearity and stability. The IL-modified LDH showed promise for use in both analytical and synthetic applications.
209. Assessing the Toxic Effects of Ionic Liquids: More Concerns for Environmental Safety

Catherine McEntee1, Placide Bisangwa1, Majid Sahin2, Xing Li3, James F. Wishart4, Jinhee Gwon3 and Sharon Lall-Ramnarine3, (1)Kingsborough Community College, Brooklyn, NY, (2)Brooklyn College, Brooklyn, NY, (3)Queensborough Community College, CUNY, Bayside, NY, (4)Brookhaven National Laboratory, Upton, NY

Ionic liquids (ILs) are fast emerging as the solvents of choice in the chemical industry. Their relative non-volatility, non-flammability, wide liquid range and high conductivity make them serious candidates as green solvent alternatives to volatile organic solvents. In order to assess the relative safety of ILs, representative organisms were tested against ILs differing only in purity (as determined by color) and/or alkyl chain length. ILs were prepared identically with the exception of the reaction temperature. Our initial studies show that the purity of the IL does not contribute to its toxicity. As expected from previous reports in the literature, the size of the alkyl side chain contributes significantly to IL toxicity. These studies also demonstrate that although the presence of a cell wall has no effect on the degree of toxicity, the presence and type of bacterial glycocalyx determines the level of IL resistance. Results of the above studies were compared to a seed germination assay to determine which screen is most useful for identifying toxic ILs. Results indicate the seed germination assay is several-fold more sensitive to the ILs than the toxicity assay using microorganisms; seeds failed to germinate at IL concentrations that did not inhibit growth of bacteria, algae and fungi. These results raise concerns regarding the potential risk to microbial and plant ecosystems if ILs are released into the environment through effluent discharges or accidental spills. This work was supported in part at BNL by the U.S. DOE Office of Basic Energy Sciences under contract # DE-AC02-98CH10886.

210. Use of Zebrafish Embryos in Assessing Ionic Liquid Toxicity

PoKay Ma1, Ayisha Munawar2, Ankita Parikh2, Hughton R. Walker1, Jee-Un Lee1 and Sharon Lall-Ramnarine2, (1)Queens College, CUNY, Flushing, NY, (2)Queensborough Community College, CUNY, Bayside, NY

The potential effects of ionic liquids (ILs) on the aquatic ecosystem are assessed using zebrafish embryos as a model. Zebrafish is a small, freshwater fish that offers many advantages as a model organism in toxicological and pharmaceutical investigations. This hardy, prolific fish is relatively small (adults approximately 30 mm in length), easy to maintain, and has a 4-month generation time. Furthermore, the eggs and embryos are transparent, facilitating greatly the detection of developmental abnormalities in both morphology and behavior. The present study examines the dose-dependent effects of ILs on the growth and survival of zebrafish eggs and embryos. Viability and discernible abnormalities are documented.

Preliminary studies on several ILs show that various compounds have a wide range of toxicity. Lethal concentrations (LC50) range between 1 to 100 mM, depending on the compound. At concentrations below the LC50, retarded embryonic growth, reduced motility and hatching rate, and inability to inflate swimbladder are commonly observed abnormalities. Many of the embryos that survive fail to hatch, suggesting a motor defect. Many of those that manage to hatch fail to inflate their swimbladder, and are therefore unable to swim and feed. At concentrations above the LC50, the high mortality rate appears to be attributable to a disruption of tissue integrity. The relationship between IL structure and toxicity, and the mechanisms underlying the graded toxic effects are unknown. (This study was supported by PSC-CUNY award # 69605-00-38.)
**Physical Chemistry, I**

**Organizer:** Jianbo Liu Queens College of the City University of New York  
**Organizer:** Ruben Gonzalez Columbia University

**Session Overview:** This session will focus on experimental physical chemistry, particularly on spectroscopy and reaction dynamics.

### 211. Cosolvent Effects on Hydrophobic Surfaces: Salts and Sugars

**Joseph M. Serafin**, Jeff Stepan, Abdul Waheed and Jonathan Patete, St. John's University, Jamaica, NY

We report on how salts from the Hofmeister series as well as common sugars alter the aqueous interfacial free energy of aliphatic and aromatic hydrophobic surfaces. We prepared self-assembled monolayers (SAMs) which present a hydrophobic group, and measured the interfacial free energy, through adhesion measurements in a chemical force microscope, for a variety of solutions at high concentrations of 1 to 5 M. The cosolvents studied range from protein stabilizing to denaturing agents. Experimental results of the interfacial free measurements are critically compared to single molecule transfer free energy measurements, as well as computational studies of hydrophobic surfaces.

### 212. Explaining "Temperature"-Dependent Vibrational Spectra of Gas-Phase Proton-Bound Complexes

**Xiaohu Li**, **David T. Moore** and Srinivasan S. Iyengar, (1)University of Indiana, Bloomington, IN, (2)Lehigh University, Bethlehem, PA

Experimental vibrational action spectra for the proton-bound dimer of dimethyl ether at different temperatures are compared with predictions based on AIMD computational simulations. Single photon spectra of argon-tagged ions in a low-temperature molecular beam are found to agree well with the dipole-autocorrelation function (FT-DAC) from AIMD simulations of the system at 68K. Similarly good agreement is found between infrared multiple photon dissociation (IRMPD) spectra of room temperature ions in an ion trap and the FT-DAC from 270K AIMD simulations. As expected, the vibrational bands in the IRMPD spectra are much broader than the lower temperature argon-tagged spectrum. A detailed analysis of this broadening is presented in terms of the contributions of the normal modes of the molecule to the velocity autocorrelation function (FT-VAC) of each spectral band at high and low temperature. Ab initio calculations predict four harmonic normal modes, all involving significant motion of the bound proton, and these “light modes” contribute the vast majority of the intensity to the spectrum at all temperatures. At 68K, the vibrational bands are narrow and show close correspondence with the harmonic spectrum, although there is a splitting of the band near 1000 cm⁻¹ into a doublet, due to coupling with a dark mode. This splitting precisely matches a similar doublet in the low-T argon-tagged spectrum. At 270K, the vibrational bands are broadened by coupling of many dark modes due to vibrational anharmonicities and the conformational flexibility of the ionic complex.

### 213. Surface Enhanced Raman Spectra in Semiconductor Quantum Dots

**John R. Lombardi**, City College of New York, New York, NY

We report on the observation of surface enhancement of the Raman signal by semi-conductor quantum dots. Until recently surface enhanced Raman spectroscopy has been observed only on metals, especially Ag and Au. One requirement for the effect is that the metal be in the form of
nanoparticles. Enhancement factors of up to six orders of magnitude and even larger have been reported. Two sometimes-competing explanations for the effect have been suggested: either plasmon resonances or charge-transfer resonances between the molecule and metal.

We have recently observed surface enhancement in molecules adsorbed on semiconductor quantum dot surfaces. We have observed these in MBE grown InAs and CdSe quantum dots, as well as colloidal quantum dots such as ZnS, ZnO and CeTe. Enhancement factors of up to four orders of magnitude are observed. It is impossible to explain these observations using plasmon resonance, which for semiconductors are in the infrared. We explore the possible application of the charge-transfer theory to semiconductor dots. Application of the Herzberg-Teller theory to such systems implicates polaron (electron-phonon) coupling in the suggested mechanism.

214. Flipping Electron Spin without Touching: Collision Induced Intersystem Crossing in CH₂

Gregory E. Hall, Brookhaven National Laboratory, Upton, NY

One in about seventy collisions of He with singlet CH₂ produces triplet CH₂, even though the spin-orbit coupling of singlet and triplet CH₂ is weak and virtually unaffected by He. Mixed-state gateways are invoked as the key intermediates in such molecules, where the level structure is sparse and the spin-orbit couplings are weak. Experimental eigenstate-resolved kinetic spectroscopy, double-resonance saturation recovery and saturation transfer experiments provide a new, direct, and detailed look at the role of mixed states in the collision-induced intersystem crossing process. Spin-preserving, rotationally inelastic collisions, along with coherent evolution of non-stationary spin in mixed state pairs, interrupted by frequent dephasing collisions provides a conceptual framework for an efficient spin changing process that never invokes the direct interaction of the collision partner with the spin of the target molecule.

215. Injecting Single Charges into Nanoscale Molecular Wires

John R. Miller¹, Andrew R Cook¹, Paiboon Sreearunothai¹, Sadayuki Asaoka², Kirk S. Schanze³, Norihiko Takeda¹, Tomokazu Iyoda⁴ and Julia M. Keller⁵, (1)Brookhaven National Laboratory, Upton, NY, (2)Tokyo Institute of Technology, (3)University of Florida, Gainesville, FL, (4)Tokyo Institute of Technology, Japan, (5)University of Florida, Upton, FL

Conjugated polymers can act as semiconducting molecular wires having diameters of 0.5-1.0 nm and lengths of 2-100 nm. Good nanoscale molecular wires must be excellent charge carriers, even at very long lengths. This research uses picosecond electron pulses to inject electrons or holes into conjugated polymers. It explores remarkable behaviors including transient terms in diffusion-controlled reactions for charge attachment, delocalization lengths, and transport of charges along the wires.

Conjugated molecules investigated here are polyfluorenes, polythiophenes and oligomers of platinum-acetylides. In some cases the molecules incorporate traps for electrons or holes, usually positioned at the ends of the chains.

These are remarkable materials have properties we are only beginning to understand and potential we are only beginning to tap.

216. The Electronic Spectroscopy and Anomalous Photophysics of Phenylacetylene

Philip M. Johnson, Stony Brook University, Stony Brook, NY

Phenylacetylene is a molecule of interest because of its role in the chemistry of combustion. It has also been discovered to have some unique photophysical properties. When excited to a single rotational level of its lowest singlet state in a collisionless environment, it rapidly chooses either to
become a species (probably an isomer) that lives for at least hundreds of microseconds, or stays in
the excited singlet state to fluoresce. Both the longevity of its photoproduct and the bifurcation of its
excited state evolution pathway are properties previously unseen in the photophysics of aromatic
molecules. This molecule has been studied using excitation with an ultra-high resolution laser,
combined with excited state photoelectron spectroscopy. Possibilities for its anomalous behavior will
be discussed.

Analytical Chemistry, General Session I
Organizer: Rosario LoBrutto Novartis Pharmaceutical Corporation
Organizer: Richard Thompson Novartis Pharmaceutical Corporation

Session Overview: This session is for general contributions in the field of analytical chemistry.

217. Development and Validation of HPLC Method for Related Compounds Test in
USP Norethynodrel Monograph
Zarema Kassymbek, Shane X. Tan, MinLi Liu and Samir Wahab, US Pharmacopeia, Rockville, MD

An HPLC method was developed and validated for related compounds test to replace both the
Ordinary Impurities and the Limit of norethindrone TLC methods in current USP Norethynodrel
monograph (USP 30, 2077). The HPLC method was developed based on the chromatographic
conditions in USP Norethindrone and Ethinyl Estradiol Tablets Assay (USP 30, 2773). It completely
separated norethynodrel from norethindrone and ethinyl estradiol. The resolution between
norethynodrel and norethindrone peaks was 7. The tailing factor was 1.1 for norethynodrel and 1.2
for norethindrone. The relative standard deviation of the peak area response of standard solution for
norethynodrel and norethindrone was less than 1.0 %. The detection limit of norethynodrone was
0.1% of the test solution. On USP Norethynodrel RS and a commercial norethynodrel sample, the
HPLC method detected three more impurities than the current Ordinary Impurities TLC method. USP
Norethynodrel RS exhibited less than 2.0% of total impurities, including norethindrone, while the
commercial norethynodrel sample exhibited more than 2% of total impurities.

218. Automated Evaluation of Novel Chiral Columns by SFC Using Standard Chiral
Compounds Library
Zainab Pirzada, Michelle Personick, Mirlinda Biba, Xiaoyi Gong, Wes Schafer and Christopher. J.
Welch, Merck & Co. Inc., Rahway, NJ

Many new chiral stationary phases (CSP) are introduced to the market each year. Evaluation of new
CSPs is typically haphazard and incomplete. To achieve quick and systematic evaluation of new
chiral CSPs, a standardized evaluation workflow was proposed in this presentation using automated
SFC screening and a standard library of racemic analytes. The SFC system is capable of automated
screening of chiral samples in 96-well plate format using 6 columns and multiple solvents. The
standard library of racemic analytes was assembled using a combination of proprietary Merck
synthesized and commercial chiral compounds. The library was screened in 96-well plate format on
6 newly available CSPs using the above mentioned automated SFC screening system. The screening
results were archived in a structure searchable ACD database. The separation performance of the
new CSPs was compared with each other and previously available chiral columns.
219. A Stepwise Strategy for Developing a Robust HPLC Separation for a Novel Diabetes Compound

Karthik Jayaraman, Frank Hu, Frank Tomasella and Merill Davies, Bristol Myers Squibb Company, New Brunswick, NJ

A stepwise method development strategy was employed in developing a robust HPLC method to resolve several closely eluting process impurities associated with a novel diabetes compound. The strategy consisted of rapid column screening, optimization of mobile phase compositions and separation temperature, DryLab modelling, and experimental verification of optimized separation conditions.

The column evaluation process involved screening of a series of 20 columns varying in bonding chemistry using four sets of mobile phases composed of water, acetonitrile and/or methanol at three different pHs. The screening process resulted in identifying two promising columns: XBridge Shield RP18 and SunFire C18. The effects of organic modifiers and separation temperatures were then evaluated to narrow down the chromatographic separation parameters. DryLab® was used to predict optimized gradient profile and separation temperature. Finally, the DryLab® predictions were verified experimentally.

The study demonstrates that factors such as stationary phase composition, organic modifiers, pH and separation temperature have profound and oftentimes complex effects on chromatographic conditions. Therefore, it is critical to adopt a rational strategy as demonstrated here to evaluate the interplay of these factors, there by greatly enhancing method development efficiency.

220. Development of DBTAA Grafted Macroporous Monolithic Stationary Phases for HPLC

Kathleen M. Ford and J. Faye Rubinson, Georgetown University, Washington, DC

Dibenzotetraaza[14]annulenes (DBTAAs) have inspired research in a variety of areas since first being synthesized thirty years ago. Studies have investigated such topics as their electropolymerization on electrode surfaces, interactions with DNA/RNA, electrochemical activity, and catalytic abilities. Their structural similarity to porphyrins makes them an exciting option for separation used as part of the stationary phase in HPLC. We have recently begun investigation into the immobilization of substituted DBTAAs onto polymer monoliths, fixed porous structures consisting of crosslinked polymer chains and pores, which have provided an alternative to beads. DBTAAs and their metal complexes can be grafted onto prepared monoliths to aid in separation of such compounds as polycyclic aromatic hydrocarbons (PAHs), amino acids, and peptides. Monoliths have been prepared with varying initiator:monomer (4,4'-azobis(4-cyanovaleric acid):4-vinylaniline) concentrations and it has been shown that the initiator concentration must be equal to or greater than the monomer concentration for polymerization to occur. Using SEM, an inversely proportional dependence between the amount of initiator to the pore size was also detected.
**221. Characterization of Major Degradation Products of An Adenosine 2a Receptor Antagonist Under Stressed Conditions by LC Tandem MS Analysis**

Li-Kang Zhang and Birendra Pramanik, Schering-Plough Research Institute, Kenilworth, NJ

Parkinson's disease (PD) is a very serious neurological disorder, and current methods of treatment fail to achieve long-term control. SCH 420814 is a potent, selective, and orally active adenosine A2a receptor antagonist discovered by Schering-Plough. The stability testing provides evidence of the quality of a bulk drug when exposed to the influence of environmental factors. Moreover, the degradation profiles are critical to the safety and potency assessment of the drug candidate for clinical trials. The use of LC/MS(/MS) has a significant impact on degradation product characterization. In this study, a rapid, sensitive and method was developed for the determination of the degradation products of the stressed SCH 420814.

**222. Enhancing the Selective Detection of Dipicolinic Acid (DPA) with a Fluorescent Dye Using a Molecular Imprinting Method**

Anne Okafor, Enju Wang, Neil Jespersen and Mostafa Sadoqi, St. John's University, Queens, NY

DPA is a useful biological agent, acting as a chelating agent of elements in the body and is a constituent of the redox coenzyme, NAD/ NADH. It is used for the quantitative detection of calcium. It is also a useful analytical indicator for the presence of bacteria spores. Thus the sensitive determination of DPA is very important in many biological processes.

A method for the selective detection of dipicolinic acid (DPA) in the presence of other analogs using a molecular imprinting method and fluorescence detection has been developed in our laboratory. We further explored detection methods by incorporating a fluorophore. The fluorophore is immobilized on an (ITO) plate tethered with a silane coupling agent. DPA is imprinted on the plate using a molecular imprinting technique developed in our laboratory. The process has been shown to be very promising for the selective detection of DPA in the presence of other analogs. Incorporating this fluorophore leads to a more versatile instrumental detection method. Comparison of the process will be made with the original parameters obtained without the fluorophore. Reproducibility selectivity, sensitivity, shelf life, real time analysis and fabrication processes will be described fully in this paper.

**Biocatalysis and Biomimetic Catalysis**

**Organizer:** Kent Kirshenbaum New York University, New York, NY

**223. Thiamine Inspired Catalysis: Not Just for Breakfast Anymore!**

Jeffrey W. Bode, University of Pennsylvania, Philadelphia, PA

Thiamine, or vitamin b1, is an triazolium cofactor responsible for remarkable chemical transformations in both primary and secondary metabolism. Although the synthetic potential of thiamine-inspired catalysis has long been recognized, particularly in the form of the benzoin reaction, recent years have witnessed a resurrance of synthetic transformations inspired by the unique ability of thiamin to activated aldehydes and related substrates for further transformation. In our own work, we have pioneered internal redox reaction of alpha-functionalized aldehydes for the azolium-promoted catalytic generation of reactive species including activated carboxylates, enolates, and homoenolates. The development of new catalytic structures inspired by thiamine has led to a new generation of azolium salts ideally suited for these powerful transformations and the identification of chiral variants for highly enantioselective reactions. The development of these thiamine-inspired catalysts, and their application to catalytic approaches to ester and amide bond
formation, inverse electron-demand Diels-Alder reactions, gamma-lactone and gamma-lactam forming annulations, and a remarkable cascade catalysis approach to enantiopure cyclopentane derivatives will be described.

224. Organocatalytic Activation Modes for the Asymmetric Alpha-Functionalization of Aldehydes and Ketones
Teresa D. Beeson and David W. C. MacMillan, Merck Center for Catalysis, Princeton University, Princeton, NJ

Over the last four decades, the capacity to induce asymmetry using enantioselective catalysis has been an area of extensive chemical research efforts. A multitude of new asymmetric catalytic reactions have been invented, mostly from a small number of established activation modes. The advent of organocatalysis has since introduced new types of chemical reactivity, which has made a substantial contribution to the advancement of the field of synthetic chemistry. This presentation will discuss our recent advances in the use of organocatalyzed enamine-activation for the direct enantioselective α-functionalization of aldehydes and ketones to create α-fluoro stereocenters. Also, the development of a new mode of asymmetric activation based on transient radical cation formation, SOMO catalysis, and its application to the direct enantioselective α-allylation of aldehydes will be discussed.

225. Folded Peptides for Asymmetric Catalysis: Some Structures and Some Functions
Scott J. Miller, Yale University, New Haven, CT

Modern organic synthesis depends heavily on the use of catalysts for selective transformations. We have discovered a class of synthetic peptides that catalyze a number of enantioselective and regioselective reactions. This presentation will describe the discovery and use of peptides containing proteinogenic and non-natural amino acids for a variety of asymmetric bond formations. The connections between peptide sequence and stereoselectivity will be explored in a range of mechanistically distinct reactions. Prospects for generalizations and eventual design of catalysts from first principles will be evaluated. The presentation will also discuss potential analogies to enzymes.

226. Peptoid Oligomers Incorporating Nitroxide Side Chains
Galia Maayan, Michael D. Ward and Kent Kirshenbaum, New York University, New York, NY

N-substituted glycine oligomers, or “peptoids”, are a family of peptidomimetic foldamers capable of adopting stable secondary structures. By employing a solid-phase synthesis protocol, a wide variety of side chains can be incorporated into peptoid sequences. Thus, the peptoid scaffold can be used as an efficient platform for different functional sites displayed in a specific manner.

Herein, we explore the use of an oligomeric peptoid as a scaffold for the incorporation of chiral side chains and an achiral nitroxy moiety for applications in biogumatic chemistry.

227. Biologically Inspired Catalyst for Ceramic Synthesis
Douglas H. Adamson, Daniel M. Dabbs and Ilhan A. Aksay, Princeton University, Princeton, NJ

Certain biological systems have long been able to form ceramics in environmentally benign conditions. The near neutral pH and ambient temperatures of biology are in stark contrast to the conditions employed commercially. These man-made systems typically involve extremes of pH and temperature in order to form condensed ceramics from alkoxide precursors. We have developed a functionalized block copolymer synthesized with inspiration from the protein Silicatein α. This protein is found in silica spicules produced by the sponge Tethya aurantia. These spicules contain proteins at their core, the most abundant being Silicatein α. Our polymer contains the chemical functional
groups shown to be active in natural protein and we have shown it to catalyze the hydrolysis of tetraethoxysilane (TEOS). In this talk we will describe the polymer, the catalysis of silica formation from TEOS and the application of the polymer system to ceramics in addition to silica.

228. Biomimetic Catalysis
Ronald Breslow, Columbia University, New York, NY

We have developed mimics of enzymes that have several important features. They operate in water solution, and one type is able to direct oxidation reactions whose selectivity is dominated by the geometry of the catalyst/substrate complex, overriding the intrinsic reactivity of the substrate. Our goal in this work is to "liberate chemistry from the tyranny of functional groups."

Another type of biomimetic catalyst is based on hydrophilic polymers with hydrophobic cores. This class is able to imitate the ability of enzymes to use the advantages of water for hydrophobic binding but use the non-aqueous interior of the protein to promote rapid catalytic reactions, producing “a drop of DMSO suspended in water.” The result is an acceleration of the synthesis of tryptophan by transamination with an acceleration of 240,000-fold caused by the polymer. Recently the system has been improved by using non-covalent complexes of coenzyme mimics to accelerate tryptophan synthesis by 725,000-fold.

Delaware Valley Chromatography Forum Student Award
Sponsor: Chromatography Forum of Delaware Valley

Session Overview: The annual CFDV Student Award Symposium provides graduate and undergraduate students with an opportunity to present their research in the field of separation science. Though many participants are pursuing separation science as their major course of study, students in the areas of medicine, biochemistry, engineering and organic chemistry have successfully presented papers describing areas of research that involve separations.

229. Separation of Water Soluble Vitamins by UHPLC
Michael J. Bozym, Michelle L Owens, Anna Glinko and Karyn M. Usher, West Chester University, West Chester, PA

Water soluble and fat soluble vitamins are vital to human health making it imperative to have a method to detect and quantify them in dietary supplements, drinks etc. Current methods of separation described in the United States Pharmacopeia are complicated and require ion pair reagents. Ion pairing irreversibly changes the chromatographic column making its use for other analyses impossible. Furthermore these methods need to be updated due to emergence of new technologies. The main goal of the project was to create a single High Performance Liquid Chromatography method that would allow separation of the water soluble vitamins: Ascorbic Acid, Biotin, Cyanocobolamin, Niacinamide, Panthothenic Acid, Pyridoxine, Riboflavin and Thiamin.

Analyses of the mixtures were performed on the Agilent 1200 LS Rapid Resolution LC system. The mobile phase was made of two components; A: 25 mM KH2PO4 buffer at pH = 2.5 and B: Methanol. The analytes were separated on Zorbax Eclipse Plus C18 (4.6 x 150 mm, 5 μm), (4.6 x 100 mm, 3.5 μm), and (4.6 x 50 mm, 1.8 μm) columns. As the column particle size decreased; the phase interaction, equilibrium, and separation became faster and more efficient. Identification of the vitamins in the standard mixture, supplements and vitamin drinks was confirmed using the Diode
Array Detector with high-speed full spectral UV-Vis detection. This separation was completed in under 3.5 minutes under the conditions stated.

230. Extra Column Effects as a Function of Flow Rate

**Casey M. Mulcahy, Scott H. Snyder and Karyn M. Usher, West Chester University, West Chester, PA**

HPLC is the most commonly used analytical technique for separation of compounds in solution. This experiment investigates the effects of extra column volume (ECV) in HPLC experiments at various flow rates. ECV is important in chromatography because understanding it and how it affects HPLC results can help scientists to develop more efficient separation of samples. As flow rate is increased, the total system variance decreases. When the variance is decreased, the peaks are narrower and more analytes can possibly be separated and identified. It was found in these experiments that as the overall variance decreased, the percent of variance due to extra column volume increased. When this occurs, the separation becomes more difficult and the chromatographer is unable to take advantage of all the benefits of newer stationary phase technology since the ECV becomes a limiting factor. In this experiment it was confirmed that minimizing ECV diminishes this phenomena, but that once the ECV has been minimized to a certain degree that this effect can be removed. Our measurements were taken at extra column volumes of 90 and 60μL. Based on this data, it appears that the extra column volume can be optimized to diminish this effect. Based on calculations, for our system, this optimal volume would be 45μL.


**James D. Vasta and Joseph Sherma, Lafayette College, Easton, PA**

Complete and uniform application of postchromatographic derivatization reagents to the layer is critical for sensitive detection and accurate and precise quantification of separated analytes lacking a chromophore in high performance thin layer chromatography (HPTLC). In this research, standards representing the five major neutral lipid classes were separated on silica gel HPTLC plates by development with petroleum ether-diethyl ether-glacial acetic acid (80:20:1) and detected as blue zones using ethanolic phosphomolybdic acid (PMA) reagent. Qualitative and quantitative results for the lipids were compared after applying PMA by the two most widely used methods, manual spraying and dipping, and with the new manual Derivapress device, followed by heating of the plate on a plate heater. The application methods were compared in terms of accuracy, precision, visible and densitometric limit of detection, calibration curves, cost effectiveness, ease of use, and safety. Samples were applied to the layer using a spray-on band applicator, and a densitometer was used for instrumental detection and quantification at 610 nm. Results showed that dipping is the best PMA application method for quantitative analysis and that spraying is best for high sensitivity qualitative analysis. The Derivapress proved to be simple and economical for application of PMA in qualitative and quantitative analysis of neutral lipids. These comparative procedures can serve as a general model for optimization of the detection step in any analyte-layer-mobile phase system using all possible postchromatographic derivatization reagent application methods: manual and instrumental spraying, manual and instrumental dipping, modified commercial printer, or Derivapress.

232. Lost Protein Technology for Proppant and Catalyst Manufacture

**Christopher J. Morrison and Gennaro J. Maffia, Widener University, Chester, PA**

Collagen dispersions are heterogeneous mixtures of collagen nanofibrils, manufactured from bovine corium, and buffered water. The dispersion is viscous and can support many times its mass in metal dust. After freezing and lyophilizing the dispersions, porous protein-metal structures are recovered.
This material is then sintered at temperatures between 600 and 1300 °C. During the sintering process the metal particles diffuse into one another while the collagen scaffold is burned away. The closer the temperature is to the specific metal's melting point the more diffusion that occurs and the stronger the resulting bridge between particles. The oxidation of the particle's surface may pose issues for the bridging between particles and the resulting strength. The void left by the removal of the collagen provides more surface area that is able to be utilized as a catalyst or allow higher rates of extraction of oil and gas from wells if utilized as a proppant. Several metals have been successfully processed with the lost protein technology. Results of this research including required processing and analysis will be presented.

233. Examining Chiral Separations with Bile Salt Micelles Using MEKC and NMR

Alyson M. Cobb, Kyle W. Eckenroad, Gregory A. Manley, David Rovnyak and Timothy G. Strein, Bucknell University, Lewisburg, PA

It has been well-documented that bile salts, including cholate and deoxycholate, can be used to form a pseudostationary phase in micellar electrokinetic capillary chromatography (MEKC) and employed for the separation of chiral isomers. However, despite many reports of bile salt micelles being used for chiral separations in chromatography and capillary electrophoresis, both the mechanism by which the micelle is formed from surfactant monomers and the molecular-level interactions between the isomers and the micelles are not well characterized. This work attempts to explore these two questions through careful and systematic characterization of both the MEKC behavior of model-drug analytes and nuclear magnetic resonance (NMR) signals obtained from the MEKC solutions. Using the model analytes 1,1′-binaphthyl-2,2′diyl hydrogenphosphate and 1,1′-binaphthyl as probes, we are able to closely examine the interactions between the micelle and chiral isomers and have begun to understand how the micelle and analytes interact. We also have further examined the interactions of bile salt monomers as they form micelles. The NMR examination of these aqueous MEKC systems has included 1H and 31P chemical shift analysis and, recently, 2D Nuclear Overhauser Effect Spectroscopy (NOESY). The data from the NMR experiments was correlated with MEKC results. We will present recent results from both MEKC and NMR that aid our increasing understanding of the complicated interactions between individual bile salt monomers, bile salt micelles and the analyte molecules.

234. Investigation of Buffering and Mixing Conditions for the Jaffe Reaction with Capillary Electrophoresis

Sarah A. Schubert¹, John W. Stahl² and Timothy G. Strein¹, (1)Bucknell University, Lewisburg, PA, (2)Geneva College, Beaver Falls, PA

Renal function is generally determined by serum creatinine levels in blood serum. Clinical determination of creatinine in blood is based on the Jaffe reaction, in which creatinine in the serum reacts with sodium picrate to produce a colored product that can be spectrophotometrically quantified. Previous work has introduced an electrophoretically mediated initiation of this reaction utilizing nanoliter volumes in a capillary column, followed by electrophoretic separation of the reactions product from excess reactant(s).

This work involves a fundamental and quantitative investigation of the factors influencing the reaction yield and the transient isotachophoretic stacking of the Jaffe product. The effect of the background electrolyte on the reaction was principally investigated, with borate, glycine, AMPSO, and CAPSO buffers used in the experimentation. The background electrolytes seem to primarily affect the flow rate within the capillary, but they also have a minimal effect on the Jaffe reaction product. Additionally, the timing of the applied voltage used to overlap the reactant zones was studied. Addition of chloride to the creatinine zone is found to yield a significant improvement in stacking behavior, presumably due to minimized electrodispersion of the product.
235. Improving the Sensitivity of Electrophoretically Mediated Micro Analysis (EMMA) for the Determination of Creatinine

Ranasinghe K. Sampath¹, John W. Stahl² and Timothy G. Strein¹, (1)Bucknell University, Lewisburg, PA, (2)Geneva College, Beaver Falls, PA

Inefficient mixing of reagents with electrophoretically mediated microanalysis (EMMA) and the degradation of the reaction product (Janovosky complex) have been previously identified as limitations associated with CE-based in-line assays for creatine. Calculations that assume constant voltage field do not accurately predict the optimal mixing parameters. Through digital simulation (freeware program Simul-5) of experimental conditions (3 mm sample zones of 20 mM creatinine and 47 mM alkaline sodium picrate, various borate BGEs at pH 9.0) local electric field intensities in the reagent zones were found to vary widely from 260 kV/m to 0.83 kV/m, indicating the consideration of non-homogeneous fields is more important than was previously realized. Correlation of experimental and calculational data will be shown. In addition, counter ions have been found to pay an important role in achieving optimal conditions for both reactant overlap and product stacking.

Secondly, the degradation of the in-line generated product was investigated. By periodic reversal of the potential, the product was electrophoresed back and forth across the detector window within an 8 cm segment of the capillary centered around the detection point. The decay of the Janovosky product peak area illustrated first order degradation kinetics (0.085 S⁻¹ to 0.153 S⁻¹). The rate of degradation increased with both elevated borate buffer concentration and pH, but was considerably slower (< 10⁻⁴ S⁻¹) when no potential field was applied. By combining conditions for both optimal overlap and minimum product degradation an optimized CE based method can be developed.

Frontiers in Nanoscience and Nanotechnology - Nanoscience, II

Sponsor: Momentive Performance Materials
Organizer: Bhanu P. S. Chauhan William Paterson University
Organizer: Kenrick Lewis Momentive Performance Materials, Tarrytown, NY
Presider: Michal Kruk College of Staten Island and Graduate Center, City University of New York, Staten Island, NY
Presider: Moni Chauhan CUNY-Queensborough Community College, Bayside, NY
Presider: Frieder Jäkle Rutgers University-Newark, Newark, NJ

236. Architectural Diversity and Elastic Networks in Hydrogen-Bonded Host Frameworks: From Molecular Jaws to Cylinders to Embedded Capsules

Michael D. Ward, New York University, New York, NY

Guest-free guanidinium organomonosulfonates (GMS) and their inclusion compounds display a variety of lamellar crystalline architectures distinguished by different “up-down” projections of the organomonosulfonate residues on either side of a two-dimensional (2D) hydrogen-bonding network of complementary guanidinium ions (G) and sulfonate moieties (S), the so-called GS sheet. Using a combinatorial library of 24 GMS hosts and 26 guest molecules, a total of 304 inclusion compounds out of a possible 624 possible host-guest combinations were realized. The GS sheets in the inclusion compounds behave as “molecular jaws” in which organomonosulfonate groups projecting from opposing sheets clamp down on the guest molecules, forming ordered interdigitated arrays of the host organic groups and guests. Both the guest-free and inclusion compounds display a variety of architectures that reveal the structural integrity of two-dimensional GS sheet and the unique ability of these hosts to conform to the steric demands of the organic guests. Certain GMS host-guest combinations prompt formation of tubular inclusion compounds in which the GS sheet curls into cylinders with retention of the 2D GS network. The cylinders assemble into hexagonal arrays.
through interdigitation of the organosulfonate residues that project from their outer surfaces, crystallizing in high symmetry trigonal or hexagonal space groups. This unique example of network curvature and structural isomerism between lamellar and cylindrical structures, with retention of supramolecular connectivity, is reminiscent of the phase behavior observed in surfactant microstructures and block copolymers. More recent results that demonstrate the introduction of molecular capsules embedded in these frameworks also will be described.

237. Molecular Network Reinforcement of Sol-Gel Glasses

Geraud Dubois1, Willi Volksen1, Teddie Magbitang1, Robert D. Miller1, David M. Gage2 and Reinhold H. Dauskardt2, (1)IBM, San Jose, CA, (2)Stanford University, Stanford, CA

The intrinsic mechanical properties of a given material strongly depend upon its chemical nature: the organics tend to be soft, but tough, while the inorganic materials, on the other hand, are hard but brittle, and are prone to fracture. The later characteristic gets even worse for porous materials and is of major concern in the microelectronics industry as porous organosilicates (mainly inorganic) will constitute the next insulating layers in future electronic devices [1]. In this presentation, we demonstrate that significantly tougher organosilicates glass thin-films prepared by sol-gel process, can be obtained by introducing carbon bridging units between silicon atoms present in the organosilicate network [2,3]. Fracture energy values of 14-16 J/m2 were measured, surprisingly higher than those for dense silicon dioxide (10 J/m2), suggesting mechanical properties that lie somewhere in between those of conventional glasses and organic polymers. We also found that the Young's modulus follows a linear decay when porosity is introduced, a unique property when compared to traditional organosilicates. As a result, crack resistant films were obtained at high level of porosity, opening potential applications in the field of low-k materials for future integrated circuits, membranes, sensors, waveguides, fuel cells and micro-fluidic channel.


238. Organic Rigid-Rods with Para- and Meta- Conjugated Bridges for Semiconductor Nanoparticles Sensitization

Olena Taratula and Elena Galoppini, Rutgers-Newark, Newark, NJ

Rigid-rods with organic chromophores (Pyrene and Coumarin 6H) having a oligophenylenethynylene (OPE) rigid linker, linear or branched, were synthesized and bound to MOx (TiO2, ZrO2, and ZnO) nanoparticle thin films through isophthalic (Ipa) groups anchoring groups (see Figure). The influence of the linker's length and branching on the photophysical properties of the compounds has been studied in solution and on MOx surface. All synthesized rigid-rods showed high quantum yields and high extinction coefficients when compared to the parent compounds. Photophysical, photoelectrochemical, and electrochemical studies been complemented with quantum mechanical calculations. The nature of the binding of the organic sensitizers to MOx was characterized by FTIR-ATR and found to be dependent on the pH pretreatment of the semiconductor surface. The aggregation phenomena of the organic dyes were studied using ZrO2 (an insulator, bandgap ~ 5 eV) films. Pyrene rigid-rods formed excimers on the metal oxide surface whereas coumarin rigid-rods produced non-emissive aggregates. Photoelectrochemical studies of the pyrene rigid-rods in regenerative solar cells showed near quantitative conversion of absorbed photons into electricity. Work in progress will be discussed.

(See Figure on Next Page)
239. Nano-Size Particles of Porous Metal Oxides and Their Applications
Steven L. Suib, University of Connecticut, Storrs, CT

This presentation will focus on the synthesis, characterization, and applications of porous nano-size particles of metal oxides. Selectivity to produce desired products in catalytic reactions is the focus of our research. Several examples of the design of catalysts to drive various reactions will be discussed. These catalysts are nano-size and designed via molecular control. The role of redox chemistry in preparation and use of such catalysts will be discussed. Catalysts for selective oxidations, production of acrolein, and activation of CO2 are of current interest in our group. Novel methods of catalyst preparation such as in situ mixing nozzle microwave methods will be mentioned. Catalysts that are porous oxides and mixed metal oxides are used in these reactions. Effects of morphology and particle size on rates of reaction have been observed. Applications in adsorption, catalysis, spintronics, and others will be discussed.

240. Molecular Grafting of Metallic Solutions
Moni Chauhan, Devendra Tilakdhari and Maninder Kaur, CUNY-Queensborough Community College, Bayside, NY

Nanosized particles are of enormous importance due to their unique chemical and physical properties. During the last two decades there has been a tremendous amount of activity in this area due to its potential for use in future applications. The primary goal of this research is to control the stability and functionality of nanoparticles using silicone based oligo-and polymers. In this presentation, we will demonstrate the use of trimethoxysilylpropyl isocyanurate as an efficient agent for generation and stabilization platinum and palladium nanoparticles. Preliminary results show that the oxidation of this molecule leads to silicone based polymer which help in stabilization of the nanoparticles. Future research will focus on the potency of using these metallic nanoconjugates as catalysts for various processes such as silaesterfication, hydrosilylation and reduction reactions of conjugated alkenes.

241. Nanostructured Organoboron Block Copolymers
Frieder Jäkle1, Chengzhong Cui1, Yang Qin1 and Edward M. Bonder Sr.2, (1)Rutgers University, Newark, NJ, (2)Rutgers University-Newark, Newark, NJ

This presentation will focus on our recent research on boron-containing nanostructured polymeric materials. The selective attachment of boryl groups to polymers provides wide-ranging opportunities in materials research where they are, depending on the specific nature of the boron moieties and the polymer scaffold, attractive as flame retardants, materials with improved thermal stability, preceramic materials, electrolytes for lithium ion battery applications, and optoelectronic materials.
Various other applications have also recently emerged, ranging from supported reagents and immobilized catalysts to separation media, sensors for anions and biologically important molecules, holographic materials, and stimuli responsive polymers.

We have introduced several new methods for the preparation of well-defined organoboron-functionalized styrene polymers. Especially interesting are block copolymers that are capable of forming self-assembled nanostructures in solution and in the solid state, and hence are expected to provide exciting new opportunities in the above-mentioned areas. We describe here the preparation and assembly properties of three new classes of organoboron block copolymers containing anionic organoborate, cationic organoboronium, and pH sensitive boronic acid moieties, respectively. The solution self-assembly properties of these novel polymers will be discussed.

242. Lab on a Chip: The Role of ProteinChip Arrays in the Discovery of Cardiovascular Biomarkers

Bishambar Dayal, William Paterson University, Wayne, NJ and Norman H. Ertel, University of Medicine and Dentistry of New Jersey, Newark, NJ

Recent studies by Barzilai et al. indicated that supersized cholesterol carriers (large particles of both HDL cholesterol and LDL cholesterol) may protect against heart disease and thus lead to exceptional longevity (J Amer. Med. Association, 290: 2030-2040 (2003). These studies attributed enhanced longevity with specific biological genetic factors. We recently demonstrated the versatility of the surface-enhanced laser desorption ionization mass spectrometry (SELDI-MS), SELDI ProteinChip MS technology as a rapid method for the identification of HDL-apoA-1, a major anti-inflammatory carrier protein in patients who have diabetic cardiovascular disease, (Dayal and Ertel J Proteome Res 1: 375-380 (2002), (ACS Abstr. 2005, 2006). Using the Weak Cation Exchanger Surface (WCX2) chip and analysis via surface-enhanced laser desorption ionization mass spectrometry (SELDI-MS), apoA-I and A-II were separated as sharp peaks at 28 and 17 kD and did not overlap with other serum protein peaks.

Present studies will describe a comparative molecular characterization and expression levels of cardiac molecular markers: specifically, high sensitivity C-Reactive Protein, HDL apolipoprotein apoA-1 using Surface-enhanced laser desorption/ionization-time of flight mass spectrometry, SELDI-TOF MS ProteinChipArray Technology.

This presentation will also highlight two recent reports namely 1) use of rectangular glass chip microscope slides holding several white dots containing human cell cultures and enzymes mimicking human reactions to test toxic drugs 2) Use of Nanostructured-Initiator Mass Spectrometry (NIMS).

We believe current use of biochips may soon replace laboratory animals routinely needed for drug testing.
Ionic Liquids III: Dynamical Effects in Ionic Liquids

Sponsor: CEM Corporation
Organizer: James F. Wishart Brookhaven National Laboratory, Upton, NY
Organizer: Sharon Lall-Ramnarine Queensborough Community College, CUNY, Bayside, NY

Session Overview: Research in ionic liquids (ILs) has exploded in recent years because of their great promise in a broad range of applications in chemistry and chemical technology for process and safety improvement and reduction in overall environmental impact. This three-session symposium features the broad spectrum of ionic liquids research conducted in the Middle Atlantic Region.

243. Electric Field Responsive Ionic Liquid Polymers

Arthur W. Snow and Holly Ricks-Laskoski, Naval Research Laboratory, Washington, DC

The electrowetting behavior of ionic liquids as well as electrolyte solutions can manifest itself in a shape change of a droplet on a surface or translational movement across that surface. The magnitude of the response depends on the strength of the electric field, the nature of the surface being wetted (surface energy, roughness) by the droplet and on the chemical nature of the ionic liquid itself (composition, structure, conductivity, surface tension, viscosity). In the work to be presented we focus on an ionic liquid monomer – liquid polymer system based on an acrylamidopropane sulfonic acid – oxyethylene amine base (depicted below) and describe comparative electrowetting measurements. The contact angle dependence on electric field and polarity as well as translational droplet motion will be illustrated. The issues of interest are comparison of a monoionic with a polyionic liquid system, the molecular weight effect of polyionic system and volume fraction effect of the oxyethylene ammonium counter ion.

244. Understanding Solvent Polarity in Ionic Liquids

Mark Kobrak, Brooklyn College and The Graduate Center of the City University of New York, Brooklyn, NY

The polarity of a solvent is a fundamental determinant of its use in chemistry. For molecular liquids, the principles that explain the relationship between molecular structure and solvent polarity are sufficiently well-understood to guide experimentalists in the proper choice of solvent. These principles are vastly different for ionic liquids. We present the results of theoretical modeling on ionic liquids that clarify this relationship, and express simple principles that researchers can use to select the appropriate ionic liquid for a given task.
245. Intermolecular Dynamics and Solvation in Ionic Liquids
Edward W. Castner Jr., Tatiana A. Fadeeva, Heather Y Lee, Hideaki Shirota and James F. Wishart, (1) Rutgers, The State University of New Jersey, Piscataway, NJ, (2) Chiba University, Chiba, Japan, (3) Brookhaven National Laboratory, Upton, NY

We will present several topics from our recent research on the physical chemistry of ionic liquids. In particular, we are interested in understanding how the atomic and molecular properties of the ions comprising ionic liquids are correlated to their properties as strongly interacting and associating liquids. We are attempting to connect the macroscopic properties such as the temperature dependence of the viscosity and the glass transition temperature of the fragile glass-forming ionic liquids with their spectroscopic properties. We have studied both the neat ionic liquids using femtosecond Raman and NMR methods, and we have studied the solvation properties using solvatochromic fluorescence probe molecules. A new project is to understand the connection between solvation and photo-reactivity in ionic liquids using a series of novel electron donor-bridge-acceptor complexes.

Work done at Rutgers was supported by the NSF and the ACS-PRF. Work at BNL was supported by the U.S. Department of Energy Office of Basic Energy Sciences, Chemical Sciences Division, under contract DE-AC02-98CH10886.

246. Solvation and Solvation Dynamics in Room-Temperature Ionic Liquids
Sergei Arzhantsev, Hui Jin and Mark Maroncelli, The Pennsylvania State University, University Park, PA

Room temperature ionic liquids (ILs) are currently being studied as new solvent media for a variety of purposes. Our interest lies in understanding solvation energetics and solvation dynamics in this distinctive environment. Steady-state and time-resolved fluorescence spectroscopy are used to measure solvation energies and dynamics in several series of imidazolium, pyrrolidinium and ammonium ionic liquids. The combination of femtosecond Kerr-gated emission spectroscopy and picosecond time correlated single photon counting are used to measure the full solvation response in ionic liquids. The observed solvation dynamics is highly non-exponential and extends over four decades in time. This non-exponential temporal response probably originates from dynamical heterogeneity similar to that found in supercooled liquids.

247. Heterogeneous Solute Kinetics in Ionic Liquids
Mark Maroncelli, Hui Jin, Xiang Li and Sergei Arzhantsev, The Pennsylvania State University, University Park, PA

Although the solvation energies in ionic liquids are often similar to those in highly polar conventional solvents, the dynamics of solvation is markedly slower. Whereas solvation energies in conventional solvents are usually completely relaxed within 10 ps, in ionic liquids relaxation extends well into the nanosecond time range. This 1000-fold difference in the solvation response times has a pronounced retarding effect on solvent-controlled reactions and gives rise to heterogeneous kinetics for reactions and other processes that occur on ps and ns time scales. This heterogeneity is manifest in both non-exponential and excitation-wavelength dependent kinetics of excited state reactions. We have been using steady-state and time-resolved emission measurements to explore a number of model intramolecular reactions that involve charge transfer and large-amplitude solute motion in order to try to understand the distinctive kinetics that occur in ionic liquids. I will speak about our most recent results on this subject.
248. Carbon Dioxide and Molecular Nitrogen as Switches Between Ionic and Uncharged Room-Temperature Liquids

Tao Yu, Georgetown University, Washington DC, DC

The properties of a new class of reversible, room-temperature, chiral ionic liquids—amidinium carbamates—which are easily made from readily available chemicals, amidines and chiral amino alcohols, are described. The ionic liquid phases are prepared by exposing a 1/1 (mol/mol) mixture of an easily synthesized amidine and an amino alcohol, obtained in one step by reduction of a naturally-occurring amino acid, to CO2 gas; one commercially available amino alcohol with two chiral centers, has been employed as well. All of the amidine-amino alcohol combinations examined, 35 in all, form ionic liquids in this way at room temperature. They are stable indefinitely under an atmosphere of CO2 and they remain liquids well below 0 oC and above room temperature. The ionic liquids can be reconverted to their non-ionic states after an inert gas (such as N2 or argon) is bubbled through them at room temperature or, more rapidly, at slightly elevated temperatures. The thermal, conductive, viscous, and spectroscopic properties of both the nonionic and ionic phases will be reported and compared. Unlike many other ionic liquids, these need not be prepared and handled under dry conditions and they can be cycled repeatedly between high- and low-polarity states.

We thank the National Science Foundation for its support of this research.

Metal Complexes in Chemotherapy and Diagnostics

Organizer: Roberto A. Sanchez-Delgado Brooklyn College and The Graduate Center, CUNY

249. Platinum Complexes as Anticancer Agents

Nicholas Farrell, Virginia Commonwealth University, Richmond, VA

Platinum compounds, such as cisplatin, carboplatin and oxaliplatin are amongst the most useful drugs in the anticancer armamentarium. DNA is considered the biological target of platinum drugs but the overall efficacy is the sum of target binding, cellular uptake and metabolic deactivation. This contribution will summarize the medical uses and biological mechanisms of the currently used drugs. The status of new agents in development, especially those such as polynuclear platinum and mononuclear transplatinum compounds acting by different mechanisms to cisplatin and congeners, will be critically surveyed.

250. Inorganic Radioisotopes for Molecular Imaging and Radiotherapy

Lynn C. Francesconi, Hunter College and the Graduate Center of the City University of New York, New York City, NY

Inorganic radioisotopes form the basis of FDA approved molecular imaging agents and radiotherapy agents. For molecular imaging, radiopharmaceuticals that emit γ rays or positrons that penetrate through the body are employed. On the other hand, radioimmunotherapy (RIT) agents employ radioisotopes that emit α or β particles that possess limited range in tissue. Technetium-99m (99mTc), a γ emitter, is currently the most widely used radioisotope in the clinic for diagnostic imaging due to its favorable physical properties (γ energy: 142 keV; half-life: 6.02 hr) and convenience (obtained from a 99Mo/99mTc generator). Recent targeted imaging agents, AcuTect (99mTc apcitide) and NeoTect (99mTc depreotide), are based on cyclic peptide targeting vectors and peptide chelators that offer amine and amide nitrogen and thiolate sulfur donor atoms to stabilize a TcV oxo moiety. The development, characterization and chemistry under physiological conditions of these agents will be discussed. Rhenium-188, the third row congener of technetium, as well as
Radiolanthanides are potentially useful for radiotherapy applications because these isotopes offer a range of $\beta$ particle energies and half-lives that may be matched to the size and disposition of tumors in the body and to the residence times of targeting vectors. Parameters that impact the stability of $^{188}$Re chelates will be elucidated.

**251. Chemically Inert Metal Complexes as Anticancer Agents**

**Eric Meggers**, Phillips-Universitat, Marburg, Germany

The presentation will illustrate how the structural properties of metal complexes can be applied to the design of molecules with unprecedented biological properties. For example, recent results from our laboratory demonstrate that organometallic compounds can function as highly potent and selective enzyme inhibitors. Along these lines, a recipe is introduced for morphing indolocarbazole alkaloids into simple and easily accessible metal complexes, leading to the discovery of picomolar and maybe even femtomolar inhibitors for protein kinases. Some of these compounds display promising anticancer properties.

**252. Ruthenium Complexes as Potential Antiparasitic and Antitumor Agents**

**Roberto A. Sanchez-Delgado**, Brooklyn College and The Graduate Center, CUNY, Brooklyn, NY

Metal complexes continue to attract considerable attention for applications in the chemotherapy of a variety of diseases. In this lecture we will provide an overview of our work on ruthenium complexes of potential chemotherapeutic value, making use of the concept of metal-drug synergism. Coordination of ruthenium-containing fragments to organic drugs like clotrimazole or ketoconazole resulted in enhanced biological activity against Trypanosoma cruzi, the causative agent of Chagas disease, by a dual mechanism of action involving inhibition of sterol biosynthesis and DNA binding; the same compounds were also active against some types of tumors by a mechanism different from that of cisplatin. Also, we have synthesized ruthenium complexes containing chloroquine as a ligand, which display activity against malaria parasites, in some cases against resistant strains. Mechanistic studies indicate that the main target is heme aggregation and that the lipophilicity of the compounds plays a key role in the activity and the lowering of resistance.

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**Physical Chemistry, II**

Organizer: Ruben Gonzalez Columbia University
Organizer: Jianbo Liu Queens College of the City University of New York

**Session Overview:** This session will bring together experimental biophysical chemists who are using advanced spectroscopies and microscopies in order to gain mechanistic insights into complex biological systems.

**253. From Liposomes to Live Nerve Cells**

**Kenneth B. Eisenthal**, Columbia University, New York, NY

Experiments of equilibrium and time dependent phenomena at membrane mimetic phospholipid interfaces and live nerve cells will be presented. The application of second harmonic spectroscopy to selectively probe these various interfacial processes will be described.
254. Biophysical Insights into the Mechanism of Viral Protein Synthesis

Dixie J. Goss, Mateen A. Khan, Artem Domashevskiy and Hasan Yumak, Hunter College CUNY, New York, NY

Plant viral diseases affect a significant number of food crops world-wide and can have severe impact on both economic conditions and food supply. Protein synthesis is a key step in viral infection, however the mechanism is not well understood. Biophysical studies have provided insight into the mechanism of this process and how viruses compete for host cell machinery to synthesize viral proteins. We have recently gained new insight into the role of the potyvirus genome-linked protein, VPg in wheat germ in vitro translation. Addition of VPg to wheat germ extracts leads to enhancement of uncapped (viral) RNA translation and inhibition of capped (host) RNA translation. To understand the molecular basis of these effects, we characterized the interaction of VPg with eIF4F, eIFiso4F, and a structured RNA derived from tobacco etch virus. When VPg formed a complex with eIF4F the affinity for TEV RNA increased more than 4-fold compared with eIF4F alone. The binding of eIF4F to TEV RNA correlates with translational efficiency. Viral RNA which is generally translated less efficiently than capped RNA, must compete for available cell components for translation. In the presence of both capped and uncapped mRNA, VPg competes with eIF4F and eIFiso4F for cap binding. Formation of a VPg-eIFiso4F complex leads to a non-productive complex that reduces host cell translation. In contrast, an eIF4F-VPg complex binds more tightly to viral RNA and enhances its translation. These complementary functions provide a significant competitive advantage for viral RNA.

255. How Does a Bacterium Secrete Folded Proteins across the Outer Membrane - a Cryo-EM Study

Chunyan Tang¹, Nadine Henderson², David G. Thanassi² and Huilin Li¹, (1)Brookhaven National Laboratory, Upton, NY, (2)Stony Brook University, Stony Brook, NY

Gram-negative bacteria use the conserved chaperone/usher pathway for assembly and secretion of a superfamily of virulence-associated surface structures. P and type 1 pili (fimbriae) are prototypical organelles assembled by this pathway in uropathogenic E. coli. These hair-like surface fibers mediate initial binding to and subsequent invasion of the urinary tract. Protein secretion and pilus biogenesis across the bacterial outer membrane are poorly understood. We captured a pilus assembly intermediate corresponding to the type 1 pilus tip fiber during secretion through the outer membrane FimD usher. 3D reconstruction of cryo-EM images revealed that the translocating usher is a dimer, with a single pilus tip fiber emerging from one of the two available usher pores. The location of the chaperone-subunit complex at the periplasmic face of the assembly intermediate likely explains the requirement of a twin pore for asymmetrical subunit translocation and pilus assembly.

256. NMR Studies of Protein Dynamics

Ann E. McDermott, Columbia University, New York, NY

NMR studies of conformational dynamics of enzymes and membrane proteins will be discussed. New solid state NMR methods allow for structural and dynamic characterization of proteins, including order parameters. Applications to several proteins including a prokaryotic potassium channel will be described.

257. Effect of Suberoylanilide Hydroxamic Acid (SAHA) on Glioma Invasion in Vitro

Zhihua An, Megan L. Choy and Laura J. Kaufman, Columbia University, New York, NY

Current treatments of high grade malignant gliomas do not significantly affect patient prognosis, in large measure because they can not curtail the diffuse invasion of single glioma cells into brain...
tissue surrounding the tumor. Here, we investigate whether SAHA affects glioma invasion, which could be of critical import clinically. Our results show that SAHA inhibits both glioma proliferation and invasion. MTT assays show that the proliferation of C6 glioma cells is arrested after treatment with 5mM SAHA for 24 hours. A Boyden chamber invasive assay as well as a 3D variation on this assay shows SAHA inhibits C6 invasion at 5mM. Multicellular tumor spheroids embedded in 3D collagen I matrices in the presence of SAHA were also monitored via microscopy. The results show that cell invasion and volumetric spheroid growth are inhibited by SAHA even though the majority of cells within the MTS remain viable. We find that SAHA independently affects both C6 glioma invasion and the reorganization of the tumor surroundings that usually proceeds glioma cell invasion into collagen I gels. Preliminary investigation into the mechanism by which SAHA inhibits invasion was undertaken. Because degradation of extracellular matrix via matrix metalloproteases (MMPs) is likely essential for tumor invasion, we investigated whether SAHA affects MMP production. Zymography reveals that MMP2 is down-regulated by SAHA. We have shown that SAHA decreases glioma cell proliferation, ability to reorganize its surroundings, and ability to invade these surroundings.

258. Coupled Proton Diffusion and Binding within Bacterial Spore Nanocompartments

Sergey V. Kazakov and Elizabeth M. Bonvouloir, Pace University, Pleasantville, NY

Method of time-resolved micro-potentiometry was introduced for probing the kinetics of proton uptake by dormant Bacillus subtilis spores. It was shown that the plurality of steps comprising the uptake of protons may be attributed to the multi-layered structure of the spores. Based on the diffusion time analysis, it was found that the effective diffusion coefficient for hydrogen ions within the spore core can be up to 3 orders of magnitude lower than that within the coats and cortex. Estimated from the coupled proton diffusion and binding model, the concentrations of binding sites inside the spore layers appeared to be comparable with the spore proton capacity found from the equilibrium binding. Together with the known facts of the low level of water content (25-55% of the mass of the hydrated spore core), the bound state of water, the high level of dipicolinic acid (5-15% of the mass of the hydrated spore core) in the spore core, the immobility of a soluble protein in dormant spores, and the inner membrane lipids immobility, the high concentration of ionizable groups found in this work supposes that the spore cytoplasm is a particular state of biological matter characterized by a high density of charge within the nanosized matrix of the spore core. In the practical point of view, regulation of the spore internal pH may be the way of its metabolic dormancy control, since the internal pH may be a contributing factor to enzymatic activity within the dormant spore.

259. Binding of Modified Alkane Polymers to Human Recombinant TLR-2 Receptor Monitored by Intrinsic Tyr Fluorescence

Cristina C. Clement, Albert Einstein College of Medicine (AECOM), Bronx, NY

Inflammatory responses to alkane/alkyl polymeric materials, extensively used to replace nonfunctional body parts, have been noted. Purification of the alkane polymers from the site of inflammation revealed extensive “in vivo” oxidation as detected by fourier transformed infra-red spectroscopy. Herein, we report the novel observation that oxidized alkane polymers could induce activation of TLR1/2 pathway as determined by ligand dependent changes in intrinsic tyrosine fluorescence intensity. Molecular docking of the oxidized alkanes designated ligand specificity and polymeric conformations fitting into the TLR1/2 binding grooves. This is the first report of a synthetic polymer that could activate immune responses through TLR binding.
260. Complex Particles and Patterned Substrates: Future Opportunities in Life Sciences and Material Science

**Joseph M. DeSimone**, University of North Carolina at Chapel Hill, Chapel Hill, NC

To translate promising molecular discoveries into benefits for patients, we’re taking a pharmaco-engineering systems approach to develop the next generation of delivery systems with programmable multi-functional capability. A key strategy is to apply manufacturing technologies from the microelectronics industry to fabricate polymeric delivery systems that are capable of multiple functions. A novel method for the fabrication of organic particles on the order of tens of nanometers to several microns will be described. Our imprint lithographic technique called PRINT (Particle Replication In Non-wetting Templates), takes advantage of the unique properties of elastomeric molds comprised of a low surface energy perfluoropolyether network, allowing the production of monodisperse, shape-specific nanoparticles from an extensive array of organic precursors. This engineered nature of particle production has a number of advantages over the construction of traditional nanoparticles such as liposomes, dendrimers, and colloidal precipitates. The nature of PRINT technology takes drug delivery for the first time into the uncharted realm of engineered drug therapies given its à la carte approach and versatility. PRINT allows for the precise control over particle size, shape, composition, cargo, modulus and surface properties. Key therapeutic parameters such as bioavailability, biodistribution, and target-specific cell penetration can be simultaneously designed into a therapy. Extensive *in vitro* and *in vivo* studies have begun focused on fundamental cellular uptake and intra-cellular trafficking of particles; *in vivo* biodistribution as a function of size, shape, surface chemistry and deformability; *in vivo* tissue and cellular targeting for autoimmune disease treatment and cancer treatment and diagnosis.
261. Carbon Nanostructures Made by Focused Ion Beams on Carbonaceous Substrates

Alexander Zaitsev, College of Staten Island, Staten Island, NY

Ion irradiation with doses exceeding the amorphization threshold converts carbonaceous materials into amorphous carbon, which may possess high electrical conductivity and considerably different chemical activity. This effect is especially pronounced in diamond, which is an insulating and chemically inert material. Because of very sharp threshold of the ion-induced diamond-carbon conversion, the interface between the amorphized carbon and the intact substrate may be as narrow as a few nanometers. Thus using controlled scanning of the ion beams focused at nanoscale, one can reproducibly fabricate complex carbon nanostructures of predetermined 2D geometry. It has been shown that the focused ion beam-written carbon nanostructures possess novel electronic properties: non-linear behavior, electronic switching, anomalously high conductivity, Coulomb blockade at elevated temperatures. These structures can also form regular hydrophobic-hydrophilic nanopatterns or functionalized nanoarrays, which may be used for 2D self-assembly of macromolecules and polymers. The FIB-written carbon nanostructures are discussed as novel devices for carbon-based nanoelectronics and sensorics.

262. Effect of Semiflexibility on the Conformational Hysteresis of a Giant DNA

Chwen-Yang Shew, CUNY-College of Staten Island, Staten Island, NY and Higuchi Yuji, Kyoto University, Kyoto, Japan

To elucidate the conformational behavior of DNA, an integrative approach by combining experimental and computational methods is developed. In the experimental part, the forward and backward titration are conducted to measure the folding and unfolding processes of a giant DNA by increasing and decreasing PEG concentration, respectively, at a high salt concentration (to screen out DNA charges). We find that these two processes form a hysteresis loop, suggesting that the folding and unfolding processes of a giant DNA undertake different pathways. The results present the very first experiment to characterize the conformational hysteresis loop of DNA. Furthermore, computer simulations are resorted to examine the role of chain semiflexibility on hysteresis loop by using a bead-spring chain model. The simulations predict that the hysteresis loop emerges only when the chain is stiff enough, but not in the case of flexible chains. Meanwhile, the compact conformation in the hysteresis loop is found to be thermodynamically more stable. Nevertheless, the elongated DNA chain, which is thermodynamically less stable, persists until the concentration of condensing agents becomes high enough. Such behavior can be attributed to the semiflexibility of a DNA molecule. Namely, an increase of chain stiffness attenuates the number of chain conformations, including most of conformations required to make a transition to compact conformation. As a result, the folding process is impeded. On the contrary, an increase of condensing agent concentration enhances monomer-monomer attraction, which facilitates the folding process by increasing the number of chain conformations.

263. ADMET (acyclic diene metathesis) Synthesis of Heteroatom Containing Polymers

Ralf M. Peetz and Narayan Mukherjee, CUNY-College of Staten Island, Staten Island, NY

Silylene- and siloxane-containing conjugated polymers and macrocycles were synthesized by acyclic diene metathesis (ADMET), starting from diene-functional monomers. In the case of silylene, linear polycondensates were observed, whereas the siloxane cases resulted in cyclic condensates. The presented systems highlight the ring-chain equilibrium inherent in ADMET reactions, and significantly expand the synthetic scope of ADMET chemistry to novel heteroatom containing polymeric systems.
264. Engineering Nanoparticles for Rendering Polymer Blends Flame Retardant:
S. Pack, SUNY Stony Brook, Stony Brook, NY, M. H. Rafailovich, Stony Brook University, Stony Brook, NY, E. Weil, University of Akron, Akron, OH and T. Kashiwagi, NIST, Gaithersburg, MD

We have previously demonstrated that large aspect ratio nanoparticles such as clays or nanotubes can form in-situ grafts which and become universal compatibilizing agents for polymer blends. Here we show how the same mechanism could be applied to producing flame retardant materials. In this case the large aspect nanoparticles also serve as potent dispersal agents for the flame retardant formulations, which greatly increase their efficiency in retarding combustion. These particles can act in multiple ways. The presence of the nanoparticles prevents phase segregation in the flame, maintains the dispersal of the FR agent in the phases which affects the heat release rate and the mass loss rates. In the case when one of the polymer is a good char former, the nanoparticles promote partial compatibilization of even highly immiscible blends.

An important concern regarding nanocomposites is the environmental impact of the nanoparticles used. This impact is minimal in the intact nanocomposite, but could be quite significant if combustion occurs and the particles become airborne or settle in the soil or water. Hence the toxicity of these particles on primary cultures was also studied and the results will be presented.

265. Synthesis of Protein-Polymer Hybrids
Krishnaswami Raja, Department of Chemistry, College of Staten Island, CUNY, Staten Island, NY
Wei Shi, Sukanta Dolai, Saadhya Averick, Jose Saltos, Francoise Sidimie, Solomon Gulayamov William L'Amoreaux, Probal Banerjee and Krishnaswami Raja*

Novel near-infrared (NIR) fluorescence dye incorporated polymers were synthesized for applications in in vivo imaging. The polymers have glucose side chains to improve water solubility and pendant NIR dyes acting as imaging agents with an azide/biotin chain-ends which serve as reactive handles for the attachment of the polymers to proteins. The polymers were synthesized via Atom Transfer Radical Polymerization (ATRP) using a novel azide initiator. Biotin alkyne was attached to the azide chain-end via "click" chemistry. The polymers were characterized using NMR spectroscopy, GPC and FPLC. Protein hybrids with streptavidin were prepared. The conjugates were characterized and potential biological applications for non-invasive imaging in mice and in 96 well plate assays were explored.

266. Soft-Template Synthesis of Conducting Polymer Hollow-Nano-Spheres and the Study of Release Control Via pH Value
I-Wei Chu¹, Kai Su² and Nan-Loh Yang¹, (1)CUNY-College of Staten Island, Staten Island, NY, (2)Ciba Specialty Chemicals, Tarrytown, NY

Conducting polymers as novel vesicles for controlled release have attracted attentions due to their unique property of substantial volume changes with the variation of doping level. Hollow conducting polymer nanostructures have promises for loading contents of interest, although relatively poor mechanical properties and limited solubility of conducting polymers lead to significant challenges in the fabrication of such structures. We report here a novel soft-template, ionic liquid micelles, used for the first time synthesis of conducting polymer nano-hollow-spheres for controlled releases. The concentration of 3, 4-ethylenedioxythiophene (EDOT) monomer plays a significant role in controlling the morphology of intact hollow PEDOT nanospheres. The nascent sizes of the nano-hollow sphere were controlled by the composition ratio of ionic liquid to surfactant (IL-to-surfactant, R) ratio. The controlled release of uncharged as well as anionic species was demonstrated through delivery from the surface with pH as tuning factor.
267. From Oligo(phenylene vinylene)S to Conjugated Polyazines
Narayan Mukherjee and Ralf M. Peetz, CUNY-College of Staten Island, Staten Island, NY

Conjugated polyazines have been receiving attention due to their semi-conducting and non-linear optical properties, making them potential candidates for electro-optical and optical applications. In this paper, an efficient polycondensation of α,ω-di-formyl functional aromats, namely 2,5-diheptyloxy-1,4-diformyl benzene and side-chain substituted α,ω-di-formyl oligo(p-phenylene vinylene) (OPV) with hydrazine afforded two novel conjugated polymers. Structurally, the resulting materials are rigid-rod type polymer chains that feature extended delocalized conjugated systems with integrated azine linkages. The polymer products were analyzed in regard to microstructure, chain length, and their optical properties. 1H/15N NMR and ATR-FTIR indicated all-trans configured C=N-N=C linkages in OPV-based azine polymers. The optical properties proved extended conjugation, and differential pulsed voltammetry showed that the OPV-based polyazine behaves as n-doped material.

268. Luminescent Polystyrene: Synthesis and Characterization
Kshitij Parab and Frieder Jäkle, Rutgers University, Newark, NJ

Incorporation of Lewis acidic boron centers into polystyrene side-chains has been realized by tin-boron and/or copper-boron exchange reactions. Arylboration compounds are of particular interest as the interaction of the empty p-orbital on the boron center with organic systems leads to interesting photophysical properties. The Lewis acidity of the boron center as well as the optical properties of the polymers can be easily fine tuned by variation of the aryl groups. The oxidative stability of these compounds has also been enhanced by the use of bulky 1,3,5-trisopropylphenyl groups. The polymers synthesized may find applications as conduction layers in OLED’s or as sensors for nucleophiles.

Synthesis of Complex Biologically Active Molecules
Sponsor: ACS Division of Organic Chemistry
Organizer: Christian Rojas Barnard College, New York, NY
Organizer: David R. Mootoo Hunter College, CUNY, New York, NY

Session Overview: Complex biologically active molecules have traditionally attracted the attention of synthetic chemists because they provide a showcase for new synthetic methodology, raise the necessity for analogs for biological studies, or simply present compelling synthetic challenges. This symposium will feature new technologies that enable the preparation of complex molecules as well as syntheses of specific molecular targets. Presentations from both academic and industrial research will provide an opportunity to compare the interests and strategies in these settings.

269. Total Synthesis Complex Galbulimima Alkaloids. Discovery of a Himbicine Based Antithrombotic Agent SCH 530348
Samuel Chackalamannil, Schering-Plough Research Institute, Kenilworth, NJ

This talk will discuss the total syntheses of complex Galbulimima alkaloids himbacine and himgaline and a case history for the discovery of SCH 530348, a thrombin receptor antagonist (TRA) that is currently undergoing Phase-III clinical trials for myocardial infarction. The lead for the TRA program was a synthetic analog of himbacine. After achieving a practical synthesis of himbacine analogs, extensive lead optimization went through several years of efforts and synthesis of thousands of
analogs. The final development candidate SCH 530348 showed potent antiplatelet effect in a number of functional assays and in a monkey ex-vivo model. The compound was subsequently progressed to clinical studies.

270. Strategies and Methods for the Synthesis of Natural Products
Kathlyn A. Parker, Stony Brook University, Stony Brook, NY

The total synthesis of natural product structures continues to fascinate and challenge creative chemists. The incentives for reaching these molecular targets are not only intellectual; many natural products provide novel leads for medicinal chemistry.

These days, total synthesis can be efficient enough to provide really useful amounts of complex drug candidates. Furthermore, the strategies and methods developed for the synthesis of natural products can be used to prepare structurally and functionally related compounds.

This lecture will present strategies for the efficient preparation of stereochemically complex small molecule natural products, describe the discovery of new methods in the context of novel schemes, and provide illustrations with examples of recent contributions from the speaker's lab at Stony Brook.

271. Multicatalysis: A Platform for Increasing Synthetic Efficiency and Inspiring Discovery
Tristan H. Lambert, Columbia University, New York, NY

Our research is focused on challenging the paradigm of iterative synthesis for the preparation of complex molecules. A major objective of this program is to advance strategies that achieve rapid generation of molecular complexity via the prosecution of multiple distinct catalytic cycles in a single reaction vessel, an area of research we call multicatalysis. In these endeavors, we aim (1) to discover new chemical technologies that are amenable to incorporation in multicatalytic processes, and (2) to develop versatile multicatalytic strategies that allow for the preparation of biologically relevant organic architectures with unprecedented efficiency. In this lecture, some of our efforts towards developing multicatalytic strategies to access complex oxygen heterocycles will be discussed, as well as our discovery of several useful new chemical technologies that enable these novel approaches.

272. COPPER-Promoted C-Heteroatom Bond Cross-Coupling Via Boronic Acids: Chan-Lam Coupling Reaction
Patrick Y. S. Lam, Bristol-Myers Squibb, Pinceton, NJ

Copper-promoted C-N/C-O bond cross-coupling between arylboronic acids and H-N/H-O containing substrates, a complementary reaction of Suzuki-Miyaura’s palladium-catalyzed C-C bond cross-coupling, has recently emerged as an important and powerful synthetic methodology. The hallmark of this new coupling methodology is the mild conditions of the reaction, similar to the well-established condensation reactions to make the amide C-N bond – room temperature, weak base and in air. Since our initial reports, we have extended the methodology to include other organometalloids such as hypervalent arylsiloxanes and arylstannanes, in place of arylboronic acids, and general catalytic copper systems. The methodology is also applicable to N-vinylation with vinylboronic acids – the mildest method for performing N-vinylation. We would like to describe the development and mechanism of this important reaction and to contrast with Buchwald/Hartwig's palladium chemistry. Background: 1. Chan, Lam. Book chapter in “Boronic Acids” Hall, ed. 2005, Wiley-VCH, 205-240. 2. Lam, Clark, Saubern, Adams, Winters, Chan, Combs. Tetrahedron Lett. 1998, 39, 2941-2944. 3. Evans, Katz, West. Tetrahedron Lett. 1998, 39, 2936-2940. 4. Chan, Monaco, Wang, Winters. . Tetrahedron Lett. 1998, 39, 2933-2936.

(See Figure on Next Page)
273. Exploring Hetero-Annulation Strategies for Complex Alkaloid Synthesis

David Y. Gin, Memorial Sloan-Kettering Cancer Center, New York, NY

Guanidine natural products comprise an intriguing class of structurally diverse marine alkaloids. Several polycyclic guanidine alkaloids have been isolated from the sponge Crambe crambe and were found to elicit varied and potent biological responses, including antiviral, immunosuppressive, and ion channel blocking activities. Current efforts directed toward the total synthesis of members of the batzelladine and crambescidin alkaloids will be presented, focusing on novel annulation strategies for the construction of functionalized pyrimidine rings.

Plenary Lecture II: Roald Hoffmann, Cornell University

Organizer: John R. Sowa, Seton Hall University, South Orange, NJ

274. The Chemical Imagination at Work in Very Tight Places

Roald Hoffmann, Cornell University, Ithaca, NY

Diamond anvil cell and shock–wave technologies now permit the study of matter under multimegabar (i.e. several hundreds GPa) pressures. The properties of matter in this pressure regime differ drastically from those known at 1 atm. Just how different chemistry is at high pressure and the role that a chemical intuition for bonding and structure can have in understanding matter at high pressures will be explored in this lecture. I will discuss in detail an overlapping hierarchy of responses to increased density, consisting of (a) squeezing out van der Waals space (for molecular crystals); (b) increasing coordination; (c) decreasing the bond length of covalent bonds and the size of anions; and (d) an extreme regime of electrons moving off atoms and new modes of correlation. Examples of the startling chemistry and physics that emerge under such extreme conditions will alternate in this account with qualitative chemical ideas about the bonding involved.
275. Structural Effects of Interstrand Crosslinks on DNA through Molecular Dynamic Simulations

Arthur J. Campbell, Angelo Guainazzi, Orlando D. Scharer and Carlos L. Simmerling, Stony Brook University, Stony Brook, NY

Nitrogen mustards (HN2) are a cytotoxic class of bifunctional alkylating agents that form various DNA crosslinks. Among the adducts that form in the reaction of these compounds with DNA, interstrand crosslinks (ICLs) cause the greatest cytotoxicity to the cell. ICLs form covalent bridges between two complementary strands of DNA inhibiting essential processes such as DNA replication and transcription. Various DNA repair pathways, including NER, homologous recombination and translesion synthesis work together to repair ICLs, but the details of how repair is achieved are not understood. In particular, the relationship between the structure of the ICL and its repair are not known. Investigating the effect due to variations of length and charge on these ICLs may lead to a better understanding of the recognition pathways involved in crosslink repair. In this work we use computational methods to investigate and predict helical distortions caused from various ICLs.

276. Exploring Structure and Biochemistry of Nitrogen Mustard Interstrand Crosslinks through Synthetic Analogs

Angelo Guainazzi and Orlando Schärer, SUNY Stony Brook, Stony Brook, NY

Despite the importance of chemotherapeutic agents that form DNA interstrand crosslinks (ICLs) during cancer therapy, it remains poorly understood how ICLs are repaired. Present evidence suggests that while the main ICL repair pathway in mammals depends on replication and homologous recombination at least one replication-independent minor pathway exists.

The limited availability of defined ICL substrates is the major impediment to studying the ICL repair mechanisms. To overcome this limitation we have developed strategies for the de novo synthesis of different analogs of the clinically-relevant nitrogen mustard (NM) ICLs to provide tools for biochemical studies. In our approach two “crosslink precursors” with reactive aldehyde groups are incorporated into complementary strands of DNA using solid phase synthesis and crosslink formation is induced by a double reductive amination.

In this project we will expand the scope of this strategy by synthesizing new crosslink precursors and using them to generate a range of relevant NM ICLs analogs by means of different amines. Moreover, we will use NMR techniques to structurally characterize various NM ICL mimics. The combination of chemical and structural approaches will provide well defined and well characterized substrates for biochemical and cell biological studies of ICL repair.

277. The Relationship Between the Ionic Structure and Viscosity in the Room-Temperature Ionic Liquids

Hualin Li, Murfat Ibrahim, Ismail Ageremi and Mark Kobrak, Brooklyn College and The Graduate Center of the City University of New York, Brooklyn, NY

We investigate the relationship between the ionic structure and the viscosity in Room-Temperature Ionic Liquids (RTILs). We build on earlier work and derive an ionic property we call the Charge Lever Moment (CLM). We compare calculation values and the CLM to experimental viscosities of RTILs, and
show a correlation between the two quantities. We also explore the important of ionic rigidity to viscosity.

**278. Synthesis of Imidazolium and Pyridinium Ionic Liquids for Toxicity Studies**

Xing Li¹, Jinhee Gwon¹, James F. Wishart², Catherine McEntee³ and Sharon Lall-Ramnarine¹, (1)Queensborough Community College, CUNY, Bayside, NY, (2)Brookhaven National Laboratory, Upton, NY, (3)Kingsborough Community College, Brooklyn, NY

Ionic liquids (ILs) are salts with melting points below 100 degree Celsius. A lot of attention has been drawn to the ILs lately because of their relative non-volatility, non-flammability, wide liquid range, and high conductivity. These properties make ILs very good candidates as potential green solvent alternatives to volatile organic solvents. We have successfully prepared a series of halide salts based on 1-methylimidazole and pyridine. The alkyl halides used to produce the corresponding quaternary ammonium halide salts include 1-bromobutane, 1-bromopentane, 1-bromooctane, 1-bromodecane, 1-bromododecane, 1-bromooctadecane. These salts were purified by washing with ethyl acetate and diethyl ether and converted to ILs bearing the phosphate and bis(trifluoromethylsulfonyl)imide anions. These liquids were prepared in different grades of purity by varying the temperature of the halide salt synthesis. Degree of color and reaction temperature was used to designate purity level. The structures of the salts were confirmed using H-1 and C-13 NMR. The grades of purity were detected by using UV-Vis and fluorescence spectroscopy. The liquids were screened for their toxicity to a variety of microorganisms. Preliminary results indicate that bacterial growth inhibition caused by ILs is dependent on concentration, alkyl chain length and bacterial strain. It was also observed that alkyl chain length affects mycelial growth. This is part of a larger collaborative research project where other similar series of ionic liquids will be prepared and tested. This work was supported in part at BNL by the U. S. DOE Office of Basic Energy Sciences under contract # DE-AC02-98CH10886.

**279. An Electrospray Ionization Guided-Ion-Beam Tandem Mass Spectrometer for Studying Gas-Phase Biological Ion-Molecule Reactions**

Fang He, Yigang Fang and Jianbo Liu, Queens College of the City University of New York, Flushing, NY

An electrospray ionization (ESI) guided-ion-beam tandem mass spectrometer (GIB MS) was developed for studying gas-phase biological ion-molecule reactions, such as reaction dynamics of amino acids and small peptides with reactive oxygen species. This poster describes the design, construction and operation of this instrument, including the development of a vacuum control system. Biomolecular ions are generated by ESI and introduced into the instrument through a heated capillary and a skimmer. Ions pass into a hexapole ion guide for collisional cooling and focusing, and then are mass-selected by a reactant quadrupole mass filter. Mass-selected ions are guided into an octopole ion guide surrounded by a scattering cell containing the neutral reactant gas. Ions are scattering from the neutral reactant gas at controlled collision energy. Product ions and the remaining reactant ions are collected by the octopole ion guide, and extracted into the product mass filter for mass analysis and detection. The instrument consists of five high vacuum chambers. A vacuum control and interlock system was developed for automatic control of various gates, foreline valves, roughing valves, pumps and pressure gauges. The system also provides various protective safety interlocks and alarm system which respond to failures of cooling water, compressed air, electrical power, etc. Results are presented to illustrate the application of this instrument for ion-molecule reactions of protonated tyrosine cations.
280. Synthesis of Pyrrolidinium Ionic Liquids for Toxicity Studies
Jinhee Gwon1, Xing Li1, James F. Wishart2, Catherine McEntee3 and Sharon Lall-Ramnarine1,
(1)Queensborough Community College, CUNY, Bayside, NY, (2)Brookhaven National Laboratory, Upton, NY, (3)Kingsborough Community College, Brooklyn, NY

Attention given to the field of ionic liquids (ILs) has been increasing because of their potential uses as green solvent alternatives, due to their relative non-volatility, non-flammability, wide liquid range and high conductivity. However, first it is critical to know and understand their toxic effect on the environment. There have not been many studies that showed the relationship between the purity of the ILs and their toxic effects. A series of halide salts based on N-methylpyrrolidine was successfully prepared in different levels of purities determined by color and achieved by temperature variation. N-methylpyrrolidine was reacted with alkyl halides including 1-Bromobutane, 1-Bromopentane, 1-Bromodecane, 1-Bromododecane, and 1-Bromoocctadecane to produce the corresponding quaternary ammonium halide salts. The structures of the salts were confirmed using H-1 and C-13 NMR spectroscopy. The salts were then converted to ionic liquids bearing the phosphate (PO43-) and bis(trifluoromethylsulfonyl)imide (NTf2) anions. Purity was also tested using fluorescence and UV Visible absorbance spectroscopy. This is a part of a larger collaborative research project where other similar series of ionic liquids were prepared and screened for their toxicity to a variety of microorganisms. Preliminary results indicate that bacterial growth inhibition caused by ILs is dependent on concentration, alkyl chain length and bacterial strain. B. subtilis appears to be more suitable for this type of analysis. It was also observed that alkyl chain length affects mycelial growth. This work was supported in part at BNL by the U.S. DOE Office of Basic Energy Sciences under contract # DE-AC02-98CH10886.

281. Instrument Control and Data Acquisition for a Guided-Ion-Beam Tandem Mass Spectrometer
Yigang Fang, Fang He and Jianbo Liu, Queens College, City University of New York, Flushing, NY

This poster describes the development of an ESI guided-ion-beam tandem mass spectrometer, along with instrument control and data acquisition. ESI generated ions are introduced into the instrument, and mass-selected by a reactant mass filter. Mass-selected ions are guided into an octopole ion guide, and react with neutral reactant in a scattering cell surrounding the octopole. Product ions and the remaining reactant ions are collected by the octopole ion guide, and extracted into the product mass filter for analysis. Using this instrument reaction cross section could be measured as a function of collision energy. A LabVIEW Virtual Instrument (VI) was developed for instrument control and data acquisition, with the utilization of a NI PCI-6229 multifunction analog and digital DAQ board installed in an Intel dual core PC. We use the 80 MHz timer/counters on the DAQ board for gating and event counting, and as the master clock to synchronize various outputs. One digital output is used to control the duty cycle of scattering cell on/off, and one analog output is used to set the collision energy for ion-molecule reactions. Various parameters, including voltages on electrical lens and ion detectors, are controlled by the DAQ board and could be manipulated through the VI front panel. The quadrupole mass filters are currently controlled by an Extrel Merlin controller, and an interface is being developed to integrate this controller to the LabVIEW VI.

282. Synthesis and Toxicity to Zebra Fish of Mono- and Diammonium Phosphate and Bis(trifyl)Imide Ionic Liquids
Ayisha Munawar1, Ankita Parikh1, Hughton Walker2, Jasmine Hatcher2, Xing Li1, Sofya Penkhasova2, Kijana Kerr1, Pokay Ma2 and Sharon Lall-Ramnarine1, (1)Queensborough Community College, CUNY, Bayside, NY, (2)Queens College, CUNY, Flushing, NY

Ionic liquids (ILs) are organic salts that melt below 100 degree celsius. Owing to their popularity in recent years as alternative solvents to volatile organic compounds (VOC’s) ILs have been receiving increasing attention. The purpose of this research is to synthesize and study the toxic effects of the
mono- and diammonium phosphate and bis(triflyl)imide ILs on zebra fish eggs. Halide salt precursors were prepared by reacting an amine with an alkylhalide bearing the desired substituent. Mono- and diammonium halide salts bearing ether, hydroxyl and alkyl substituents were prepared this way. The halide salts were converted to the desired IL by metathesis with a metal salt or protic acid of the desired anion. The ILs were purified using different techniques depending on the anion. The structures of the ILs were confirmed using 1H, 13C and 31P NMR. The toxicity of the ILs was tested by immersing freshly collected zebra fish eggs into aqueous solutions of ILs of varied concentrations. The development of the eggs was studied over a period of one week and was used to gauge the toxicity of the IL. Preliminary results indicate that ILs with longer alkyl chains tend to be more toxic than those with shorter chains. This project was supported by PSC-CUNY award # 69605-00 38.

283. Nitroxide-Mediated Polymerization of Poly(ethylene glycol) Acrylate Comb-Like Polymers

Milan Maric and Benoit Lessard, McGill University, Montreal, QC, Canada

Poly(ethylene glycol) methyl ether acrylate (PEGA) nitroxide-mediated polymerizations in bulk were studied at two temperatures (115°C and 125°C) and at concentrations of 5.2-20.7 mol% of added free nitroxide (N-tert-butyl-N-[1-diethylphosphono-(2,2-dimethylpropyl)] nitroxide (SG1) relative to the unimolecular initiator 2-[N-tert-butyl-2,2-(dimethylpropyl)-aminoxy] propionic acid (BlocBuilder”). Polymerizations were more controlled at 115°C with SG1/BlocBuilder” ratios from 10.4-20.7mol% giving polymers with polydispersity indices ($M_n/M_w$) as low as 1.17 and a linear increase in number average molecular weight $M_n$ with conversion up to about 50%. Chain extension of a comb-like poly(PEGA) ($M_n=8.1$ kg/mol, $M_w=1.20$) with styrene in 50 wt% dimethylformamide (DMF) at 115°C indicated sufficient “livingness” of the poly(PEGA) chain ends as observed by the linear increase in $M_n$ and monomodal molecular weight distribution as determined by gel permeation chromatography ($M_n=62.3$ kg/mol and $M_w=1.53$). 1H nuclear magnetic resonance confirmed the final block copolymer composition to be 23 mol% EG and differential scanning calorimetry revealed two distinct glass transition temperatures $T_g$ indicative of the PPEGA ($T_g=-70^o$C) and PS ($T_g=98^o$C) segments.

284. Synthesis of Mixed-Valence Compounds with Metal-Metal Bonds

Amy Schauss and Jack Lu, University of Houston-Clear Lake, Houston, TX

The diversity of the structures and new topology discovered in metal-organic compounds are attributed to the selection of metal centers and organic compounds. Numerous recent reports demonstrated that copper ions form complexes with organic ligands with versatility, in which copper atoms have +1, +2, mixed-valence state, and/or Cu-Cu bonds. Although mixed-valence copper coordination compounds may be generated from either oxidation or reduction reactions of copper ions, most known examples were obtained from the reduction route. The oxidation reaction routes for the synthesis of new mixed-valence compounds with metal-metal bonds will be presented.

285. Determination of Methamphetamine and Amphetamine in Urine Using Ionic Liquid Based Headspace Solid-Phase Microextraction (HS-SPME) and Gas Chromatography-Mass Spectrometry (GC-MS)

Yi He, Jeremy Pohl and Stephanie Petch, John Jay College, City University of New York, New York, NY

A simple sample preparation method for determination of methamphetamine (MA) and its major metabolite, amphetamine (AP), in urine was developed using ionic liquid based headspace solid-phase microextraction (HS-SPME) and gas chromatography-mass spectrometry (GC-MS) with electron impact ionization working at selected ion monitoring mode. SPME fiber was prepared by coating ionic liquid (IL) on a bare silica fiber. Factors that affect extraction performance, including the base used, the concentration of the base, salt concentration, stirring rate, extraction
temperature, and extraction time were investigated and optimized. The extraction performance of IL based SPME has been compared with the commercially available SPME fiber with 100um and 7um polydimethylsiloxane (PDMS) coating. The feasibility of the method was demonstrated by analyzing spiked urine samples donated by volunteers.

286. Properties of DABCO Containing Ionic Liquids
Kijana Kerr1, Marie Thomas2, Gopal Subramaniam2, James F. Wishart3 and Sharon Lall-Ramnarine1,
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We report here on the synthesis of DABCO (diazabicyclo[2.2.2]octane) containing ionic liquids (ILs) using thermal and microwave assisted reaction methods. ILs were synthesized using several alkyl halides including ethoxyethyl, ethoxymethyl, hydroxypropyl and butyl. Structures were confirmed using H-1 and C-13 Nuclear Magnetic Resonance (NMR) spectroscopy. The halide salts were converted into NTf2 ILs using anion exchange. These new ILs were characterized for their thermal properties using Differential Scanning Calorimetry (DSC). NTf2-containing ILs melt at lower temperatures than halide-containing ILs, as expected. Many of the disubstituted compounds are high-melting salts and not ILs. However some species such as the dihydroxypropyl NTf2 IL exhibits melting points below 100 °C. This work was supported in part at BNL by the U. S. DOE Office of Basic Energy Sciences under contract DE-AC02-98CH10886 and the Louis Stokes Alliance for Minority participation.

287. The Quantitative Determination of the Minimum Inhibitory Concentration of Silver Ions to Bacterial Growth
David E. Marx and John J. Mercuri, The University of Scranton, Scranton, PA
The antimicrobial use of silver has had a remarkable history, beginning with the use of silver nitrate by the Romans as a medicinal agent and extending to the present time, where silver is employed in a wide range of antimicrobial consumer products and wound care dressings. While the efficacy of silver ion as an antimicrobial agent has been firmly established, little reliable data concerning its minimum inhibitory concentration (MIC) has been collected. In this study, we demonstrate the use of modified Szybalski density gradient plates coupled with silver analysis by Graphite Furnace Atomic Absorption Spectrometry to determine quantitatively the MIC of silver ion for Escherichia coli, Pseudomonas aeruginosa, Methicillan-Resistant Staphylococcus aureus, Staphylococcus epidermidis, and Actinobacter baumannii.

288. Preparation of Some Novel Dithioether-Diketones and Chelating Derivatives of Them
Molly A. O’Connor and Anthony W. Addison, Drexel University, Philadelphia, PA
Novel alkyl- and aryl-bridged dithioether-diketones were prepared via an N,N,N-triethyl-N-(propan-2-onyl)ammonium ion and several dithiols. These dithioether-diketones were then used as templates to make derivatives with other N, O, and S donor groups. Some ortho-functionalized anilines formed polydentate metal-chelaters with N2O2S2-donor sets. Structural, spectroscopic, and electrochemical data for these ligands and complexes will be presented.

289. Carbon Nanotubes Filled with Copper Nanoparticles
James Giammarco1, Patricia Valenzuela1, Sebastian Oswald1, Vadym Mochalin1, Farhad Forohar2 and Yury Gogotsi1, (1)Drexel University, Philadelphia, PA, (2)NSWC, Indian Head Division, Indian Head, MD
Over the past decade, there has been an increased interest to filling the interior of carbon nanotubes with nanoparticles for trapping gases, magnetic control of the tubes, and catalytic applications. This
study focuses on filling commercial carbon nanotubes with copper. Conventionally, suspensions or colloidal solution of nanoparticles are used for nanotube filling. In our research, we filled nanotubes with a copper salt (CuCl2) and conducted subsequent hydrogen reduction to obtain metal particles. This process helps to avoid problems with agglomeration of the metal nanoparticles in dispersion. If the metal particles in question are oxidized easily, as is the case with copper, oxides can also be reduced under hydrogen. Filling the tubes with a salt solution occurs by capillary forces. Boiling and vacuum assisted infiltration were used as two alternative filling techniques. After filling, the samples are rinsed with water to eliminate salt from the exterior of the tubes and prevent particle formation on the outer surface. SEM and TEM images show that the interior walls of carbon nanotubes are covered with a thin layer of copper chloride. XRD results confirm that copper chloride is present. After reduction under hydrogen atmosphere at 300°C for 90 min, XRD shows no copper chloride peaks and indicates presence of metallic copper.

290. Synthesis and Characterization of Transition Metal Complexes of Pendant Arm Macrocycles and Tripodal Ligands

Savitri Chandrasekhar, Rick Chen, Jeff Chan and Amanda Lee, University of Toronto Scarborough, Toronto, ON, Canada

Tripodal ligands and macrocyclic ligands have been known to stabilize less common oxidation states e.g. Ni (III) and Pd (III) have been stabilized in complexes containing macrocyclic ligands. Both macrocyclic and tripodal ligands are known to mimic biologically active molecules, in that, they provide a strained geometry for the metal ions mimicking the entatic state. In the present study a mixed donor macrocycle containing aza and oxa donor ligands has been successfully synthesized. Ni(II) and Pd(II) complexes of this ligand have been synthesized and characterized by IR, UV-visible spectroscopy, elemental analysis and electrospray mass spectroscopy. Both complexes have been shown to have syn conformation showing interaction of metal ions with the axial ligands as opposed to the normal anti conformation found in many of these complexes. The Ni(II) complex of a pendant arm macrocycle has been synthesized and characterized and the results will be presented.

291. Ruthenium(II) Complexes of Some Tripodal Amine Ligands

Gordan T. Reeves1, Anthony W. Addison1, Vitaly V. Pavlishchuk2, Allen Hunter3 and Matthias Zeller3, (1)Drexel University, Philadelphia, PA, (2)Institute of Physical Chemistry, Kiev, Ukraine, (3)Youngstown State University, Youngstown, OH

Several new Ru(II) complexes of tris(2-aminoethyl)amine (Tren) and diethylenetriamine (Dien) have been prepared using Ru(PPh3)3Cl2 and (Me4N)2[Ru(Phen)Cl4] as starting complexes. The Tren-based complexes are significant in that only one other Ru(II)-Tren complex has been reported previously. The reaction of Tren or Dien with Ru(PPh3)3Cl2 leads to the formation of either the [Ru(Tren)(PPh3)Cl]Cl or the [Ru(Dien)(PPh3)Cl2] complex, of which the latter then reacts further with a heterocyclic diimine (N–N) ligand to yield [Ru(Dien)(PPh3)(N–N)Cl2]. Addition of Tren or Dien to solutions of the (Me3N)2[Ru(Phen)Cl4] complex replaces the coordinated chlorides with the N-donor ligand, forming [Ru(Tren)Phen](ClO4)2 and [Ru(Dien)(Phen)Cl]Cl respectively. All of the complexes are luminescent with several emitting in the visible region. Their redox chemistry shows a single-electron Ru(II)→Ru(III) oxidations over a wide range of potentials. Additionally, we have synthesized two Ru(II) complexes from the heterocromatic Tren analogue, tris(1-ethyl-2'-benzimidazoly)methylamine (EtNTB). Due to the alkylation of the EtNTB ligand, benzimidazolate-based NTB-bridging is thwarted, and so [Ru(EtNTB)(Phen)](ClO4)2 and [Ru2(EtNTB)2(mu-Cl)2]Cl2 are formed.
292. Colloidosomes: "Smart" Materials for Biomedical Applications

Rachel Rosenberg, Drexel University, Philadelphia, PA

Colloidosomes have a wide range of applications including cell encapsulation, imaging and diagnostics, and drug delivery. They consist of an aqueous polymer core with a shell of colloidal particles adsorbed to the surface by electrostatic interactions. The distribution and packing of the colloidal particles determine the pore size. Poly (N-isopropylacrylamide) (PNIPAAm) and alginate hydrogels are used as two different aqueous gel scaffolds, synthesized via microfluidics. The shells consist of packed polystyrene spheres which are functionalized to yield the appropriate charge. Temperature and pH sensitive polymers allow the packing of the colloidal particles to be tuned. Modifying the pore size can be particularly useful in drug delivery applications that require localization.

293. Organogold (III) Iminophosphorane Complexes and Study of Their Cytotoxicity against Solid Tumor Cells

Neha Shaik, Idline Augustin and Maria Contel, Brooklyn College and the Graduate Center, The City University of New York, Brooklyn, NY

Cancer chemotherapy is dominated by platinum-based compounds that are currently the world's best-selling anticancer drugs. However, platinum compounds have drawbacks that include side effects and intrinsic or acquired resistance. There is a renewed interest in the study of gold compounds as an alternative to platinum drugs. While the mechanism of action for platinum relies on covalent binding to DNA purine bases, it seems that gold compounds behave in a different way (most plausibly by interference with mitochondrial functions).

We present here the synthesis of organogold(III) compounds containing iminophosphorane ligands with a pincer C,N backbone (figure 1) that stabilize the oxidation state III and a phosphine fragment very useful to study reaction mechanisms by $^{31}$P NMR. Reactions of the precursor $[\text{Au}\{k_2-C,N-C_6H_4(PPh_2=N(C_6H_5)-2}\}Cl_2]$ (1) with dithiocarbamates (Na$S_2$CNR$_2$; R = Me, Ph) and NaPF$_6$ afford stable cationic compounds $[\text{Au}\{k_2-C,N-C_6H_4(PPh_2=N(C_6H_5)-2)(S_2CNR_2)\}]PF_6$ (2, 3) that are soluble in dimethylsulfoxide. Water-soluble compounds of the type $[\text{Au}\{k_2-C,N-C_6H_4(PPh_2=N(C_6H_5)-2)Cl(PR_3)\}]BF_4$ (4, 5) have been also prepared by reaction of 1 with AgBF$_4$ and a water soluble phosphines (P(C$_6$H$_4$SO$_3$Na)$_3$; PR(C$_6$H$_4$SO$_3$Na)$_2$; R = Cp).

![Figure 1](image)

Preliminary studies on the cytotoxicity of these compounds against cis-platin sensitive and resistant cell lines will be presented along with studies on their interaction with DNA.

294. Ground State Association of Benzo[B]Fluorenone with Ethanol and Trifluoroethanol

Aaron Halpern and Brian Williams, Bucknell University, Lewisburg, PA

Emission from the solvatochromic fluorophore benzo[b]fluorenone (BF) is much less quenched by alcohols than emission from the structurally related ketone 9-fluorenone (9-FL) [1]. Previously, the quenching effect of alcohols on 9-FL has been examined in terms of a model scheme involving hydrogen bonding to 9-FL in both ground and excited states. Equilibrium constants for 9-FL association with alcohols in ground and excited state 9-FL for some binary mixtures have also been reported. Here, we investigate the effect of ethanol and 2,2,2-trifluoroethanol on BF absorption in binary cyclohexane, methylene chloride, and acetonitrile mixtures. Equilibrium constants for the association of ethanol and trifluoroethanol with ground state BF in these solvents were then determined where possible.


295. Butterfly Wings, Crustacean Shells, and Squid Pens: Studies on Chitin Sources

Jessica D. Schiffman and Caroline L. Schauer, Drexel University, Philadelphia, PA

Chitin, a high molecular weight (MW) linear polymer composed of N-acetyl-D-glucosamine (N-acetyl-2-amino-2-deoxy-D-glucopyranose) units linked by β-D (1→4) bonds is the second most abundant organic material after cellulose. Chitosan is the N-deacetylated derivative of chitin. Both of these biopolymers are intrinsically biocompatible and biodegradable, have aqueous adsorption capabilities, and chelate metals. Depending on the source of extraction, chitin exists in two crystalline polymorphic forms. Crustacean shells and butterflies contain α-chitin, whereas the polymorph β-chitin is more rare and found in squid pens. Electrospinning these biopolymers or biopolymer-composite mats could create flexible, affordable filtration membranes sensitive to metal ions or gas permeation. We have electrospun practical grade α-chitin as well as practical grade, low MW, medium MW, and high MW α-chitosan into non-woven mats. Two methods of cross-linking through the amine groups of chitosan were also employed to obtain an improved chemical stability. Chemical, morphological, and crystallinity analyses have been conducted utilizing FTIR, SEM, and XRD. To determine the metal absorption and mechanical properties of the mats, EDS and Kawabata microtensile testing were utilized, respectively. Despite the initial success with α-chitin, β-chitin has yet to be electrospun. Conductivity and rheology analysis, as well as the previously mentioned techniques are utilized to investigate and understand the differences between the polymorphic forms.

296. Arene-Ru-Chloroquine Complexes as Potential Antimalarial Agents

Chandima S.K. Rajapakse¹, Alberto Martinez², Becky Naoulou² and Roberto A. Sanchez-Delgado², (1)Brooklyn College, CUNY, Brooklyn, NY, (2)Brooklyn College, Brooklyn, NY

Malaria is one of the most important parasitic diseases causing over nine million deaths annually. Chloroquine diphosphate (CQDP) was the most widely used drug against malaria but resistant strains of the parasite (Plasmodium falciparum) have emerged throughout the world. Complexation of CQ to metals has been previously shown by us to enhance the activity against resistant strains of the malaria parasite, for instance [RuCl₂(CQ)]₂.

Here we report the synthesis of new Arene-Ru-Chloroquine complexes and their characterization by NMR techniques and DFT calculations. The new complexes are heme aggregation inhibitors, and intercalate in DNA. Preliminary results indicate antimalarial activity and the main mechanism of action is most likely related to the heme aggregation inhibition activity and the lipophilicity of the metal complexes.
297. Greening the Organic Chemistry Laboratory at Widener University
Kaitlyn Gerhart and Loyd D. Bastin, Widener University, Chester, PA

In the past, the problem of waste disposal in the sophomore organic chemistry laboratory was combated by using microscale experiments. While the microscale approach reduces the amount of waste generated, it introduces several pedagogical problems. First, the microscale experiments require "special" glassware to deal with the small amounts of material used and produced in an experiment that are not always similar to comparable mini- and macroscale equipment. Second, the microscale experiments routinely result in little or no yields. This result is disheartening to students and leads to an unnecessary anxiety in the organic chemistry laboratory. Third, rescaling a reaction does not fully address the issue of hazardous waste disposal or the need for environmentally friendly methods. Therefore, in order to teach students about alternative solvents, reagents, and reactions, we redesigned the organic chemistry I laboratory. Here we describe our process of redesigning the organic chemistry I laboratory from a microscale into a green organic chemistry laboratory. Our approach involved an investigation of the current labs performed in the organic chemistry I and II laboratories to determine their pedagogical value. We also discussed the skills/knowledge that students should obtain from organic chemistry I and II laboratories with science faculty. From this information, we outlined the knowledge/skills that a student should gain in an organic chemistry laboratory and searched the current literature for "green" organic chemistry labs that met the developed course goals. We also developed a three step inquiry-based, green synthesis as a capstone experience for the organic chemistry I laboratory.

298. Mechanism of Antimalarial Action of the Ruthenium(II)-Chloroquine Complex [RuCl2(CQ)]
Alberto Martinez, Chandima S.K. Rajapakse, Becky Naoulou and Roberto A. Sanchez-Delgado, (1)Brooklyn College, Brooklyn, NY, (2)Brooklyn College, CUNY, Brooklyn, NY, (3)Brooklyn College and The Graduate Center, CUNY, Brooklyn, NY

The mechanism of antimalarial action of the ruthenium-chloroquine complex [RuCl2(CQ)]2 (1), previously shown by us to be active against CQ-resistant strains of \textit{P. falciparum} and \textit{P. berghei}, has been investigated. This compound is stable in aqueous solution, binds to hematin and inhibits aggregation to \(\beta\)-hematin at \(pH \sim 5\) to a slightly lower extent than chloroquine diphosphate (CQDP); more importantly, the heme aggregation inhibition activity of complex 1 is significantly higher than that of CQ when measured at the interface of n-octanol/aqueous acetate buffer mixtures under acidic conditions modeling the food vacuole of the parasite. Partition coefficient measurements confirm that complex 1 is considerably more lipophilic than CQ in n-octanol/water mixtures at \(pH \sim 5\). This suggests that the principal target of complex 1 is the heme aggregation process, which has been recently reported to be fast and spontaneous at or near water/lipid interfaces. Furthermore, the activity of complex 1 against CQ-resistant strains of \textit{P. falciparum} is probably related to its greater lipophilicity, in line with previous reports indicating a lowered ability of some membrane proteins to promote the efflux of highly lipophilic drugs. The metal complex also interacts with DNA by intercalation, to a comparable extent and in a similar manner to uncomplexed CQ and therefore DNA binding does not appear to be an important part of the mechanism of antimalarial action in this case.

299. Incorporation of Cisplatin, Carboplatin and Oxaliplatin into a Trinuclear Iron-Platinum Intervalent Charge Transfer Complex: Options for the Photochemical Delivery of Drug to Targeted Sites
Kate Keets and Andrew Bocarsly, Princeton University, Princeton, NJ

Cisplatin is a highly effective and widely used chemotherapeutic treatment with severe negative side effects. Incorporation of the drug into the trinuclear intervalent charge transfer complex \([\text{L2(CN)}2\text{FeII}-(\text{CN})-\text{PtIV(Cl2(NH3)2})(\text{NC})-\text{FeII(CN)2L2}]^{2+}\) (\(\text{L= 2,2'-bipyridine or 1,10-}

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phenanthroline) allows for the release of cisplatin upon irradiation into the IVCT band of the trinuclear complex. Thus, these trinuclear compounds can be used as molecular masking agents for drug delivery, minimizing side effects. Complexes containing the second and third generation platinum drugs carboplatin and oxaliplatin have also been synthesized. Excitation of the broad absorption band ranging from 460 to 500nm in these complexes results in complex degradation and the photoproducts \([\text{FeIIIL2(CN)2}]^+\) and \([\text{PtII(NH3)2(OH2)2}]^2+\). Photoproduct identity has been obtained using IR spectroscopy and cyclic voltammetry.

300. **Parvalbumin in Fish Muscle: Cation Binding Properties and Its Role in Muscle Relaxation**

Mohit Sirohi, Steven Youseff, Kristen Sands, David Coughlin and **Loyd D. Bastin**, Widener University, Chester, PA

Parvalbumin, a myoplasmic protein with multiple isoforms in fish muscle, is a low molecular weight protein (9-11 kD) that appears to aid in relaxation from contraction. Parvalbumin aids in relaxation by binding free Ca\(^{2+}\), which reduces the intracellular concentration of the ion. Since Ca\(^{2+}\) plays a necessary role in contraction by binding to the myofibrillar protein troponin, a decrease in its intracellular concentration will result in relaxation of the muscle fiber. Mechanics measurements have shown that there is a correlation between muscle relaxation and the total amount of parvalbumin as well as the relative expression of the two isoforms (Parv1 and Parv2) in a variety of fish including sheepshead and rainbow trout. Muscle with relatively high relaxation rates expresses more parvalbumin and relatively more of the Parv2 isoform. These physiology results suggest that there are differences in the cation binding properties of each isoform. Since parvalbumin is bound to Mg\(^{2+}\) in its native state, Mg\(^{2+}\) ions must dissociate for parvalbumin to bind Ca\(^{2+}\) ions. Therefore, the dissociation rate for Mg\(^{2+}\) is believed to determine the physiological properties of parvalbumin and its ability to aid in relaxation. To test these suggestions we are studying the Ca\(^{2+}\) and Mg\(^{2+}\) binding characteristics of parvalbumin isoforms in several fish. Here we report on our isolation and characterization of parvalbumin isoforms from sheepshead (*Archosargus probatocephalus*), rainbow trout (*Oncorhynchus mykiss*), scup (*Stenotomus chrysops*), and dogfish shark (*Squalus acanthias*).

301. **Trinculear Iron-Platinum Complexes as Chemotherapeutic Agents: Increasing Water Solubility**

**Amanda Tricarico** and Andrew B. Bocarsly, Princeton University, Princeton, NJ

Cisplatin is a leading chemotherapy agent; however its effectiveness is limited by its severe side effects. Photoreducible complexes incorporating cisplatin, of the general formula \([L_2(CN)_2\text{FeII}-(CN)\text{-PtIV}-(Cl_2(NH_3)_2)-(NC)\text{-FeII(CN)L}_2]^{2+}\) (where \(L=2,2'\)-bipyridine or 1,10-phenanthroline) have been synthesized. These complexes contain an intervalent charge transfer band that when irradiated with visible light undergo a charge transfer reaction forming cisplatin. These complexes can act as masking agents for photoaction therapy as a way to decrease side effects of cisplatin treatment. However, these complexes have limited solubility in water. In order to increase water solubility, substitution of the 2,2'-bipyridine or 1,10-phenanthroline ligands is undertaken. Systems containing 2,2'-bipyridine-5-carboxylic acid or bathophenanthrolinedisulfonate as ligands are evaluated as potential chemotherapeutic agents.

302. **Light Activated De Novo Proteins Using Phthalocyanines**

**Andrew C. Mutter** and Ronald L. Koder, The City College of New York, New York, NY

Phthalocyanines (PC) have long been used for their photophysical properties namely as dye stuffs due to their high molar absorptivities. Due to their colorful nature PC have been the center of research into their photochemistry, this has lead to specific interest in PCs as agents for photo-induced electron transfer. In order to obtain control over these properties the PCs must be isolated in order exclude aggregation of the PCs. Utilize the tools of protein design to construct a scaffold for
precise control of PC derivates their properties can be exploited and modular protein designs can be made and inserted into natural or designed protein systems. Reengineering a previously designed maquette protein that binds two heme molecules, we have designed a scaffold that can bind either heme or phthalocyanine derivates. In experiments, we have been able to bind iron phthalocyanine and ruthenium phthalocyanine in the same protein with positional control. This construct has also been used to make mixed species of one heme and one PC in order to demonstrate light-activated charge transfer. The ultimate goal lies in biomaterials which utilize the photochemistry of PCs in solar energy conversion and light-gated ET wires..

303. Electrocatalytic Reduction of Carbon Dioxide with Dibenzotetraaza[14]

**Annulene-Coated Platinum Electrodes**

**Daniel J. Dooley**¹, J. Faye Rubinson¹ and Richard Hotz², (1)Georgetown University, Washington, DC, (2)College of Mount St. Joseph

Dibenzotetraaza[14]annulenes (DBTAAs) have the potential for application in a variety of fields, including catalysis and chromatography. These macrocyclic ligands are characterized by their ability to effectively bind transition metals, making them useful candidates for electrocatalytic reduction of carbon dioxide. Platinum electrodes coated with a polymer of the Me2[(p-t-butyl)Ph]2N4-Co complex have been created using cyclic voltammetry in acetonitrile, facilitated in some trials by copolymerization with poly-3-methylthiophene. These modified electrodes were found to be effective catalysts for the reduction of carbon dioxide, as evidenced by differences in cyclic voltammetric behavior under nitrogen and under a carbon dioxide atmosphere at ambient temperature and pressure.

304. The Properties of the Amyloid Beta Protein Coated Gold Colloidal NANOPARTICLES

**Sophia H. Hahn**, Hyunah Cho, Nicole Briglio and Kazushige Yokoyama, State University of New York at Geneseo (SUNY Geneseo), Geneseo, NY

Proteins immobilized at an interface are expected to behave differently from their counterparts in bulk solutions, and understanding the interactions of the proteins on the interface surface is crucial to designing a bio-composite device. Extensive studies of gold colloidal nanoparticles have been applied to biomaterial- nanoparticle conjugations. Our particular interest is in conformational changes in the conjugation of various sequences of the Amyloid Beta (A-Beta) protein on the surface of gold colloidal nanoparticles. A-Beta is involved in the reversible process of fibrillogenesis, a key hallmark of Alzheimer's disease. Absorption spectroscopy was utilized to identify changes in the optical properties of the gold nanoparticles coated with various A-Beta sequences (1-11, 12-28, 31-35, 1-40, and 1-42) for a pH range of 2 to 10. We have discovered that the surface net charge of the gold colloid became less negative due to the conjugation of A-Beta protein. Quite interestingly, a reversible color change was found only in A-Beta1-40 conjugated on 20 nm gold colloid between pH 4 and pH 10. This reversible process may involve a key intermediate of fibrillogenesis. Further details of pH dependence and the reversibility of A-Beta will be discussed.

305. Benzyl Imidazolium Porphyrins

**Weici Fang**, Maung-Tin Htoo Kyaw, Rukya Ali, Virginia Seng, Xiulan Wang and Alison Hyslop, St. John's University, Queens, NY

Our research interests lie in the formation of porphyrin arrays through novel binding modes to metal centers. We have recently synthesized and characterized a series of porphyrins with imidazole groups incorporated onto the porphyrin periphery. The imidazole ring affords two binding sites, with one nitrogen bonded to the porphyrin, the other one can act as a Lewis base to coordinate to metal centers. The other binding site comes from the formation of an imidazolium group and the formation
of the N-heterocyclic carbene. This will allow the carbon atom between the nitrogens to coordinate to a metal center. We will describe the formation and the electronic properties of these imidazole porphyrins.

306. Synthesis of Porphyrin-Imidazolium-Ferrocene Complexes

Jennifer Chabra, Rukya Ali, Virginia Seng and Alison Hyslop, St. John's University, Queens, NY

Porphyrins and metalloporphyrin compounds are used in energy conversion and in the molecular-scale as electronic devices. The synthesis of asymmetric porphyrin derivatives is of great interest for the development of new molecular structures. We are interested in the synthesis of porphyrin arrays in which a ferrocene moiety is attached to the porphyrin through an imidazole ring. A bis-porphyrin imidazolium compound has been synthesized and characterized, however, different routes are being taken to recreate this compound and to incorporate a ferrocene onto the imidazole ring.

307. Synthesis of Porphyrin-Heterocycle-Osmium Complexes for Use as Light Harvesting Compounds

Elissa Ramcharitar, Samantha Blondel, Carina Hernandez, Elise Megehee and Alison Hyslop, St. John's University, Queens, NY

Porphyrins and osmium metal complexes absorb light and can be used in energy transfer reactions. Having published studies on an osmium-porphyrin dyad, the first examples of an osmium attached through coordination directly to the porphyrin periphery, we are expanding this study to include modified porphyrins and modified osmium complexes. By joining together these two moieties, the ability of the complexes to absorb light and transfer the energy can be modified. We have found that the osmium portion absorbs the light and transfers the energy to the porphyrin fragment. A new series of osmium-porphyrin compounds are being synthesized and studied to explore their light harvesting capabilities. These alterations change the light absorbing and emitting properties of the complexes and will affect the energy transfer reactions that may occur.

(See Figure on Next Page)
308. Theoretical Calculations of C60 Isomers: A New Stable? or Unstable? Isomer C60[3,4,5]

John R. Sowa Jr., Jacqueline Rodriguez, Johnna Campbell and Theresa Wertheimer, Seton Hall University, South Orange, NJ

The well known and stable isomer of C60 consists of five and six-membered aromatic rings. We have successfully built computer models of two other C60 isomers; a previously reported C60[3,10] isomer and, to our knowledge, a previously unreported C60[3,4,5]. As shown below, this isomer consists of 3, 4 and 5 membered rings. Semi-empirical calculations indicate that this isomer is very unstable with a heat of formation of 5,500 kcal/mol compared with C60[5,6] which is 810 kcal/mol.

309. Does the Chain Length of Alkyl 4-Hydroxybenzoates Alter Phenolic Pka Values?

John J. Sczepanski1,2, Leopold May1, Jason R. Kinder2 and Francis B. Pedersen2, (1)The Catholic University of America, Washington, DC, (2)Hood College, Frederick, MD

The alkyl esters of 4-hydroxybenzoic acid (parabens) are widely used as preservatives and antimicrobial agents. Significant variability in Kₐ for phenol hydrogen dissociation of different alkyl 4-hydroxybenzoates has been reported in the literature. The literature also indicates no variation in Hammett’s sigma values for all esters, regardless of size. Since sigma is calculated from the dissociation constants for substituted benzoic acids (Kₓ) and of benzoic acid (Kₓ): sigma = log(Kₓ / Kₓ), it is reasonable to expect that all the parabens would have the same (or nearly the same) Kₓ. One possible explanation for the discrepancy is a solvent effect, the s data was obtained in water, but the parabens data were obtained in 95% ethanol. Previously, we presented information demonstrating that the Kₓ values for three of the parabens were different in largely aqueous media.
Limits from instrumentation and solubility have been addressed and we are reporting Ka values for additional parabens.

310. Polyaniline Nanofibers and Composites with Polymer-Stabilized Gold Nanoparticles

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The conducting polymer polyaniline can be synthesized in high yields as nanofibers with diameters less than 100 nm and lengths of up to several micrometers. Though typically carried out in acidic media, the polymerization can also take place in aqueous solution. We have investigated the formation of these materials by removing aliquots from the solution at timed intervals and then quenching the reaction with ammonium hydroxide to produce a sequence of “snapshots” throughout the synthesis. Scanning electron microscopy reveals a morphological evolution from non-fibrous to fibrous materials. This transition can be roughly correlated to UV-Vis and FTIR spectroscopy and suggests that nanofibers are not formed until the emeraldine state of polyaniline is reached. These nanomaterials have also been synthesized in the presence of polysiloxane-stabilized gold nanoparticles. The resulting nanocomposites may offer enhanced electrical conductivity and additional reactivity relative to the well-characterized conducting polymers alone. They are being explored for use as components in biosensors and other electronic devices.

311. Morphological Effects of Ring-Substitution on Polyaniline Nanomaterials

Carolina Chaves Prado and David M. Sarno, Queensborough Community College - CUNY, Bayside, NY

For decades, the conducting polymer polyaniline was known as a material with an irregular granular morphology. In recent years, methods such as electrospinning and templating on micelles have been used to impose a regular nanoscale structure on the polymer. Most notably, a simple modification of the “conventional synthesis” based on rapidly mixing the reagents has proven to be an extremely effective way of producing high yields of uniform nanofibers. We have extended this technique to mono and di-substituted analogs of aniline to examine the influence of variations in molecular structure on the nanoscale morphology of the resulting material. Scanning electron microscopy has revealed both discrete and interconnected nanofibers; nano/microspheres; and highly porous materials.

312. Effects of Commonly Used Cosmetic Industry Preservatives on Water Activity

Karen Root Caldwell¹, Michael A. Lull² and Janet R. Bass², (1)Pace University -- Westchester, Pleasantville, NY, (2)San-Mar Laboratories, Inc., Elmsford, NY

Preservatives are used in consumer cosmetic products in order to stop microbial growth and to provide product stability, thereby helping to ensure safe products for the consumer. The water activity of a system can be useful for determining microbial contamination risk and preservation factors. For example, decreasing water activities by adding water-binding agents tends to reduce microbial growth in a product. The water activity of several commonly-used industry preservatives was measured at supplier-recommended levels of preservatives using a commercially available water activity meter (Decagon Aqua Lab Series 3TE). Previously created products were also tested for water activity, and the results were compared with their USP micro-challenge test results. It was determined that most commonly-used industry preservative systems did not affect the water activity of the products they were in. Also, known water-binding agents, e.g. glycerin, affected water activity more than the preservative, itself.
313. Identification of Clinical Candidate OSI-906 as a Potent, Selective and Orally Bioavailable IGF-1R Inhibitor

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The insulin-like growth factor receptor (IGF-1R) is a transmembrane tyrosine kinase which has been implicated as a key driver in certain forms of cancers. Receptor over-expression and/or over-stimulation through either of its cognate ligands, IGF-I or IGF-II, leads to signal transduction processes which synergize to promote cellular proliferation, inhibit apoptosis, and increase cell survival. The validated role of IGF-1R in tumors such as colorectal, NSCLC and ovarian, has made it an attractive candidate for molecular targeted therapy. Here we present our efforts which led to the identification of the clinical candidate, cis-3-[8-amino-1-(2-phenyl-quinolin-7-yl)-imidazo[1,5-a]pyrazin-3-yl]-1-methyl-cyclobutanol (OSI-906) as a potent, selective and orally bioavailable IGF-1R inhibitor. Initial efforts focused on optimizing substituents at the C1 position of the imidazo[1,5-a]pyrazine core and establishing SAR around a benzyloxyphenyl moiety. Through structure based design efforts utilizing IGF-1R and IR co-crystal structures, the benzyloxyphenyl substituent was replaced with a bioactive, conformationally constrained 2-phenylquinolinyl moiety which resulted in a 10x boost in cellular potency. The progression towards OSI-906 continued with optimization of the partially solvent exposed C3 imidazopyrazine substituent, optimizing for favorable DMPK properties (i.e. blocking key sites of metabolism and incorporating functionality to improve solubility). Upon optimization of both the C1 and C3 imidazopyrazine substituents for IGF-1R potency and ideal DMPK and physiochemical properties, efforts shifted to exploring a novel imidazo[5,1-f][1,2,4]triazine core, as a potential bioisostere to the imidazo[1,5-a]pyrazine series. In summary, the general SAR around the benzyloxyphenyl substituent, progression to the quinolinyl series, optimization of the C3 substituent, and comparison of the two cores will be presented.

314. Synthesis of C-Glycosides of Glycoinositols Pseudodisaccharides

Sunej Hans and David Mootoo*, City University of New York, Hunter College, New York, NY

Glycosylinositosls make up the framework of the glycosyl phosphatidyl inositol (GPI) anchor that covalently links certain proteins to the outer leaflet of eukaryotic cell membranes. GPI’s are also attached to high mannose oligosaccharides in the cell wall of mycobacteria. Glycosylinositols are also believed to function as secondary messengers in important cellular processes, such as the mediation of insulin action. C-linked glycoinositols because of their greater hydrolytic stability and different conformational behavior compared to their native O-glycosides have attracted interest as biomechanistic probes.

The synthesis of 6 and 8, the C-glycosides of 6-O- (a-mannosyl)-myo-inositol 5 and 4-O- (2-amino-2-deoxy-b-D-galactopyranosyl)-3-O-methyl-D-chiro-inositol 7, will be presented. Pseudodisaccharide 5 is an important subunit of microbacterium cell wall, and < >7=">7">is putative insulin mediator. The key step in the synthesis of C-glycosides 6 and 8 is the formation of glycals like 4 from enol-ether via an oxocarbenium ion-alkene cyclization. Enol ether was prepared by Tebbe olefination of the ester derived from thio-acetal 1 and acid 2.

(See Figure on Next Page)
315. Single Molecule Study of Dynamics near the Glass Transition
Tobias K. Herman, Stephan A. Mackowiak and Laura J. Kaufman, Columbia University, New York, NY

We are investigating the rotational dynamics of single fluorescent molecules in supercooled liquids near the glass transition to elucidate the presumed heterogeneous dynamics in these systems. We have collected preliminary data on the behavior of rubrene, and of nile red, in glycerol. These data show a broad range of diffusion times, demonstrating that these probes experience at least a subset of the heterogeneities in supercooled glycerol. Furthermore, a subset of molecules appear to exhibit changes in dynamics, possibly related to exchange of local environment.

316. Absolute Configuration Determination of a Light Harvesting Porphyrin by Circular Dichroism Tweezer Methodology
Troy, M. McCord¹, Alicia Canzusi¹, Gloria Proni¹, Ana G. Petrovic², Nina Berova² and Teodor S. Balaban³, (1)John Jay College of Criminal Justice, New York, NY, (2)Columbia University, New York, NY, (3)Karlsruhe Institute of Technology, Forschungszentrum Karlsruhe, Karlsruhe, Germany

A circular dichroism (CD) exciton chirality method based on a host-guest chiral recognition has allowed the absolute configuration of 10,20-bis(3',5'di-tert-butyl-phenyl-13-acetyl-3-(hydroxyethyl)porphyrin, a self building light harvesting porphyrin. Computational studies have provided a strong theoretical basis for the assignment.

317. Analysis of Vitamin "C" in Fruits and Vegetables
Rana Said, Syamala Ranganathan, and Pedro Irigoyen, Queensborough Community College, Bayside, NY

Vitamin C is found in many vegetables and fruit. Its deficiency in the diet causes scurvy, a fact known very early in history. Various fruits and vegetables can give the daily recommended dose of vitamin C. In this experiment vitamin C is extracted from different fruits and vegetables. These juices are
analyzed with via High Pressure Liquid Chromatography (HPLC). The reverse phase C-18 column is used. UV absorption is used to monitor the Vitamin C content. Since ascorbic acid is stable in acidic pH range a buffer prepared from disodium hydrogen phosphate is used.

318. Analysis of Vitamin "C" in Commercial Juices

Shaun Bruney, Syamala Ranganathan, and Pedro Irigoyen, Queensborough Community College, Bayside, NY

Vitamin "C" is one of the essential nutrients whose daily recommended dose by World Health organization (WHO) is 20-30 mg. Several commercial juices indicate in their label "100% vitamin C". Do they really mean 100% of the recommended dose by WHO? In this experiment the juices are filtered and samples are injected into High Pressure Liquid Chromatography (HPLC). The amount of vitamin "C" is calculated from the standard graph obtained that uses standard ascorbic acid. The amount of vitamin C in different brands of various juices are compared using the standard graph.

319. Comparison of Hemoglobin in Thin Films and in Hydrogels Formed by Photo Initiated Polymerization on Glassy Carbon

Amos Mugweru and Christian Schnarr, Rowan University, Glassboro, NJ

Hemoglobin (Hb) was immobilized on a glassy carbon electrode using a photo-initiated polymerization of polyethylene glycol molecules and using the 1-phenyl-2-hydroxy-2-methyl-1-propanone molecule as initiator. UV-visible absorption spectra, circular dichroism (CD) and electrochemical studies indicated native three dimensional hemoglobin structure was preserved. Thin film sensors of the same protein and poliyons were also constructed using layer by layer technique and film growth was monitored using cyclic voltammetry(CV), quartz crystal microbalance (QCM). The electrochemistry from both type of sensors were compared. Reversible pairs of oxidation-reduction peaks for the two types of sensors were observed using cyclic voltammetry corresponding to the HbFeIII/HbFeII redox couples at -0.3 V vs Ag/AgCl. Catalysis of the two types of sensor assemblies is discussed.

320. Peptide Folding Dynamics and Their Implications in Neurodegenerative Diseases

Gregory Siroky, Marsiyana M. Henricus, Melanie P. Dabakis, Evan M. Smoak, Robert Tamayev and Ipsita A. Banerjee, Fordham University, Bronx, NY

Misfolding of proteins leads to insoluble protein deposits, which eventually causes neurodegenerative diseases such as Alzhiemers and Parkinsons. We are investigating the molecular basis of peptide aggregation and protein deposition. The transformation process from α-helices to β-sheet structures appear to play a major role in the fibril formation and aggregation of such peptides. In addition, their binding properties with metals and other proteins are considered to play a significant role, in particular because there is an abundance of certain metal ions in brain tissue. In lieu of this, we have studied the binding properties of β-amyloid and α-synuclein peptides with several metal ions including Pd, Ni, Cu, Zn, Mg, Al and Cd ions. The studies may further shed light on the metallochemistry associated with Alzhiemer's disease and the impact of secondary structure transformation at the molecular level. In addition to metal ions, in order to further decipher the mechanism of aggregation, we have also examined their interactions with synthetic peptide nanovesicles and nanotubes as a function of pH, and solvent polarity.

The interactions of the aggregating systems were studied using atomic force microscopy, circular dichroism, transmission electron microscopy, zeta potential measurements, dynamic light scattering and infrared spectroscopy. Our studies reveal that at certain pH, the α-synuclein can bind to the nanovesicles leading to a reduction in fibril formation. Similar studies are ongoing with the β-amyloid peptides as well.
321. Design, Synthesis and Applications of Metal Oxide Nanocomposites

Christopher P. Avanzato¹, Marsiyana M. Henricus¹, Karl R. Fath² and Ipsita A. Banerjee¹,
(1)Fordham University, Bronx, NY, (2)Queens College, Flushing, NY

The efficacy of formation of different nanocomposites of germania was examined in the presence of several biocatalysts such as sequenced peptides and specific amino acids to selectively mineralize germania. Studies related to germanium dioxide are relatively uncommon even though many properties of germanium are similar to those of silicon and thus open new avenues for investigation at the nano level. The shapes and sizes of the nanocomposites formed were found to be dependent upon the pH of the growth solutions, temperature, concentrations of the precursors and the types of precursors used. In some cases highly crystalline materials with high surface areas were formed. The growth of the nanocomposites was monitored by dynamic light scattering (DLS), transmission electron microscopy and atomic force microscopy. Calcination of the products led to highly crystalline materials. The optical properties of the nanocomposites were characterized by fluorescence, and ultraviolet-visible spectroscopy. Depending upon the types of the nanocomposites prepared, we also examined several applications of the nanocomposites such as antibacterial activities, sensors and catalysis. We have further extended our methods for preparation of diverse nanocomposites comprising of metal-doped silicate materials, alumina and titanium oxide extensively due to their enhanced properties and applications. Such new materials could be potentially useful for the development of highly sensitive sensors, catalysts and optical devices.

322. Design and Synthesis of Nanotube Bound Biocompatible Hydrogels

Evan M. Smoak and Ipsita A. Banerjee, Fordham University, Bronx, NY

In this work, peptide nanotubes have been used as templates for the growth of poly(ethylene glycol) diacrylate based hydrogels via photopolymerization. The nanotubes were covalently bound to specific dyes before the start of the photopolymerization process. In some cases, albumin was bound to the nanotube bound dyes before irradiation with visible light. When PEG is cross-linked with proteins such as albumin, the biomaterials obtained have higher biocompatibility due to reducing platelet adhesion and this property may be further enhanced on the surface of nanotubes. These characteristics along with high hydrophilicity allow the PEG-albumin-nanotube based hydrogels to be good candidates for several biomedical applications. We have explored the possibility of formation of a system based on photocuring involving BSA, different families of dye-bound nanotubes and PEG-diacrylate in the presence of visible light. The efficacy of gel formation was tested by varying the concentrations of the dyes as well as that of the PEG-diacrylate and the BSA used. Swelling studies were carried out on the products and swelling factors were obtained. The thermal properties of the gels were examined using DSC and TGA analysis. The morphologies were examined using TEM and AFM analyses. We are currently exploring this methodology for the formation of different classes of polymers as well.


Yongyi Zhang and Elena Galoppini, Rutgers-Newark, Newark, NJ

Tert-butylcalix[4]arenes were used to encapsulate organic chromophores to form Dye@Host systems bound to colloidal TiO₂ thin films via carboxylic acid anchor groups in different pH environments. The calix[4]arenes hosts are designed to insulate organic chromophores from each other to prevent aggregation effects, which could lower the efficiency of organic dye/semiconductor solar cells. The FT-IR-ATR spectra of Dye@Host systems bound to the TiO₂ films showed the binding mode of the -COOH anchor groups in different pH environments. The UV-vis absorption and fluorescence emission of Dye@Host systems in solution and bound were compared at room temperature.

(See Figure on Next Page)
324. Xanes Study of Cross Sectional Distribution of Charge States and Local Structural Environments of Iron in Porous Vycor Glass

S. Amarasinghe, D Sunil and H.D Gafney, Queens College, Flushing, NY

Photo-patterning iron oxide particles derived from Fe(CO)5 adsorption on to porous Vycor glass (PVG) yield refractive index gradient capable of guiding, focusing and diffracting light. The present study focuses on the charge state and local structure of the photo-deposited iron and their cross sectional distribution within the porous matrix. High resolution XAFS corroborate previous Mossbauer studies, which indicated Fe(0) and Fe(III). XANES pre edge analysis confirms Fe(III) and no formation of Fe(II). Elemental iron found in the PVG immediately after photolysis is concentrated in the interior of the glass. Although some elemental iron is found on the surface of the glass they are covered with a protective layer of Fe(III). This protective layer is strong enough to prevent further oxidation of elemental iron particles during the annealing process at 650C. The elemental iron found in the interior of the glass oxidized during the annealing process until the protective layer of Fe(III) is formed. The results suggest that once the Fe(III) / Fe(0) ratio reaches a critical value further oxidation is prevented.

325. Hf(IV) and Zr(IV) Porphyrins as Dyes on Semiconductor Surfaces

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The structure of Hf(IV)porphyrins and Zr(IV)porphyrins with polyoxometalates (POM) occupying the remaining coordination sites serve as models for binding these porphyrins to defect sites on oxide surfaces. Thus, Hf(IV)-tetraphenylporphyrin di-acetate, Hf(TPP)OAc2, and Zr(IV)-tetraphenylporphyrin di-acetate, Zr(TPP)OAc2, have potential applications for the sensitization of oxide band gap materials for solar cell devices. The hypothesis is that dyes such as porphyrins that complex oxophilic metals will bind better to the oxide surface via the ligated metal ion upon displacing OAc ligands, and this mode of binding will improve the efficiency of electron injection from the excited state dye to the conduction band of semiconductor. The deposition and optical characterization of these metalloporphyrins on ITO surfaces and TiO2 nanoparticles will be discussed in comparison to the absorption and emission spectra of the metalloporphyrin in solution.
326. Porphyrinoid Derivatives and Fullerene C60 for Light Harvesting Materials

Alessandro Varotto, Charles Drain and Joao Tome, Hunter College and Graduate Center of the City University of New York, New York, NY

Porphyrin and phthalocyanine derivatives are promising building blocks for the fabrication of inexpensive light harvesting materials. Porphyrins exhibit a strong absorption in the blue region of the visible spectrum, whereas phthalocyanines absorb strongly in the red. Additionally, porphyrins and phthalocyanines can form long lived separated states complexes with C60, thanks to the small reorganization energy of the latter. We herein describe the synthesis of a heterodyad which contains a porphyrin and a phthalocyanine to capture the breadth of the solar spectrum. This dyad is a supramolecular host for fullerene C60 and can form a donor-acceptor charge transfer triad useful in the conversion of solar energy.

327. The Analysis of the Interactions and Complexation of Polycyclic Aromatic Hydrocarbons and Cyclodextrin Using Electrospray Ionization Mass Spectrometry

Andrew Harron¹, Catherine Bentzley¹, Preston Moore¹, Zhiwei Liu¹, Jhenny Galan¹ and Darryl Davis², (1)University of the Sciences in Philadelphia, Phila, PA, (2)Centocore, Radnor, PA

Polycyclic aromatic hydrocarbons (PAHs) are formed during the incomplete burning of organic substances, and due to their toxicity have been classified as carcinogens. PAHs are commonly introduced into the human body via the inhalation of particulate matter that has been contaminated, and absorbed onto the surface lining of the lung tissue, leading to lung cancer. Cyclodextrins, our host complex, form complexes with a multitude of hydrophobic molecules and are ideally suited to be representative of particulate matter since they noncovalently complex with PAHs based on size and structure. An investigation of the inclusion complex formed by PAHs and particulate matter will provide essential information to the reduction of carcinogenic risks associated with the inhalation of the contaminated matter.

Our primary goals in this investigation are two fold, to measure the relative abundance of multiple PAH: CD inclusion complexes retained during the ESI process and generate an index of PAH inclusion complexes. This will provide comparative information about PAH inclusion processes. Our secondary goal is to determine the binding energies between the PAH:CD complex via ESI-MS titration and molecular modeling to gain a more comprehensive understanding of how PAHs bind to particulate matter in the gaseous phase.

The PAHs examined include Pyrene, Chrysene, Benzo(alpha) Pyrene, Phenanthracene and Antracene. In addition Alpha, Beta and Gamma cyclocodextrin will all be tested as potential complexing hosts for the PAHs. The instrumentation utilized is a Thermo LTQ Orbitrap with nano esi capability and system optimization preformed using PAH.

328. New Approach to 3,5-diamino-sugars from 4,6-dodeoxy-1, 2-O-isopropylidene-D-glycero-pent-4-enopyranos-3-ulose

Zbigniew J. Witczak, Arthur Jankowski and David Lorchak, Wilkes University, Nesbitt School of Pharmacy, Wilkes-Barre, PA

Our stereoselective enones functionalization approach was first developed by the utilization of the Michael addition of reactive thiols (SugSH) to various carbohydrate enones (levoglucosenone (1) [1-4] and expanded to iso-levoglucosenone (2) [5]) and new functional L-arabinose enone [6]. These approaches constitute a new entity in the variety of new 1, 4-, 1-2-thio-linked S-disaccharides previously not easily available as well as rare 3-amino-sugars as components of various classes of carbohydrate antibiotics. In this context, extension of our synthetic strategy to amino functionalized analogs as biological targets requires stereoselective fuctionalizations at C-3, or C-5 positions respectively. Convenient functionalizations of the C-3 keto by oximation and C-5 by 1, 4 Michael addition of hydroxylamine to C-5 of enone moiety, followed by stereoselective reduction of
oxime/hydroxylamine functionality with 9-BBN produce new 3, 5-diamino analogs. These new analogs of 3, 5 diaminosugars are convenient precursors suitable for further peptidomimetics construction that will be presented and discussed.

329. Synthesis of 3-Substituted Coumarins by the Knoevenagel Condensation Reaction

Mariam N. Israiel, New Jersey City University, Jersey City, NJ

The preparation of heterocyclic compounds under solvent-free conditions offers several key advantages and represents an important class of compounds with elevated biological activity and industrial importance. The microwave-assisted synthesis of a series of 3-Substituted Coumarins via the condensation of a series of 2-hydroxyaldehydes and dimethylmalonate on silica gel is explored.

330. The Synthesis of Biodiesel

Shane E. Smith1, Josh M. Gesford1, Kathleen M. Halligan1, Gregory P. Foy1 and Gary A. Sigel2, (1)York College of Pennsylvania, York, PA, (2)Armstrong World Industries, Lancaster, PA

The Synthesis of Biodiesel

The primary objective of this project is to synthetically convert waste oil from the York College of Pennsylvania cafeteria to biodiesel. Currently, efforts have been concentrated on analysis of the waste oil to determine water content, free fatty acid concentration and general viability. Although many procedures for biodiesel synthesis exist, the exploration of both heterogeneous and homogeneous catalysis as well as a base catalyzed two-phase synthesis will be the focus of this investigation. The short term goals include development of small-scale biodiesel syntheses, comparison of viable methodologies and ASTM analysis of the products. It is envisioned that future collaborations with engineers may lead to the development of a cost efficient large scale production.

331. New Synthetic Probes for Understanding Molecular Recognition during Olfaction

Yadi Li1, Zita Peterlin2, Stuart Firestein2, Grant Sun1 and Kevin Ryan1, (1)City College of New York, CUNY, New York, NY, (2)Columbia University, New York, NY

The nose is a sensitive chemical detector able to register a wide variety of low molecular weight hydrophobic compounds, or odorants. The sense of smell begins with the molecular recognition of the odorants by G-protein coupled receptors (GPCRs) expressed in the cellular membrane of olfactory neurons. The human genome encodes almost 400 different GPCRs but little is known about the recognition strategies they employ to detect, and discriminate among, detectable odorants. The difficulty in obtaining structural data on the membrane-bound GPCR-odorant interactions has prompted us to make novel probes designed to understand the binding preferences of a representative olfactory receptor, the rat OR-I7, whose natural ligand was previously found to be octanal. We will present the design, synthesis and initial testing of a series of conformationally restricted octanal analogs, each containing eight carbons but constrained in various ways. These compounds are designed to reveal the shape requirements of OR-I7, and to enable us to understand which octanal carbon-carbon bonds must remain freely rotatable in order to be recognized by OR-I7.
332. Formation of Novel Fused-Ring System by Rhodium-Catalyzed Cycloaddition Reactions
Yu Han Gary Teng, Joseph Jr. Kaloko and Iwao Ojima, State University of New York at Stony Brook, Stony Brook, NY

We have investigated the Rh-catalyzed [2+2+2+1] and [2+2+2] cycloaddition of triynes and cyclohexenylidynes. The cycloaddition of triynes gave 5-7-5 and 5-6-5 tricyclics and the cycloaddition of cyclohexenylidynes gave 5-7-5-6 and 5-6-5-6 tetracyclics. These ring systems are of interest due to their presence in natural products and biologically relevant compounds. The Rh-catalyzed [2+2+2+1] tricyclization of triynes took place to give tropones, which should provide a potentially useful method for the synthesis of interesting troponoids. On the other hand, the Rh-catalyzed [2+2+2] cycloaddition of triynes gave annulated benzenes, an important class of synthetic intermediates in natural product synthesis.

333. The Synthesis and Rearrangement of Carbazole Sulfonamide and Imidobibenzyl Sulfonamide to the Corresponding Sulfones
Taylor W. Meek, James R. Mckee and Murray Zanger, University of the Sciences in Philadelphia, Philadelphia, PA

The spread of HIV has become a global epidemic. The need for an effective drug to combat this disease has become increasingly important. Drugs such as AZT have been effective, but due to the virus's ability to mutate, more potent compounds are needed.

Currently in our laboratories, the preparation of a group of aminosulfones that have been shown to be active are being investigated. These sulfones are being prepared using a rearrangement of the sulfonanilide to the sulfone. Previous research had focused on derivatives of tetrahydroquinoline and tetrahydrobenzazepinone. The current work is concerned with the preparation of sulphones derived from carbazole and imidobibenzyl. Currently methods for the preparation of the sulfonanilides from the starting amines have been developed. Future work will be concerned with exploring the scope of the rearrangement and isolating the product sulphones for testing.

334. Sodium Ion Dependence and Deuterium Solvent Isotope Effect Studies of the Inhibition of Human α-Thrombin by Hirudin and NAPAP
Idiko M. Kovach, John Paul Sheehy and Krystal Dole, The Catholic University of America, Washington, DC

The dissociation constant and the second-order-rate constant for the slow-tight-binding inhibition of human α-thrombin with r-hirudin are 1.9 ± 0.4 pM and (7.14 ± 0.07) x 10^7 M^-1 s^-1 at Na^+ = I = 0.19 M (I = ionic strength) in pH 8.06, 0.05 M barbital buffer, and 0.56 ± 0.07 pM and (1.50 ± 0.06 ) x
$10^8 \text{ M}^{-1} \text{s}^{-1}$ at $\text{Na}^+ = I = 0.31 \text{ M}$ in pH 8.12, 0.02 M Tris buffer at 25.0 ± 0.1 C. These parameters are similar at $\text{Na}^+ = 0.03 \text{ M}$ and in the identically prepared deuterium oxide buffered at pD 8.6. Hirudin is the most potent thrombin inhibitor and interacts non-covalently at the exosite of the enzyme. The binding efficiency of r-hirudin is contingent upon a $\text{Na}^+$-dependent conformational adjustment of thrombin to the "fast" form, which is predominant in hemostasis. A non-covalent, slow-binding, active-site inhibitor, $\alpha$-[(2-naphthyl-sulfonfyl-glycyl)-DL-p-amidinophenyl-alanylpiperidine, (NAPAP), inhibits thrombin with a dissociation constant of $4.8 \pm 0.8 \text{ nM}$ and a second-order rate constant $(1.1 \pm 0.2) \times 10^6 \text{ M}^{-1} \text{s}^{-1}$ when $\text{Na}^+ = I = 0.19 \text{ M}$ at the pH optimum, 8.0 to 8.3, in 0.05 M barbital buffer, and 25.0 ± 0.1 C. The deuterium solvent isotope effect for the association of enzyme and inhibitor is unity, which is consistent with the non-covalent nature of the process. The determination of the buffer-independent effects of sodium and deuterium oxide on the inhibition constants are now in progress.

**335. Determination of Conditions for the Dimerization of Pokeweed Antiviral Protein**

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Pokeweed Antiviral Protein (PAP), isolated from the leaves of the Phytolacca americana plant, is classified as a Ribosome Inactivating Protein (RIP). RIPs can depurinate rRNA and therefore can inhibit protein synthesis. It has been previously seen that an inactive form of PAP exists in vivo. This form could be the result of dimerization of PAP within the plant cell, prior to viral exposure.

The appearance of a PAP dimer has been confirmed through gel electrophoresis of the fractions collected of several PAP purifications. However, once the fractions are combined in order to determine concentration of the prep, the dimer dissociates. Here we present data as to whether or not PAP will form a dimer if subject to various conditions after initial purification.

Three factors that were studied were the concentration of the protein, potassium chloride concentration in the sample buffer, and pH of the sample buffer. After varying these conditions, the resultant fractions were separated using gel electrophoresis. Here we present the results of concentration of PAP via microcon, addition of buffer of various salt concentrations, and varying the pH of the sample buffer.

**336. Expression Levels of PKC Substrates in Human Breast Cancer Cells**

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Protein kinase C is a serine-threonine kinase that is exists as a family of 12 isoforms. Numerous studies have linked the PKC isoforms to the maintenance of a malignant phenotype, however the direct substrates and downstream targets of PKC are largely unknown. Specifically, the alpha isoform is reported to be involved in the motility signaling pathways of MDA MB-231 cells, a metastatic human breast cancer cell line. This study was designed to investigate the expression levels of PKC alpha, PKC substrates and the PKC substrate MARCKS in human breast cancer cell lines. The cell lines were reported to be of varying metastatic potential. Immunoblot analysis and immunohistochemistry revealed differences in expression levels of PKC alpha, PKC substrates and MARCKS. In MDA 468 cells, the expression level of PKC alpha is low, however the expression level of MARCKS was high. These results indicate the role of the PKC isoforms in malignant phenotypes may be cell line specific. Further studies will be directed toward establishing PKC isoform profiles in each cell line and identification of substrates. The results from these studies could be useful when designing cancer drug therapies.
337. Investigations into the Conversion of Cellulose to Simple Sugars for Ethanol Production

Lisa A. Williams, York College of Pennsylvania, York, PA

Ethanol can be produced from any source that contains sugar. Traditional sources, such as sugar cane and corn, lack efficiency or proper climate for growing in certain areas of the United States. Cellulose can be converted into monomer sugars through enzymatic breakdown, but this is often inhibited by lignin. Corn stover and paulownia wood were treated with supercritical CO2 (SFE) to break down the lignin. SFE-treated samples were put through enzymatic breakdown to convert the cellulose into monomer sugars. The final sugar product was detected using High Performance Liquid Chromatography (HPLC). The increase in sugar yield, due to SFE treatment, was observed for each of the samples.

338. Study of the Characteristics of Modified PF Resins from Microwave Synthesis

Meghan M. MacIntyre, David Irwin and Adango Miadonye, Cape Breton University, Sydney, NS, Canada

The characteristics of different cresol and urea modified phenol formaldehyde (PF) resins synthesized by conventional heating and microwave irradiation were evaluated. Phenol-formaldehyde (PF), cresol-formaldehyde (CF) and urea/cresol (20, 50 and 80 percent) modified PF resins were polymerized in autoclave for three, five and seven hours with oxalic acid catalyst. The syntheses were repeated by microwave irradiation at different power levels (176.5, 315.1, 454.0, and 592.7W) for reaction times between 15 and 90 minutes. Equimolar amounts of the pre-polymerized PF and CF resins were further heated at various heating times in a post-polymerization process.

Analysis with FT-IR, GC-MS and uv/visible spectroscopy showed strong similarity in characteristics of the products synthesized by microwave irradiation and conventional methods. The concentration of unreacted phenol in the resins decreased with reaction time by 3.8% (in 3hrs), 7.4% (in 5hrs) and 22.1% (in 7hrs), while in microwave synthesis significant decrease in phenol concentration was observed, particularly at higher power levels. Similar observations were made on the modified PF resins containing different ratios of phenol to urea/cresol (80:20, 50:50 and 20:80).

The melting points and gel time of the post-polymerized PF-CF resins were lower and decreased with longer heating time. Microwave irradiation process reduced the polymerization time significantly and produced resins with shorter gel times, improved yield and similar physical and chemical characteristics. The FT-IR spectra analyses for the products showed strong similarity in their chemical structures. Resins of PF-CF post polymerization process showed significant improvement in chemical and thermal stability than the urea/cresol modified PF resins.

339. Sugarcane as An Energy Crop for USA

Sohan L. Jindal, Punjab Agricultural University, Ludhiana, India

Sugarcane is grown in the tropical regions of USA to manufacture refined sugar for human consumption. The molasses are used to manufacture ethanol by fermentation. The bagasse and sugarcane tops are used as fuel or feed for animals. Energy input and output ratio of the various operations involved in growing the sugarcane crop, harvesting, transportation, unit operations for processing of sugarcane, molasses, ethanol are discussed.
340. Engineering Fluorinated Phosphotriesterases to Detoxify Organophosphates

Peter James Baker and Jin Kim Montclare, Polytechnic University, Brooklyn, NY

Organophosphates (OPs) are a synthetic class of compounds used in a variety of functions ranging from mild pesticides to potent nerve agents. These compounds inhibit acetylcholinesterases, resulting in toxicity to a wide range of animals, including humans. Several phosphotriesterases have been reported in the literature to hydrolyze and detoxify these agents. We have globally replaced phenylalanine with para-fluoro-phenylalanine into a phosphotriesterase from Pseudomonas diminuta. The enzyme bearing the fluorinated amino acid is shown to have an enhanced thermostability as compared to the wild-type enzyme, potentially making this a useful for bioremediation application.

341. Modified Gum Acacia in Emulsions and Spraydried Flavors

Florian M. Ward and Stephen A. Andon, TIC GUMS, Inc., Belcamp, MD

Modified gum acacia derived from a plant exudate (Acacia species) was modified by esterification, covered by US Patent 6,455,512 to enhance its emulsifying properties. The functionality of the modified hydrocolloid was evaluated in oil-in-water beverage emulsions and spraydried or encapsulated flavors. Stability tests included centrifugation, particle size distribution, oil retention and sensory methods. Results indicate that the modified gum acacia is superior in performance to the traditional gum, even at lower levels of usage. As a GRAS-approved ingredient, it may be used as emulsifying agent and soluble fiber source for food and beverage applications.

342. Protection of Enzymes in Harsh Aqueous and Organic Environments

Andreas Mylonakis, Indraneil Mukherjee, Sudipto Das, Shuxi Li and Yen Wei*, Drexel University, Philadelphia, PA

A method to maintain residual enzyme activity for prolonged time in harsh aqueous media such as high pH and organic solvents is presented. As an example, horseradish peroxidase (HRP) was encapsulated into a silica matrix using the nonsurfactant templated method for producing sol-gel mesoporous materials that has been invented by our group. Fructose was used as the nonsurfactant template. The porous silica containing the enzyme was then coated with a mixture of acrylic monomer (triethylene glycol dimethacrylate) and polyethylene glycol (PEG) followed by photopolymerization and crushed to get the doubly encapsulated enzyme powder. This double encapsulation ensures that the enzyme remains active and that it is not in direct contact with the harsh media. The activity of the encapsulated HRP was tested after being submerged in ethanol, laundry detergent and buffer solution of pH=10 for 24 hours and the data were compared to those of native unprotected HRP under the same conditions. Results indicate the doubly encapsulated enzyme shows much higher activity compared to the native enzyme. Our studies suggest that this new double encapsulation system could maintain the activity of various enzymes and other biomacromolecules, while they are stored and/or used in harsh environments, and may have potential applications in health care, medicine, biosensors and biocatalysis.

343. Platinum and Palladium Metallic Solutions

Moni Chauhan and Devindra Tilakdhari, CUNY-Queensborough Community College, Bayside, NY

There is a lot of research presently on synthesis of nanosized particles because of their unique chemical and physical properties. We will present the synthesis of nanoparticles using silicone based functional molecules, which could be converted to cross linked matrixes. We are using trimethoxysilylpropyl isocyanurate for stabilizing platinum and palladium nanoparticles. Preliminary results show that this molecule could be hydrolyzed to silicone based cross linked material. Further research will focus on potential application of these particles as catalyst for various chemical transformations.
344. The NYSTAR Sponsored Center for Engineered Polymeric Materials
Andrew Auerbach, CUNY-College of Staten Island, Staten Island, NY

The Center for Engineered Polymeric Materials (CEPM) is a NYSTAR designated CART Center. NYSTAR supports technology development, innovation and commercialization leading to economic growth in New York State. NYSTAR (NYS Office of Science, Technology and Academic Research) has sponsored 15 Centers for Advanced Technology (CATs) and 2 College Applied Research and Technology Centers (CARTs) in NY State. CEPM’s mission is to foster the development of complex polymeric materials (such as nanoscale materials) and material understanding that will be of value to technology based companies in NY State. This value can take the form of job creation, increased sales, cost savings, or increased capital spending. Beyond a primary mission of fostering research in polymers, the faculty takes an active role in the education and training of professionals, industrial outreach and fostering networking among interested parties.

The Center participates in interactions with NYS industry in four ways:
- Service projects based on analytical, microscopic and physical testing capabilities
- Development projects based on defined industry needs and our novel research
- Demonstration projects based on leveraging our industry contacts and our in-house capabilities
- Consulting, market support, education, networking and industrial outreach.

This poster will review case histories of industrial interactions in project work and networking. Economic impact to NYS will be estimated. The poster will also present a list of CEPM instrumental capabilities and typical research / project work that has been done at the Center.

345. Rational Design Methodology for Porphyrin Binding Proteins
Christopher Negron, Christian Fufezan and Ronald Koder, The City College of New York, New York, NY

De novo protein design stands to usher in an era of extremely promising biomedical procedures. One of the current hurdles hindering the development of de novo protein based therapies is the implantation of high affinity cofactor binding sites, where there is particular interest in developing heme binding. The method suggested for the construction of strong porphyrin binding sites is through consensus analysis of natural occurring non-homologous porphyrin binding sites, which are related by secondary structure, and most importantly subdivided by the various rotamers of the ligated amino acid. Determination of the rotameric distribution of heme ligated helical histidines was carried out by in lab PERL scripts that analyze Protein Data Bank structures. Sequence preferences, not subdivided by rotamer, yielded very small percentages, which are in sync with previous observations. Yet, sequence preferences subdivided by rotamer yielded strikingly high percentages, with particular residues, such as a glycine in position 4 of the t73 rotamer, reaching preferences of nearly 50%. Computational modeling illuminates the structural basis for some of these findings. Molecular simulation conducted with a single histidine residue placed in the center of an all-alanine helix, agreed with the natural rotameric distribution, with very important exceptions that demonstrate the importance of complimentary residues in the heme histidine ligation, and reinforcing the structural claims of the computational model. These preferences have allowed the derivation of helical consensus for each rotamer. These findings thus promise to guide the creation of higher affinity heme and porphyrin binding sites.
346. Synthesis and Self-Assembly of Boron-Containing Block Copolymers
Chengzhong Cui, Yang Qin, Edward M. Bonder and Frieder Jäkle, Rutgers University-Newark, Newark, NJ

Here we discuss an efficient preparation of well-defined boron-functionalized styrene polymers. Atom transfer radical polymerization (ATRP) has been used to polymerize silylated styrene monomer to give poly (4-trimethylsilylstyrene) (PSTMS), which was chain-extended with styrene to obtain well defined diblock copolymers (PSTMS-b-PS). After borylated with BBr3 to replace the trimethylsilyl groups, different methods were applied to obtain a series of new boron-containing diblock copolymers, which we anticipate to be valuable new hybrid materials with many potential applications. The amphiphilic properties of the resulting anionic (borate) and cationic (boronium) diblock copolymers lead to interesting self-assembly behavior in selective solvents. Different morphologies are observed depending on the nature of the solvent and the pH in the case of the related boronic acid polymer, PSBA-b-PS.

347. When Is the Histone Protein Bound to a Chain End of a Giant DNA Molecule?
Chwen-Yang Shew and Andy Khoo, CUNY-College of Staten Island, Staten Island, NY

In gene, the giant DNA molecule forms a compact structure in the presence of oppositely charged histone proteins, through strong electrostatic interaction. The recent experiment has shown that while one histone protein binds with a giant DNA, this histone protein exhibits a greater probability to emerge at chain ends than in the middle of a DNA molecule. To better understand the electrostatic interaction involved in such a complex, a simple lattice model is developed. First, an ionic chain, consisting of identical charged monomers, is placed in the three-dimensional cubic lattice under the dilute solution without excess salt. To model the bound histone (wrapped up by DNA), one charged monomer in this ionic chain is substituted with a monomer unit of a different charge. The exact enumeration is then conducted to calculate all the possible chain conformations and to determine the thermodynamic stability of a given location of the bound histone in the model. Our finding shows that the net charge of a bound histone is essential to determine its stable position. For the bound histone containing the net charge opposite to chain monomers, the most stable location of the histone is in the middle of the ionic chain. While the net charge of the bound histone has the same sign as that of chain monomers, the histone becomes stable at near chain ends under appropriate conditions.

348. A New Catalyst for Efficient and Selective Conversion of Silanes to Silanols
Moni Chauhan*, 1, Abhshek Roka1, Alok Sarkar2 and Bhanu P. S. Chauhan*, 2, (1)CUNY-Queensborough Community College, Bayside, NY, (2)William Paterson University, Wayne, NJ

It is well known that the formation of silanols is always accompanied by generation of various side products. In this presentation, we will present a new methodology, in which silanes are converted to silanols in high yields using water as reactant and with Pt-nanoclusters as the catalyst. Our catalysts lead to selective formation of silanols, expect in some cases, where only trace amounts of side products are observed. The methodology is tolerant to several functional groups such as alkenes and alkynes, where it is noteworthy that in the presence of platinum metal complexes alkenes and alkynes are known to undergo hydrosilylation reaction. The methodology is equally effective even in the presence of bulky groups. A comparative study was also undertaken to examine and compare the catalytic activity of platinum complexes with Pt nanoclusters. The nature of the true catalytic species was investigated via TEM, UV-vis and Poisoning Studies during the catalysis and the products were confirmed using NMR and Mass Spectroscopy.
349. Synthesis and Characterization of Chromophore-Grafted Polybutadienes
Bhanu P. S. Chauhan*, Alok Sarkar, Esra Cinar and Mauhanad (George) A. Bittar, William Paterson University, Wayne, NJ

In recent years, research from our laboratory have demonstrated that metal nanoparticle polysiloxanes conjugates can provide means for marrying profitable behavior of homogeneous and heterogeneous catalysts. We have also shown that such catalysts are very selective, efficient and regiospecific. In this presentation, we will present a new and efficient route to chromophore containing-polymers which synthesized via the catalytic functionalization of polybutadiene. A through study of the chain-length property of the synthesized polymers using Gel Permeable Chromatography (GPC), IR and multi- nuclear NMR experiments such as H, 13C and 29Si NMR shows a very tight control over the side reactions and very selective loading of the chromophores.

350. Chemical/Thermal Reduction of Gold and Silver Salts: A New Route to in-Situ Nanoparticle Synthesis and Stabilization
Moni Chauhan and Maninder Kaur, CUNY-Queensborough Community College, Bayside, NY

Stable silver and gold nanoparticles are of quite importance due to their applications as antibacterial carriers, tracers and staining agents. In recent years, we have been exploring ways to mildly reduce gold as well as silver salts in presence of stabilizing agents, which may prevent aggregation during the reduction process. In this presentation, we will present our results on the synthesis as well as stabilization studies of silver and gold nanoparticles in organic and aqueous media stabilized by a new stabilizing agent TTPi [tris (trimethoxy silyl propyl) isocyanurate]. In this presentation, we will also compare our method with other known methods for synthesis and stabilization of noble metal nanoparticles. We will present our preliminary study of the kinetics of the formation of particles and analysis of the nanoparticles via SEM and TEM.

351. Synthesis and Characterization of Polystyrene Supported Borane Complexes PS-BH₂•D
Ami Doshi, Yang Qin and Frieder Jäkle, Rutgers University, Newark, NJ

Boron-containing polymers have been widely used for applications such as catalysis, sensors, flame retardants, intermediates in the synthesis of functionalized polymers and device materials. Their preparation generally involves either direct polymerization of boron containing monomers or functionalization of the polymers. We have recently developed a highly efficient method to incorporate boron into the organic polymers via controlled polymerization of silylated monomers and a subsequent silicon boron exchange reaction. The polystyrene derivative with functionalized BH₂ moieties (PS-BH₂) has been prepared from poly(4-trimethylsilyl styrene) via post polymerization modification reactions. The polymer was successfully isolated in the form of its polymeric acid-base complexes PS-BH₂•D (D = ⁵BuPy, PPh₂Me). Both polymers were fully characterized by multi-nuclear NMR spectroscopy and IR spectroscopy. Their thermal properties were studied by differential scanning calorimetry and thermogravimetric analysis. These polymers may find application as precursor to other functional polymers or as supported reducing agents.

352. High-Yield Acyclic Diene Metathesis (ADMET) Synthesis of Easily Accessible PPV Oligomers
Narayan Mukherjee and Ralf M. Peetz, CUNY-College of Staten Island, Staten Island, NY

Poly(phenylene vinylene)s (PPVs) are well known for their applications in electro-optical and photonic devices. An efficient ADMET reaction using a 4th generation Ru-based initiator (Grubbs-Hoveyda 2nd generation) afforded dimeric and trimeric units with high yields, starting from 1,4-dimethoxy-2,5-divinylbenzene. Both NMR and FT-IR showed that products have all trans-configuration at the vinylene bonds. The short methoxy side group caused pronounced differences in
solubilities, especially for oligomers larger than the trimer, allowing for high yields in trimer and dimer, which then could easily be isolated and purified. Both dimer and trimer have vinyl end functional groups, which can further be modified for future applications.

353. Formation and Characterization of Donor-Acceptor Complexes of Polyamide 6 as a Mean to Modify the Morphology and Extensibility

Hsin Ho and Nadarajah Vasanthan, Long Island University, Brooklyn, NY

Polyamide 6 (PA6) has been complexed with the Lewis acid GaCl$_3$ for the purpose of disrupting the interchain hydrogen bonded network. FTIR and 13C-NMR observations suggested that Ga metal cations form a 1:1 complex with the carbonyl oxygens of the PA6 amide groups. PA6-GaCl$_3$ film appears to be amorphous from our x-ray diffraction and DSC data. These PA6-GaCl$_3$ complex films may be drawn at low drawing speeds (0.01s$^{-1}$) to draw ratios (DR) of ~17, and then decomplexed, or regenerated, by soaking in water. Regeneration of PA6 from the complex drawn at all draw ratios yielded gamma crystal form of PA6 with high crystallinity, conformed by FTIR spectroscopy and DSC. Drawing prior to regeneration increases the crystallinity for DRs up to 17 without changing crystal form. Complexation with GaCl$_3$ offers a means to draw PA6 well beyond the levels normally obtained (DR ~ 5). Highly drawn PA6-GaCl$_3$ may be readily regenerated to yield highly crystalline PA6, which can hopefully lead to PA6 fibers with improved tensile modulii.

354. Cationic Polymerization of Norbornadiene

Narmandakh Mijid-Taylor and Ralf M. Peetz, CUNY-College of Staten Island, Staten Island, NY

The carbocationic polymerization of norbornadiene (NBD) using the 2-chloro-2,4,4-trimethylpentane (TMPCl)/ diethyl-aluminium chloride (Et$_2$AlCl) initiating system in ternary solvent mixtures (CH$_3$Cl/CH$_2$Cl$_2$/hexane) lead to soluble poly(norbornadiene)s (PNBDs) with molecular weights Mn ranging up to ~6,000 g/mol and polydispersities (Mw/Mn) down to ~1.3. Slow initiation and coupling reactions between PNBD chains were observed, but the polymerization was controlled overall. After longer reaction times, multimodal weight distributions could be observed. More control could be achieved by using proton traps, e.g. di-tert-butyl pyridine.

355. Functionalization of Si(100) Surfaces with Rigid-Rod Oligo(p-phenylenevinylene)S

Chivin Sun and Ralf M. Peetz, CUNY-College of Staten Island, Staten Island, NY

Department of Chemistry, Center for Engineered Polymeric Materials/City University of New York, Staten Island, NY, USA.

Rigid-rod-type conjugated oligo-p-phenylene vinylenes (OPVs) with terminal hydroxide (-OH) and alkyne (-C$_n$H$_{2n+1}$CH) functionality were attached to Si(100) surfaces via a covalent Si-O-C bonds. One approach involved the reaction of -OH functional oligomers with Si(100)-H and/or Si(100)-Cl functionalized surfaces. Subsequent reaction of the Si(100)-OPV-OH surface with p-tolyl isocyanate produced urethane containing monolayers in a "click chemistry" reaction. A second approach involved the synthesis of Si(100)-OCH$_2$CH$_2$N$_3$ functionalized surfaces starting from the Si(100)-H and/or Si(100)-Cl functionalized surfaces and HOCH$_2$CH$_2$N$_3$, and then using more "click chemistry" to react these Si(100)-OCH$_2$CH$_2$N$_3$ functional surfaces with -C$_n$H$_{2n+1}$CH functional OPV. The monolayers were characterized by means of XPS, FTIR/ATR, and AFM. The results represent a further advance in the controlled functionalization of Si-surfaces and lead to implications for a wide variety of potential applications that can use the combination of an inorganic and organic semiconductor.
356. **n-Stacking of Soluble N-Type Semi- Conductors**

*Min Zhi Chen, Yingfeng Tu and Shi Jin, CUNY-College of Staten Island, Staten Island, NY*

Two novel soluble organic n-type semi-conductors (PDI-C20 and PDI-Gly-C20) have been successfully synthesized. Their n-Stack formation was characterized by NMR, X-ray diffraction and FT-IR. The equilibrium constants K between free and n-stacked molecules, which were deduced from NMR, exhibit a stronger tendency of forming n-stacks for PDI-Gly-C20 than PDI-C20. The X-ray diffraction results also suggest a significantly shorter intra-stack separation between two adjacent molecules in PDI-Gly-C20. Stronger n-stacking interaction in PDI-Gly-C20 will lead to enhanced charge transport performance, which makes it a promising material in the field of optoelectronics.

357. **Synthesis and Characterization of Oxazoline Block Copolymers for Photovoltaic Devices**

*Hongmei Li and Morton Litt, Case Western Reserve University, Cleveland, OH*

The synthesis of 2-(3-(N-carbazolyl) propyl-2-oxazoline and 3-(N-3, 6-dimethoxycarbazolyl) propyl-2-oxazoline are described. The oxazoline monomers are basic heterocycles that undergo ring-opening cationic polymerization with an initiator of methyl p-toluenesulfonate to form a linear N-acyl polyethylenimine. This is a living polymerization, so one block can be polymerized and then the second monomer added to make the second block. Very sharp molecular weight distributions were obtained. Demethylation of the polymer with boron tribromide gave 3, 6-dihydroxycarbazole blockpolymer in quantitative yield. The dihydroxycarbazole polymer was oxidized by potassium periodate. The polymers crystallize and the aromatic side chain shows a good n-stacking. The ends of the molecules can be tailored to have cationic, anionic or non-polar substituents by using different terminators. It is easy to deposit a layer of polymers on a conducting surface. The proposed work has potential application in solar cell. Studies of photovoltaic devices based on the new materials and their current-voltage characteristics are underway.

358. **High Performance Size-Exclusion Chromatography (SEC) Column for Water Soluble Polymers**

*Ken Tseng¹, Ryuji Takahashi², Ritsuko Ohno² and Masatoshi Murakami², (1)Shodex, New York, NY, (2)Showa Denko, K.K., Kawasaki, Japan*

We are introducing OHpak SB400 series semi-micro columns for gel filtration chromatography (GFC) analysis. They have similar calibration curves as our popular SB-800 series. In addition, the SB400 columns have better sensitivity and higher theoretical plate number, while using less sample amount and solvent.

The packing material is polyhydroxymethacrylate gel with controlled surface hydrophilicity and pore distribution. The operational pH range is 3 to 10, and the temperature range is 5 to 70 oC. Water soluble organic solvents such as methanol, acetonitrile and DMF can be used.

SB400 series are available with 4 different exclusion limits ranging from 1,000, to 1,000,000. Specifically, the SB401-4E column with the lowest exclusion limit (1,000) is completely new, and not available in the SB-800 series.

We will introduce basic features of SB400 series and their applications in cationic, anionic, and non-ionic polymers.
359. DNA Functionalized Carbon Nanotubes as Active Stabilizers: Conducting Polymer Nanocomposites with Enhanced Stability

William Cheung¹, Yufeng Ma¹, Guangru Mao¹ and Huixin He², (1)Rutgers University, Newark, NJ, (2)Rutgers University, Newark Campus, Newark, NJ

Short lifetime has been a thorny problem for chemical and biosensors, and light emitting devices consisting of organic (polymer) materials. In this work, a water-soluble self-doped polyaniline nanocomposite was fabricated by in-situ polymerization of 3-aminophenylboronic acid monomers in the presence of single-stranded DNA dispersed- and functionalized- single-walled carbon nanotubes. For the first time, we found that carbon nanotubes act as novel active stabilizers. This is possibly due to DNA functionalization: they reduced the polyaniline backbone from the unstable, degradable, fully oxidized pernigraniline state to the stable, conducting emeraldine state, which significantly improves the chemical stability of the self-doped polyaniline against the harsh UV irradiation.

360. Synthesis and Characterization of Fluorene-Based Organoboron Quinolate Polymers

Haiyan Li and Frieder Jäkle, Rutgers University, Newark, NJ

Two types of luminescent fluorene-based organoboron quinolate polymers, PFB2Q2 and PFBQ, have been prepared by boron-induced ether cleavage reaction. PFBQ has a structure with quinolato substituted boron embedded in the main chain, while in PFB2Q2, both the quinolato moieties and the boron atoms are placed in the main chain. All the resulting polymers are readily soluble in common organic solvents and have been characterized by multinuclear NMR spectroscopy. They show good chemical stability and are thermally stable to >300 °C. The photoluminescence properties of PFB2Q2 are strongly dependent on the conjugated bridge connecting the two quinolato groups. With a biphenyl linker yellow green emission was observed, whereas the Th-Ph-Th linker gave (weak) orange emission. The polymer with the Th-Ph-Th linker shows an unusual wavelength and concentration-dependent emission.

361. Preparation and Characterization of Nano-Hollow Spheres of Conducting Polymer by “Micro-Interfacial Polymerization” and the Study of Controlled Release from Them

I-Wei Chu¹, Kai Su², and Nan-Loh Yang¹, (1)College of Staten Island/CUNY, Staten Island, NY, (2) Ciba Specialty Chemicals, Tarrytown, NY

In recent years, controlled releases by using conducting polymers as novel vesicles have attracted attentions due to their unique property of substantial volume changes with the variation of doping level. Hollow conducting polymer nanostructures have promises for loading contents of interest, although relatively poor mechanical properties and limited solubility of conducting polymers lead to significant challenges in the fabrication of such structures. We report here a novel soft-template synthesis of conducting polymer nano-hollow-spheres for controlled releases. These hollow spheres were readily prepared by using a “micro-interfacial polymerization” approach under mild reaction conditions. The concentration of 3, 4-ethylenedioxythiophene (EDOT) monomer plays a significant role in controlling the morphology of intact hollow PEDOT nanospheres. The size of nano-hollow sphere can also be readily tuned from 75nm to 400nm by ionic liquid to surfactant (IL-to-surfactant, R) ratio. Furthermore, the behaviors of controlled release were studied by tuning pH.
362. Biocompatible, Hydrogen-Bonded Multilayers of a Polyphenol with High pH-Stability

Irem Erel Unal and Svetlana Sukhishvili, Stevens Institute of Technology, Hoboken, NJ

We report on layer-by-layer (LbL) deposition of tannic acid (TA)/neutral polymers and their stability in the pH scale. The neutral polymers used for hydrogen-bonding with TA were poly(N-vinylcaprolactam) (PVCL), poly(N-vinylpyrrolidone) (PV Pon), poly(ethylene oxide) (PEO) or poly(N-isopropyl acrylamide) (PNIPAM). LbL film deposition and pH-stability were followed by phase-modulated ellipsometry and in situ Fourier transform infrared spectroscopy in attenuated total reflection mode (ATR-FTIR). Hydrogen-bonded films of TA with PVCL, PVPON, PEO, and PNIPAM were constructed at pH 2 and did not dissolve until a critical dissolution pH of 9.5, 9, 8.5 and 8 (measured in 0.01 M buffer solutions) for PVCL/TA, PVPON/TA, PEO/TA, and PNIPAM/TA, respectively. Incorporation of a polyacid with a low pKa, such as poly(aspartic acid) (PLAA), as the third polymer component into these films results in TA/PVCL/PLAA hybrid films, whose pH destruction profile can be tuned by varying film architecture, i.e. by depositing alternating or stacked PVCL/TA and PVCL/PLAA sublayers. High pH-stability of hydrogen-bonded TA films, as well as the capability of tuning the critical dissolution pH close to physiological pH values makes such multilayer systems promising candidates for biomedical applications.

363. An Odd Couple: A Designed Protein:Natural Protein Chimera

Jessica A. Norman, Andrew C. Mutter and Ronald L. Koder, The City College of New York, New York, NY

Designed proteins capable of electron transfer are of interest as tools to accomplish many applications including industrial chemical applications, solar energy, and nanochemical therapeutic devices. However, these proteins require a source of electrons and interfacing them with the endogenous electron-providing proteins of a cell is a difficult task. To avoid this compatibility and stoichiometry problem, we take advantage of the natural catalytic function of phthalate dioxygenase reductase, a flavoprotein which transforms the paired reducing equivalents of NADH into sequential single electrons by fusing it to a de novo designed diheme helical bundle domain. This two-part module is intended for use in varied applications such as a prodrug activating enzyme for cancer therapy or in solar energy conversion.

364. De Novo Designed Safranine Enzymes

Gheevarghese Raju, Graduate Student, New York, NY and Ronald L. Koder, The City College of New York, New York, NY

Safranines have the ability to catalyze electron transfer reactions similar to those catalyzed by flavins without the oxygen activation side reactions that flavins are also structured to perform. We are constructing a series of de novo-designed helical bundle enzymes in which safranines act as the cofactors which catalyze the NADH-dependent reduction of nitroaromatics. A novel chemical synthesis has been developed which allows the rapid generation of many safranine derivatives, each of which has differing reduction potentials, visible and fluorescent spectra. Selection of the appropriate derivative will allow the tuning of the catalytic activity towards particular nitroaromatic substrates. These novel proteins are intended for use in explosives sensing, chemotherapeutic prodrug activation and 'green' chemical catalysis.

365. Multi-Responsive Polyelectrolyte Diblock Copolymer Micelles

Zhichen Zhu, Li Xu and Svetlana Sukhishvili, Stevens Institute of Technology, Hoboken, NJ

We report on synthesis, self-assembly and response to variations of pH, temperature and ionic strength of the polyelectrolyte diblock copolymer micelles in aqueous solutions. Well defined poly[2-(dimethylamino) ethylmethacrylate –block-(N-isopropylacrylamide)] (PDMAEMA-b-PNIPAM) and
poly[2-(diethylamino)ethyl methacrylate)-b- poly(N-isopropylacrylamide)] (PDEAEMA-b-PNIPAM) block copolymers with different block ratios were synthesized using atomic transfer radical polymerization (ATRP) technique in methanol solutions using BIEE/CuBr/Bpy as initiator/catalyst/ligand, respectively. Micellization of the copolymers was monitored using dynamic light scattering (DLS). In PDMAEMA-b-PNIPAM solutions with low salt concentrations and at room temperature, the copolymer was molecularly dissolved in a wide range of pH values, due to insufficient hydrophobicity of the PDMAEMA block. However, micellization of PDMAEMA-b-PNIPAM copolymers could also be induced at room temperature by salting-out the PNIPAM block in NaH2PO4 buffer. The unimer/micelle transitions were also pH-dependent, and could be observed in the temperature scale. Such transitions reflect the effect of the polycation charge density on the critical micelle concentration of the PDMAEMA-b-PNIPAM copolymers. The copolymer composition strongly affected the unimer/micelle transitions, i.e. shortening the PNIPAM block length resulted in an increase of the critical micellization pH and/or temperature. In contrast to PDMAEMA-b-PNIPAM micelles, which were stabilized by PDMAEMA corona, PDEAEMA-b-PNIPAM copolymers self-assembled into PDEAEMA/PNIPAM core/corona micelles with strongly associated PDEAEMA core, which were stable at room temperature in solutions with both low and high salt concentrations.

366. Rheology and Confocal Reflectance Microscopy as Complementary Probes of the Kinetics of Collagen and Collagen/hyaluronan Gelation

Yali Yang and Laura J. Kaufman, Columbia University, New York, NY

Three dimensional collagen/hyaluronan (HA) composite gels are prepared, and their gelation at 32°C and 37°C is studied by rheology and confocal reflectance microscopy (CRM). By varying collagen concentration, gelation temperature and adding HA, we can change the gelation kinetics and manipulate structural and mechanical properties of collagen at equilibrium. We demonstrate that HA can both deposit on collagen fibers as well as remain dispersed throughout the gel. Varying the gelation temperature alters the HA distribution and therefore also varies HA's effects on collagen fibrillogenesis kinetics and equilibrium properties of the gels. CRM and rheology are used complementarily to investigate gelation kinetics. Four dynamic parameters are studied: the arrest time (t_a) measured by CRM, the lag phase time (t_{lag}), the slope of the growth phase (k_{growth}) and the crossover (gelation) time (t_c) determined by rheology. t_{lag} and k_{growth} describe the nucleation and growth phases of collagen self-assembly, respectively. They are affected by properties of the dispersing medium and thus by the dispersed HA. t_c, which defines the sol-gel transition, is mainly affected by the deposition and viscosity of HA. t_a, which describes the arrest of microstructures during gelation, is affected by both dispersed and deposited HA. Together our data indicate that HA can modulate the equilibrium mechanical properties of collagen matrices subtly, but changes the kinetics of their self-assembly and their non-equilibrium structure substantially. This work also shows new ways in which rheology and microscopy can be used complementarily to reveal details of gelation processes.
**367. Living Photocontrolled and Living Supramolecular Polymerizations as Routes to Functional Metallopolymers**

**Ian Manners**, University of Bristol, Bristol, United Kingdom

Polymers containing metal atoms are attracting increasing attention as they offer access to new functional macromolecular and supramolecular materials with novel properties. Our group has developed ring-opening polymerization routes to metallopolymers such as polymetallocenes with high molecular weights which allows easy processing.

Controlled architectures (e.g. block copolymers) are available through living polymerization processes, including a remarkable recently developed photocontrolled method. This talk will focus on recent efforts to use these metallopolymers to create, for example, photonic devices, and self-assembled supramolecular structures, which can be used in nanolithographic applications and catalysis.

References:

**368. Tightening the Belt**

**Colin Nuckolls**, Columbia University, New York, NY

Department of Chemistry and The Nanoscience Center

This presentation details metathesis reactions on strained [8]-annulenes. One annulene, where one of its double bonds is kinked into a trans-configuration, is found to wind into helical conformation and is spring-loaded with ~18kcal/mol strain energy to act as an active monomer for ROMP. The polymerization produces a living phenylene vinylene with all ortho-linkages. The polymer has equal number of cis and trans double bonds.

**369. In-Situ Polymerization of a Thin Skin of Self-Doped Conducting Polymer to Improve the Electronic Performance of Carbon Nanotube Networks**

**Huixin He**, Rutgers University, Newark Campus, Newark, NJ

The overall conductivity of SWNT networks is dominated by the existence of high resistance and tunneling/Schottky barriers at the intertube junctions in the network. Here we report that in-situ polymerization of a highly conductive self-doped conducting polymer “skin” around and along single stranded DNA functionalized- SWNTs can greatly decrease the contact resistance. The polymer skin also acts as “conductive glue” effectively assembling the SWNTs into a conductive network, which decreases the amount of SWNTs needed to reach the high conductive regime of the network. The conductance of the composite network after the percolation threshold can be two orders of magnitude higher.
magnitude higher than the network formed from SWNTs alone. In addition, the polymer skin also provides a powerful functionality for biosensor applications.

However, we found that only in-situ polymerized conducting polymers were able to effectively interlink the SWNTs to form a highly conductive network. The pre-formed conducting polymer dramatically decreased the conductivity and increased the percolation threshold of the SWNT networks. Surprisingly, the conducting polymer formed by in-situ polymerization with pre-oxidized SWNTs (“seed” method) did not assemble the nanotubes into a conductive network either. Instead, the polymer induced severe aggregation of the nanotubes into large particles. Consequently, the percolation threshold of the composite formed by the seed approach is much higher and the conductance after the percolation threshold is three orders of magnitude lower than the network formed by SWNTs alone. Various techniques were applied to understand the mechanism for the different enhancement in nano and molecular scales.

370. Poly(ferrocenylenes) with Three- and Four-Coordinate Boron Bridges

Matthias Wagner, J. W. Goethe-Universität, Frankfurt (Main), Germany

The development of ferrocene-containing polymers is a highly active field of research which originates from the quest for novel materials showing useful electronic and optical properties. Polymers featuring ferrocene as an integral part of the main chain are particularly interesting, but their synthesis proves to be a major challenge. Our group has recently developed a condensation polymerization approach to borylene-bridged poly(ferrocenylenes) \([-\text{fcB}(\text{Br})^-]_n\) starting from \(\text{fc}(\text{BBr}_2)_2\) and HSiEt$_3$ \([\text{fc} = (\text{C}_5\text{H}_4)_2\text{Fe}]\). The reaction proceeds with liberation of B$_2$H$_6$ and gives polymers with up to 40 repeat units. The bromo derivative can be transformed into the corresponding mesityl polymer or the 2,2'-bipyridylboronium salt. The mesityl polymer \([-\text{fcB}(\text{Mes})^-]_n\) is interesting because it features three-coordinate boron atoms which, due to their empty p-orbital, are well-suited for the promotion of electron delocalization along the polymer chain. The 2,2'-bipyridylboronium salt \([-\text{fcB}(\text{bipy})^-]_n^{n^+}\) possesses four-coordinate boron bridges which are reminiscent of the organic electron acceptor Diquat. As a consequence, charge-transfer interactions between the ferrocene donor fragments and the bipyridylboronium moieties are observed leading to a very deep purple color of the material.

This lecture deals with the synthesis and purification of \([-\text{fcB}(\text{Mes})^-]_n\) and \([-\text{fcB}(\text{bipy})^-]_n^{n^+}\) and with an investigation of their physical properties ((spectro)electrochemistry, femtosecond laser spectroscopy).

371. Iridium Containing Phosphorescent Polymers for OLED Applications

Marcus Weck, New York University, New York, NY and Alpay Kimyonok, Georgia Institute of Technology, Atlanta, GA

The design and synthesis of polymeric organic light-emitting diodes (OLEDs) has been a major research focus in academia and industry due to the potential stability, processability, and tunability of these materials in comparison to their inorganic counterparts. In particular, phosphorescent metal complexes are at the center of recent research emphases on OLEDs. We recently reported the covalent functionalization of iridium complexes onto poly(norbornene)s. We demonstrated that the poly(norbornene) backbone does not interfere with the photophysical properties of the iridium complexes studied. In the presentation, we will discuss the synthesis of random copolymers containing host moieties and various iridium complexes in the side-chains that emit in various regions of the visible spectrum. Furthermore, we will discuss their solution and solid-state photoluminescence properties and their solid-state electroluminescence properties. Finally, we will report some preliminary results on the incorporation of these copolymers as the emissive layers in OLED devices.
372. Selective Olefin and Polyolefin Stiching to Silicon

Bhanu P. S. Chauhan*, Alok Sarkar and Bharthi Balagam, Engineered Nanomaterials Laboratory, William Paterson University, Wayne, NJ

Nanoparticle synthesis is a very fascinating and fast developing field of research due to the applications of resulting materials. One of the major difficulties in this endeavor is to obtain isolable and catalytically active nanoparticles in multigram scale. In the field of catalysis, nanoparticles have gained interest due to their vital characteristics such as redispersibility and recyclability.

Recently, our laboratory has been developing new strategies for the generation of catalytically active metal nanoparticles.1, 2, 3 We have been able to generate and stabilize a fair number of late transition metal nanoparticles via this strategy. In this presentation, we will present catalytic utility of nanoparticles to tailor olefins to silicon molecules via hydrosilylation reactions. We will demonstrate that a fair number of electronically and sterically varied olefins were quantitatively and regioselectively grafted to Si-H containing silicone molecules and oligomers. Furthermore, hybrid nanoarchitectures were generated by selective incorporation of olefin based polymers on predefined nanostructures, such as Octakis(dimethylsiloxy)-T8-silsesquioxane (Q8M8H) and 1,3,5,7 Tetramethylycyclo-tetrasiloxane (D4H).


373. Nanoparticle Applications to Wool Part I: Synthesis and Characterization

Justin J. Martin, Jeanette M. Cardamone and Peter Irwin, USDA ARS Eastern Regional Research Center, Wyndmoor, PA

Wool, composed of keratin protein, has complex morphology and chemistry. Wool is easily damaged by conventional processing methods at all stages of its fabrication from yarn to fabric, and through dyeing and finishing. To obviate these effects and improve the properties of wool, we have been exploring nanoparticle systems that can strongly adsorb to wool without the need for chemical pre-treatments. Nanoparticle wool stands to benefit from the myriad of exciting properties that exist in the nano-domain that are not observed for bulk materials. Recently, we have prepared colloidal silver nanoparticles of varying diameter and structure using solubilized proteins as stabilizers. Initial testing of the colloidal nanoparticles has shown a marked antimicrobial efficacy toward Staphylococcus aureus. Furthermore, we observed that the stabilized nanoparticles are easily applied to wool and cotton, they impart the yellow-orange color associated with surface plasmon resonance and remain adsorbed after rinsing. These discoveries lay the foundation for extending our investigation to antimicrobial wool. Our approach, using functional stabilizers to deliver nanoparticles to materials, can be extended to other nanoparticle systems and offers an exciting opportunity for integrating nanotechnology and textiles. Here we will discuss the morphology of our colloidal silver nanoparticles, the characterization of our materials, their antimicrobial efficacy, and their sorption to wool.
Applications of Organometallic Chemistry
Sponsor: Strem Chemicals, Air Products, Boulder Scientific
Organizer: Chip Nataro Lafayette College

Session Overview: Organometallic chemists from inorganic and organic backgrounds will discuss how organometallic compounds are being used to solve new and interesting problems in their labs.

374. Tuning the Electronic and Structural Properties of a Ferrocene Based Bifunctional Lewis Acid
Thilagar Pakkirisamy, Krishnan Venkatasubbaiah and Frieder Jäkle, Rutgers The State University Newark, Newark, NJ

The development of sensor systems for ionic and neutral molecules is a promising field of research in Lewis acid chemistry. We have been interested, for some time, in developing appropriate synthetic routes for ferrocene based bifunctional Lewis acids. Our initial discovery of the diboracycle $(\eta^5-C_5H_5Fe)_2[\mu-C_{10}H_6(BPh)_2]$ has spurred us to investigate the electronic communication between the two ferrocenyl moieties by changing the aryl substituents on boron center. In this presentation, we will discuss the synthesis and characterization of a series of diboradiferrocenes with different aryl substituents on boron center. In addition the binding behavior of $(\eta^5-C_5H_5Fe)_2[\mu-C_{10}H_6(BPh)_2]$ toward different pyridine derivatives as the Lewis base has been investigated.

375. Anchored Wilkinson's Catalyst: Comparison with the Homogeneous Catalyst and Supported Rhodium with Respect to Reaction Selectivity
Robert L. Augustine, Setrak K Tanielyan, Norman Marin and Gabriela Alvez, Seton Hall University, South Orange, NJ

A series of Anchored Wilkinson's Catalysts (AWC's) were prepared by reacting the homogeneous Wilkinson catalyst with several alumina/heteropoly acid support materials. These catalysts were used to promote the model hydrogenations of cyclohexene, 1-hexene and limonene. The results were compared with those obtained using the homogeneous Wilkinson and a Rh/Al2O3 catalyst with respect to catalyst stability, reaction selectivity and the amount of isomerization observed. The effect which the nature of the heteropoly acid exerted on the reaction was also examined.

The results of these hydrogenations will be discussed along with data relating to the composition of the anchored catalyst before and after hydrogenation as well as the application of these catalysts to continuous reactor systems.

376. Novel Approaches to the Cross-Coupling Reactions
Jing Liu, Yingsheng Zhao, Xiancai Luo and Aiwen Lei, Wuhan, China

During the past three decades, the bond formations (C-C, C-X) promoted by transition metals are extensively studied, and widely applied in the organic syntheses as the most successful, and reliable methods. In general, this transformation includes three elementary reactions: (1) oxidative addition, (2) Transmetallation, (3) Reductive Elimination. Herein, we would like to introduce a new approach: the oxidative cross-coupling, which involves double transmetallation, $^{1-3}$ and reductive elimination (Scheme 1). Using desyl chloride as the oxidant, a Csp-Sn reagent and a Csp3-Zn reagent can couple together with surprisingly high selectivity. $^4$ When the Csp3-Zn reagents have b-H, the coupling can take place well in high yield as well as the selectivity. The coupling of Csp-Sn and Csp2-Zn was also examined, and high yield of the desired cross-coupling products were
obtained. Our kinetic data from ReactorIR, $^{13}$C NMR indicate that the organozinc reagents are highly oxophilic, and the organotin reagent might be halophilic.

References:

377. Regioselectivity of Platinum-Catalyzed Hydrosilylation of Alkynes in Silyl-Substituted Ferrocenes and Related Sandwich Compounds
John B. Sheridan and Rhyan Terrado, Rutgers University, Newark, NJ

Hydrosilylation reactions between dimethylsilyl- and 1,1'-bis(dimethylsilyl)ferrocene; dimethylsilyl- and 1,1'-bis(dimethylsilyl)troticene (troticene = η-cyclopentadienyl(η-cycloheptatrienyl)titanium); dimethylsilyl- and 1,4-bis(dimethylsilyl)benzene and selected terminal alkynes were performed and the product distributions analyzed. In all cases, mixtures of α- and β(E)- isomers were formed. In general β(E)- isomers are preferred, however in the cases of the disubstituted metallocene complexes the the α isomers predominate. The selectivity is rationalized based upon the unique geometry constraints of the metallocene derivatives.

378. Microwave Heating: A Tool for Fast Preparation of Organometallics
Nicholas Leadbeater, University of Connecticut, Storrs, CT

While synthetic organic chemists have taken advantage of microwave heating in their work, there have been relatively few reports of application in preparative organometallic chemistry. Microwave heating offers several advantages over conventional methods include significant rate acceleration and, in many cases, improved product yields and selectivity. A major problem with performing organometallic chemistry using microwave heating is that, in ligand exchange reactions, stopping a reaction after a
desired number of substitutions is difficult if the reaction cannot be continually monitored. With in-situ Raman apparatus we can monitor reactions in real time and can carefully control the synthesis of organometallic compounds. In addition, by using gas-loading equipment we can perform reactions under an atmosphere of reactive gases. This has allowed us to prepare a number of key organometallic compounds very quickly and efficiently. Our results will be presented here.

379. New Transition Metal Catalyzed Carbon-Carbon Bond Forming Reactions
John D. Chisholm, Syracuse University, Syracuse, NY

Catalysis of organic reactions is of special interest as modern catalysts are not limited to simple rate acceleration, but can be modified to control the relative and absolute stereochemistry of the reaction products. The development of new catalysts for organic reactions is therefore a major goal. We have been exploring a number of alkyne addition reactions catalyzed by palladium and rhodium complexes. Recent efforts in the development of these processes will be presented.

380. Catalysis as Means to Perform Organic Synthesis: Cheaper, Cleaner and Greener
John R. Sowa Jr., Seton Hall University, South Orange, NJ

This seminar will cover our research on the following reactions that occur through organometallic intermediates.

- Suzuki Coupling

\[
\begin{array}{c}
\text{X} \text{H(OH)₂} + \text{Br} \text{Y} \\
\text{PdC} \\
\text{Heterogeneous Catalyst}
\end{array}
\]

- Asymmetric Transfer Hydrogenation

\[
\begin{array}{c}
\text{Hydrogen Free?} \\
\text{OH}
\end{array}
\]

381. Tandem Asymmetric C-C Bond-Forming Reactions
Patrick J. Walsh, University of Pennsylvania, Philadelphia, PA

We have developed several highly enantio- and diastereoselective one-pot methods for the efficient synthesis of synthetically useful cyclopropyl alcohols. Our methods take advantage of a highly enantioselective C-C bond-forming reaction to set the initial chirality. The resulting allylic zinc alkoxide intermediate is then subjected to either cyclopropanation or halocyclopropanation. This method allows generation of up to 4 stereogenic centers in a one-pot procedure from achiral precursors.

382. Use of Vanadium Hydrides to Effect Radical Cyclizations
Jack Norton, Mary E. Pulling and Deborah M. Smith, Columbia University, New York, NY

The vanadium hydrides HV(CO)₄(P–P) (P–P = dppe, dpp, dppp, dppb) transfer H• rapidly to the methylene carbon of appropriate 1,6-dienes, and thereby bring about radical cyclizations.
Chemistry and the Arts
Organizer: Sasan Karimi Queensborough Community College, Bayside, NY

383. Color Science Laboratory Exercises in Art and Theatre
Maria C. Gelabert, Wagner College, Staten Island, NY and Christopher Mustakas, Wagner College, Wagner College, NY

For a non-science majors' course entitled Color Science, four interdisciplinary laboratory exercises are presented that involve fields outside the sciences. Two of the labs focus on art, where the students investigate the chemistry of fresco art and make their own encaustic paint. The other two labs involve theatre lighting and scene design; for these the students mix light colors, use gel filters and test paint colors with different sources of light. The fresco lab, based on a published exercise from Juniata College, and the other three labs were developed last summer with the intent of branching the science of color out to other disciplines in a meaningful way.

384. Chemical and Materials Analysis of Copper-Alloy Artifacts from High Status Burials at the Pyramids at Moche Site, Peru
Marc L. Richard1, Elizabeth Myers Cooney2 and Heather Lechtman2, (1)The Richard Stockton College of New Jersey, Pomona, NJ, (2)Massachusetts Institute of Technology, Cambridge, MA

The Moche were a people who created one of the most accomplished societies of the pre-Columbian Americas. Centered about the Moche River Valley on the North coast of Peru, from approximately 100-800 AD the Moche flourished, building monumental pyramids, vast irrigation systems, and creating new forms of metallurgy, ceramics, and textiles. Metal was an ideological symbol of power, and Moche metal workers experimented with many materials, creating a wide variety of metalworking techniques. Moche metal workers were the most sophisticated and creative metal artisans of the pre-Columbian Andes, and subsequent Andean societies relied on their technological achievements.

Eight metal objects of the Moche IV period, excavated by Donnan and Mackey in 1978, have been chemically and structurally analyzed to understand their construction and possible ritual uses. The gold content of several objects indicates a deliberate addition of gold to the alloy, however in amounts insufficient to alter the surface color of the objects. Lead-isotope analysis shows that local copper ore sources were used in the object production.

Two unique objects, a metal staff and tumi (ritual knife) have been subject to detailed structural characterization. The fact that these artifacts are constructed in unique ways and intact increases the likelihood that these objects were ritually important. It was also determined that this particular tumi could not have been used as an actual cutting tool, indicating its ritual importance over practical use. Overall, these objects increase our understanding of Moche metallurgy in their terminal period.

385. An Intersession Science & Art Course for Non-Science Majors

The January intersession term, a distinctive feature of the Washington & Jefferson College academic calendar, features sharply focused topics courses and a change of pace from the standard curriculum. “Science & Art” is a course designed to engage non-science majors in an innovative fashion. This course includes introductory topics from inorganic chemistry, organic chemistry, optics, neuroscience, and the history of science. Students are encouraged to recognize the role that these fields play in the art world and to develop an appreciation of the interconnectedness between
seemingly disparate disciplines. The structure of the course and its development through four iterations will be discussed.

### 386. Teaching Science of Art in Italy

**Robert Richman**, Mount Saint Mary's University, Emmitsburg, MD

The author was the first scientist from his institution to win (or even attempt) the university-wide competition to run a semester-abroad program. This success is attributed to his proposal to teach the Science of Art. The course was taught in the spring semester of 2008 in Florence, Italy, to a group of 31 sophomores and juniors from a broad spectrum of liberal arts majors, including chemistry. The prerequisite was either non-majors' Physical Science or General Chemistry I. Texts were Patricia Hill's non-majors' book (The Molecular Basis of Color and Form) and Ken Schuman's Anatomy of a Restoration. Topics included light, color, dyes and pigments, paint, frescos, glass, and art conservation and restoration. Field trips included the Brancacci Chapel in Florence, the Sistine Chapel in Rome, a mosaics school in Ravenna, and a glass-blowing shop in Venice.

### 387. Teaching An Interdisciplinary Course on the Art and Science of Color

**Catalina Achim**, Carnegie Mellon University, Pittsburgh, PA

This presentation will describe an interdisciplinary course on The Art and Science of Color taught at Carnegie Mellon University. The course is offered to Chemistry and Art students and focuses on the intersection of painting with chemistry. The course activities are designed to expand the expertise of students in each discipline, while exposing them to the methods, demands, and aims of the other. Historically, the craft of painting was linked to the practice of pigment preparation, with painters procuring their materials in raw form from chemists/apothecaries, and performing themselves the final purification and grinding of the minerals into pigments. With the advent of mass-produced art materials in the nineteenth century, the distance between chemist and artist increased until the two worlds have little to do with one another. This class aims to reconnect the two disciplines for a study of their common ground. Students learn about the origin of the color of minerals with primary focus on colors that originate from electronic transitions. They work collaboratively in the chemistry laboratory to synthesize and characterize inorganic pigments. In the studio, they make their own egg-tempera paints, and use them in painting projects designed to increase color skills as they learn about the history of pigment use. Students collaboratively work on final projects that involve research, experiments, and creative work. Researchers who work at the boundary between art and chemistry give guest lectures, and the class makes field trips to local research labs and museums.

### 388. Chemistry in Art: Seventeen Years of Courses and Workshops

**Patricia S. Hill**, Millersville University, Millersville, PA

Since 1991 the speaker has taught a general education, lab science course to hundreds of non-science majors. The course, entitled The Molecular Basis of Color and Form: Chemistry In Art, addresses science concepts crucial to the preparation, use, and long-term care of artists' materials from metals, glass and ceramics to pigments, dyes, paints and photography. Developing directly as a result of the experience of teaching this course has been a series of workshops for chemistry and art faculty, first sponsored by the NSF Chautauqua program, then funded by an NSF-DUE grant, and currently under the auspices of the Center for Workshops in the Chemical Sciences (CWCS). Over 200 faculty members from chemistry, geology, biology, physical science and art have participated in a CWCS workshop in Chemistry and Art since 2002. The next workshop is scheduled to take place on the campus of Washington & Lee University in June of 2008. This presentation will provide an overview of both the course content of the speaker's general education course and the workshop as well as some of the broader lessons learned along the way.
389. Why Chemistry and Art?

Michael Henchman, Brandeis University, Waltham, MA

Why should we teach Chemistry and Art? We teach it to promote an attitude of mind, an approach to solving problems that is disappearing today. As scientists, we assemble all available evidence and we evaluate it critically: that done, we draw those conclusions that fit the evidence and we reject others that do not. That is what we must teach.

Art is treasured everywhere: science increasingly is not. Nevertheless we can teach non-scientists how the scientific examination of art increases their understanding of art. They witness science in action and what a scientific approach can achieve. Scientists, too, studying chemistry and art, see how science benefits art, as they themselves are introduced to art.

Art provides the lure to teach scientific reasoning. Our society faces a crisis in values. We must insist on honest reasoning and teach it widely. How else are we to evaluate global warming?

390. Uncovering the Secrets of Ancient and Medieval Artists through Chemistry

Mary Virginia Orna, College of New Rochelle, New Rochelle, NY

This paper consists of a discussion of how modern chemical methods can be used to examine both ancient and medieval artifacts. Archaeological work in Israel involved analysis of ancient pigments and dyes found on excavated materials from caves in the Judean desert and the ancient fortress of Masada. Pigments in medieval manuscripts formed the basis of further work on colorants. In addition, medieval artists' manuals were examined for recipes for blue pigments which were then carried out and characterized with some surprising results.

391. Reaction Coordinates in Enzymes - Promoting Vibrations

Steven D. Schwartz, Albert Einstein College of Medicine, Bronx, NY

The mechanism by which enzymes catalyze chemical reactions is still in many cases unclear. One controversial suggestion is that picosecond vibrations in the protein backbone form part of the reaction mechanism. Using Transition Path Sampling and Committor distributions we show that such promoting vibrations are indeed a central part of the mechanism of a number of enzymatic reactions.
392. A Computational Study of Changing Intramolecular Interactions in Serine and Threonine, at Different Phs

Mihaela D. Bojin, Queensborough Community College, CUNY, Bayside, NY

Amino acids are excellent targets for theoretical investigations, because of their small sizes and remarkable role in our lives. Yet, their flexibility leads to multiple conformations that stem from the many possibilities for intra- and intermolecular hydrogen bonding interactions, which control secondary and tertiary structures of proteins and affect enzymatic activity. We analyze conformers of serine (Ser) and threonine (Thr), in different pH, using DFT methods. We also compute chemical shifts, and compare them to currently available experimental data. Hydrogen bonds’ strength, as well as the strain they impose on these systems are strongly influenced by pH. By examining these intrinsic bonding elements in Ser and Thr, we aim to identify similar hydrogen bonding motifs in complex biological systems.

393. Enhanced Conformational Sampling and Free Energies Via Novel Spatial-Warping Transformations and Adiabatic Dynamics

Mark E. Tuckerman, New York University, New York, NY

One of the computational grand challenge problems is to develop methodology capable of sampling conformational equilibria in systems with rough energy landscapes. If met, many important problems, most notably protein structure prediction, could be significantly impacted. In this talk, I will present a new approach [1,2] in which molecular dynamics is combined with a novel variable transformation designed to warp configuration space in such a way that barriers are reduced and attractive basins stretched. The new method rigorously preserves equilibrium properties while leading to very large enhancements in sampling efficiency. The performance of the method is demonstrated on long polymer chains and simple protein models and is shown to significantly outperform replica-exchange Monte Carlo with only one trajectory [2]. Finally, a new molecular dynamics approach for generating multi-dimensional free-energy surfaces that employs adiabatic dynamics [3,4] combined with multiple time-step integration to drive a set of extended phase-space variables as a means of enhancing the sampling of a subspace of collective variables will be presented.

References:
394. The Transition State for Formation of the Peptide Bond in the Ribosome

Lou Massa, Hunter College, City University of New York, New York, NY

Using quantum mechanics and exploiting known crystallographic coordinates we have investigated the mechanism for peptide-bond formation in the ribosome. The calculation is based on a choice of 50 atoms assumed to be important in the mechanism. We used density functional theory to optimize the geometry and energy of the transition state (TS) for peptide-bond formation. The calculated TS activation energy, $E_a$, is 35.5 kcal/mol, and the increase in hydrogen bonding between the rotating A-site tRNA and ribosome nucleotides as the TS forms appears to stabilize it to a value qualitatively estimated to be 18 kcal/mol. The optimized geometry corresponds to a structure in which the peptide bond is being formed as other bonds are being broken, in such a manner as to release the P-site tRNA so that it may exit as a free molecule and be replaced by the translocating A-site tRNA. At TS formation the 2' OH group of the P-site tRNA forms a hydrogen bond with the oxygen atom of the carboxyl group of the amino acid attached to the A-site tRNA, which may be indicative of its catalytic role, consistent with recent biochemical experiments.

395. Efficient, Transformation-Free, Conformational Sampling Via Driven Adiabatic Free Energy Dynamics

Jerry B. Abrams and Mark E. Tuckerman, New York University, New York, NY

Adiabatic Free Energy Dynamics, introduced by Rosso et al. (J. Chem. Phys. 2002, 116, 4389) for computing free energy profiles quickly and accurately using adiabatic dynamics, has been used for such problems as conformational sampling of peptides (J. Phys. Chem. B 2005, 109, 4162) and computing alchemical free energies such as solvation free energy (J. Chem. Phys. 2006, 125, 074115). In both cases, the use of adiabatic dynamics has been shown to lead to significant speed increases versus traditional methods such as Umbrella Sampling, Thermodynamic Integration, and Free Energy Perturbation. The most significant drawback to the AFED approach is the need to transform the coordinate system into generalized coordinates.

Here we present an extension of the AFED method that circumvents such transformations. In this approach, additional degrees of freedom, $s_i$, are used to drive the collective variables of interest, $s_i(r)$ via a harmonic potential coupling. The driving variables are given temperature sufficient to cross any significant barriers and mass sufficient to maintain adiabatic decoupling. The free energy surface along the collective variables is then constructed using the adiabatic probability distribution of the variables, $s_i$. This driven AFED approach (d-AFED) is employed to compare the conformational preferences of small peptides for three force fields. The results show that d-AFED accurately and efficiently computes the free energy surfaces of interest using radius of gyration, $R_g$, and number of hydrogen bonds, $N_h$, as collective variables.

396. Successes, Challenges, and Prospects of Time-Dependent Density Functional Theory for Bio-Molecular Processes

Neepa T. Maitra, Hunter College of CUNY, New York, NY

In recent years there have been increasing applications of time-dependent density functional theory (TDDFT) to describe optical spectra and response of biomolecules, with implications for processes such as photosynthesis and radiation damage. In this talk I will discuss some of the successes and failures of currently available functional approximations, and challenges in designing accurate functionals for these processes.
397. DNA: Not Merely the Secret of Life

Nadrian C. Seeman, New York University, New York, NY

Structural DNA nanotechnology is based on using stable branched DNA motifs, like the 4-arm Holliday junction, or related structures, such as double crossover (DX), triple crossover (TX), and paranemic crossover (PX) motifs. We have been working since the early 1980's to combine these DNA motifs to produce target species. From branched junctions, we have used ligation to construct DNA stick-polyhedra and topological targets, such as Borromean rings. Branched junctions with up to 12 arms have been produced. We have also built DNA nanotubes with lateral interactions.

Nanorobotics is a key area of application. PX DNA has been used to produce a robust 2-state sequence-dependent device that changes states by varied hybridization topology. We have used this device to make a translational device that prototypes the simplest features of the ribosome. A protein-activated device that can be used to measure the ability of the protein to do work, and a bipedal walker have both been built. We have also built a robust 3-state device.

A central goal of DNA nanotechnology is the self-assembly of periodic matter. We have constructed 2-dimensional DNA arrays from many different motifs. We can produce specific designed patterns visible in the AFM. We can change the patterns by changing the components, and by modification after assembly. Recently, we have used DNA scaffolding to organize active DNA components, as well as other materials. Active DNA components include DNAzymes and DNA nanomechanical devices; both are active when incorporated in 2D DNA lattices.

398. Nanoparticle Based Therapeutic Agents for Brain (Rhabdoid) Tumor

Bhaskar C. Das, Albert Einstein College of Medicine, Bronx, NY

The union between nanotechnology and small molecule chemistry can facilitate development of a wide range of nanomaterials for biomedical applications as diagnostic and therapeutic agents. As a goal of our research we are developing nanoparticle conjugated libraries of N-(4-hydroxyphenyl)-retinamides (4-HPR) and utilizing it as therapeutic and diagnostic agents for brain tumors, especially focusing on rhabdoid tumors. The basic objective of our research is to use nanoscience and nanotechnology in chemical biology, for drug discovery and development. Nanotechnology has potential application in brain tumor research. The main hurdle to develop and discover new therapeutic agents and diagnostic agents for brain tumor is the Blood Brain Barrier (BBB). Often a therapeutic agent or diagnostic small molecule that is effective in vitro is not efficacious in vivo partly because of its inability to cross BBB. It is possible to overcome this difficulty by use of nanoparticle based molecular agents. By combining medicinal chemistry and nanotechnology to synthesize small molecular weight therapeutic agents conjugated to nanoparticles can greatly facilitate the study the biology, diagnostic and therapeutic intervention of brain tumors.

I will describe the Chemical Synthesis and analysis of nanoparticle conjugated 4-HPR and other derivatives of 4-HPR compound libraries, Screening of nanoparticle libraries to test their effect on rhabdoid cell lines. The in vitro and in vivo studies of lead nanoparticles to assess their biodistribution, efficacy and use of microPET for diagnosis using genetically engineered rhabdoid tumor models.
399. Target Co-Delivery of Nanoheaters and siRNAs for Cancer Therapy

Oleh Taratula¹, Ronak Savla¹, Ipsit Pandya¹, Andrew Wang², Tamara Minko³ and Huixin He¹,
(1)Department of Chemistry, Rutgers University, Newark, NJ, (2)Ocean NanoTech, Fayetteville, AZ,
(3)The Ernest Mario School of Pharmacy, Rutgers, the State University of New Jersey, Piscataway, NJ

The long term aim of this project is to develop a multifunctional nanomedicine platform for targeted
delivery of nanoheaters and short inference RNA (siRNA) to cancerous tumors as well as the use of
magnetic resonance imaging (MRI) as a noninvasive strategy to monitor the therapeutic outcome of
the drug therapy. The main obstacle to siRNA therapy is in delivering RNA to the cytoplasm where it
can guide sequence-specific mRNA degradation. It has been recognized that a prerequisite for the
facile transport of siRNA through the cell membrane is their condensation to discrete nanoparticles.
Furthermore, new methods for invasive and in-situ monitoring therapeutic responses of the RNAi are
highly desirable for optimization of the therapeutic strategies. Superparamagnetic iron oxide (SPIO)
nanoparticles exhibit superparamagnetic behavior, magnetizing strongly under an applied field, but
retaining no permanent magnetism once the field is removed. Due to such intrinsic properties,
increasing efforts have been devoted to the potential application of magnetic nanoparticles as
nanoheaters for hypothermia therapy and as contrast agent for magnetic resonance imaging (MRI).
In order to design efficient, multifunctional, and nontoxic siRNA delivery agents for cancer therapy,
different sizes of SPIO nanoparticles were fabricated. The SPIO nanoparticle surface was modified so
that the SPIO nanoparticles can efficiently provoke siRNA condensation and largely facilitate siRNA
internalization into cancer cells. Modifying the surface of the formed siRNA complex with targeting
peptides, the siRNAs can be specifically internalized by cancer cells and the internalized siRNAs can
efficiently silence their targeting mRNA expression.

400. Controlling Self-Assembly Reactivity in DNA- and Protein-Nanoparticle Systems

Mathew M. Maye, Brookhaven National Laboratory, Upton, NY

The use of bio-inspired approaches for nanoparticle self-assembly takes advantage of the natural
tunability and addressability of encoded biomolecular interactions between particles. Using the
tunable structural properties of DNA, and the addressable symmetry of genetically engineered
proteins, we have investigated the ability to tailor self-assembly kinetics, assembly morphology, and
interparticle distances in nanoparticle systems. With DNA at nanoparticle interfaces, we are able to
fine-tune assembly kinetics, relative aggregate size and aggregate morphology by controlling the
type, number, and the rigidity of the nanoparticles DNA-capping. In protein systems, we have
utilized the novel three-fold symmetry of a series of genetically expressed knob domains of
Adenovirus, for controllable particle assembly and functionalization. The observed control over
assembly morphology and interparticle spatial properties in these systems may aid in the design and
construction of increasingly complex nanosystems with desirable biomedical, optical and electronic
applications.

401. GdDTPA-TAA Functionalized Nanoparticles as MRI Contrast Agents

Talha S. Siddiqui and Marc Walters, New York University, New York, NY

Magnavist™ a complex of diethylenetriaminepentaacetic acid (DTPA) and Gd³⁺ is a clinically
approved contrast agent for magnetic resonance imaging (MRI). We have formed a derivative of
DTPA that allows it to bind to silver or gold nanoparticles through a thiocystic acid linkage (GdDTPA-
TAA). The resulting contrast agent, GdDTPA-TAA, was bound to a 10nm diameter Ag nanoparticles.
The ligand and its Gd complex were characterized by 1H and 13C NMR spectroscopy, electrospray
ionization mass spectrometry (ESI-MS) and IR spectroscopy. The production of this type of construct
opens the way for engineering increased specificity in a MR contrast agents.
402. Towards a SERS-Based Nanobiosensor for Organophosphorus Compounds

Melek Erol, Henry Du and Svetlana A. Sukhishvili, Stevens Institute of Technology, Hoboken, NJ

We report on Surface-enhanced Raman Spectroscopy (SERS) based detection of p-nitrophenol (PNP), the end product of an enzymatic reaction of the acetylcholinesterase and the paraoxon (an organophosphorus insecticide), in a ppt/ppm concentration range using surface-immobilized Ag nanoparticles. Ag nanoparticles were synthesized by a modified Lee and Meisel method, and immobilized on the glass cover slips using the intermediate layer of an adsorbed polycation. Our XPS results indicate that significant oxidation of the Ag nanoparticle surface occurred when the substrate was kept in water under ambient conditions, and that such oxidation could be inhibited by purging the aqueous solutions with argon gas. We found that the oxidation of the Ag nanoparticle surface strongly affected the adsorption and orientation of PNP molecules. Specifically, vibrational spectra of argon-purged substrates indicated flat orientation of PNP molecules at sparse surface coverages, which was not observed with oxidized substrates. The oxidation state of Ag nanoparticles also had a dramatic effect on the limit of detection (LOD) of PNP, with the LOD of ~1 ppt and ~10 ppb for the argon-purged and the oxidized Ag surfaces, respectively. Significantly lower detection limit and the flat orientation of PNP molecules at unoxidized Ag surface both reflect stronger binding of PNP with the pristine Ag surface, probably due to charge transfer interactions between the aromatic ring of PNP molecules and the metal surface.

403. Tailored Bionanocomposites for Applications in Tissue Engineering, Drug Delivery and Bone Materials

Karen T. Johnson and Ipsita A. Banerjee, Fordham University, Bronx, NY

Nanostructures were self-assembled in various media from the newly synthesized bolaamphiphiles, bis(N-alpha-amido-threonine)-1,3-propane dicarboxylate and the corresponding 1,7-heptane dicarboxylate. The self-assembly process was examined under varying pH conditions as well as in organic and mixed solvent systems. The nanostructures obtained were analyzed by various analytical methods. The range of sizes of the self-assembled structures were examined used dynamic light scattering. In particular, the nanotubular structures obtained were then functionalized with mucin, a highly glycosylated protein. The main goal of this work was to design mucoadhesive nanotubes and nanovesicles based on specific biological and physicochemical properties to achieve optimal mucoadhesion in the aqueous buccal environment. Since adhesion to the buccal surface is dependent on many conditions including hydrophilicity and charge, the bionanocomposites obtained after binding mucin to the nanostructures were examined. The samples were analyzed by AFM, TEM as well as via infrared spectroscopy. The nanotube to mucin ratio was also varied. It was found that the mucoadhesion was maximum when the ratio of mucin to nanotube was 2 to 1, after pre-hydration. Such biomaterials can be potentially useful as scaffolds for tissue engineering and for drug delivery.
**Session Overview:** HPLC separations are accomplished when there are significant differences in the interactions of analytes with the stationary and mobile phases. There are numerous options that can be undertaken in accomplishing a successful separation with respect to choice of separation mode, mobile phase components, and particularly stationary phase. However, the availability of so many options can in itself be an encumbrance. This symposium will address current means to facilitate, expedite, and optimize both chiral and achiral separations including the use of high throughput screening methodology and the implementation of software optimization and peak tracking tools.

### 404. Comprehensive LCxLC for the Analysis of Semi-Volatile Compounds

**Luigi Mondello**, University of Messina, Messina, Italy

Single column chromatographic procedures are widely applied in the analysis of complex matrices. Although such approaches often provide satisfactory results, the complexity of many samples exceeds the separative capacity of any monodimensional system.

A typical comprehensive analysis is achieved, generally, on two independent columns connected by means of a special transfer system located between them. The type of interface used is linked to the specific methodology (comprehensive GC, comprehensive LC, etc.). The function of the transfer system is to isolate and then “inject” continuous primary column fractions onto a fast second dimension. In order to achieve comprehensive analysis and to preserve the 1D resolution, the bands injected onto the secondary column must undergo elution before the following 2D analysis. During the development of each 2D separation, the interface is engaged in the following isolation process.

Various comprehensive chromatographic applications on different natural matrices will be presented. LC x LC applications will regard the development of a MD normal-phase (NP)-reversed-phase (RP)-HPLC system. Also in this case, the relative location of the components in the 2D plane is correlated to the chemical structure of the components, and allows positive identification. The contribution is focused on the most advanced multidimensional chromatographic techniques today employed. A series of applications on different samples will be described in order to demonstrate the effectiveness of these approaches.

### 405. Automated Chromatographic Method Screening and Development in Support of High Throughput Pharmaceutical Process Research


The increasing pace of drug discovery and development in recent years demands 'high throughput' pharmaceutical process research. Chromatography is an increasingly valuable tool for enabling and expediting pharmaceutical process research. In this presentation, a variety of automated tools for chiral and achiral chromatographic method screening and development to support in-process monitoring, high throughput analysis, cGMP release testing, and preparative chromatography will be presented. Topics to be covered include automated SFC and HPLC screening, fast chromatography approaches for high throughput analysis, multiparallel method screening and development using microfluidic HPLC, as well as automated databasing and data mining of chromatographic screening results.
406. Chromatography, Mass Spectrometry, Chemometrics, and Intelligent Automation

Michael McBrien, Andrey Vazhentsev and Alexey Galin, Advanced Chemistry Development, Inc., Toronto, ON, Canada

The principles of computer-assisted optimization of chromatographic systems are well established. The elution response for a given parameter/component is modeled according to defined response curves, and an optimum value for the parameter is produced based on the success criteria of the user. In theory, the combination of a modeling toolset with modern automation can produce tremendous power to create optimal chromatographic methods with little onus on the chromatographer. In practice, there are considerable challenges that must be overcome by any approach to the efficient combination of modeling and automation. Perhaps most notable of these challenges is the problem of component detection and tracking in the context of changes in chromatographic variables. As modern instrumentation offers opportunities for exploration of new selectivities due to extremely fast run times, it introduces more challenges with regards to efficient reduction of data to a manageable amount of elution data.

This paper will describe a new system that incorporates experimental design principles, chemometric data extraction of LC/MS and LC/UV hyphenated traces, chromatographic modeling, and automation. Several real-world examples will be used to illustrate the practical application of both MS and UV detection, good experimental design principles, and user interaction with method development projects.

407. Computerized Design of Robust Gradient HPLC Methods

Imre Molnar and Hans-Jürgen Rieger, Institute for Aplied Chromatography, Berlin, Germany

The development of gradient methods in HPLC is a difficult task. The transfer of the method requires deep understanding the process in the column and the factors, which are required for a safe operation in the routine lab. The talk will discuss the aspects, how to make reliable methods using computerized design in the development.

408. Rapid Automated HPLC Method Development

Ahmed Aced, Iris Technologies International Ltd / The ChromSword Group, Roswell, GA and Sergey Galushko, Dr. Galushko Software Entwicklung/ The ChromSword Group, Muehltal, Germany

The chromatographic separation of unknown sample mixtures can be challenging for the HPLC method developer if impurities or degradation products are present in the sample. Peaks of these compounds must be resolved from the peaks of interest, thereby increasing the complexity of the method development. In addition, when several methods need to be developed in a relatively short time, the analyst usually does not have enough time to achieve his goal with adequate accuracy.

ChromSwordAuto method development software integrated with LC, LC-MS and SFC instruments enables a rapid and unattended separation of complex mixtures in the reversed phase, normal phase, and chiral separation mode. In the off-line mode a chromatographer can start from structural formulae and properties of reversed-phase columns or from data of two runs. In the on-line mode the software controls HPLC amd SFC instruments and searches for optimal isocratic or(and) gradient conditions fully automatically.
409. Strategies and Systematic Processes to Develop Efficient, Sensitive and Robust HPLC Methods for Pharmaceutical Analyses

Jinjian Zheng and Abu Rustum, Schering-Plough Corporation, Union, NJ

Development of an efficient, sensitive and robust HPLC method for pharmaceutical analysis could be very challenging due to the sample complexity and stringent regulatory requirement. Here we reported the systematic strategies and processes to develop HPLC methods for pharmaceutical applications. These include: 1) Define separation goal; 2) Collect sample information; 3) Search for similar methods; 4) Design initial experiment; 5) Develop a preliminary method; 6) Screen HPLC columns to identify the most suitable stationary phase; 7) Optimize the HPLC parameters on the most suitable stationary phase; 8) Identify an alternate column; 9) Verify method validation characteristics; and 10) Assess column lifetime. An example was used to demonstrate successful method development by following the above approaches. We believe that systematic approach using ChromSword® and LC-Spiderling™ column switcher significantly improves the efficiency of HPLC method development, and ChromSword® simulation improves the possibility of developing a more efficient, sensitive, and robust method.

410. Automated Chiral Application, Databasing, Evaluation and Selection (ACADES)

Frank Riley, Pfizer, Groton, CT

Synthetic chemistry groups can produce a large number of compounds per year, putting a significant time pressure on support lines to avoid bottlenecks in method development and purification of compounds. The typical approach to development is chiral stationary phase (CSP) selectivity screening for a given sample followed by optimization of promising systems. This approach is efficient in terms of human effort, but incurs a cost in terms of instrument and compound time. In addition, when compounds are found to be problematic for the standard CSPs, considerable time can be spent investigating alternative systems. If a process can be used to target given selectivities in advance, initial screens can be tailored to the compound in question based on appropriate structural queries, increasing the probability of success initially.

Industrial Chemistry Symposium, I
Organizer: Steven R. Carlo Exponent, Bowie, MD

Session Overview: A forum for industrial or government chemists from any chemistry discipline, to present their work. The emphasis will be on the applicability of chemistry and your work to the real world.

411. Sugarcane Extract-- An Excellent Phytochemical Functional Foods

Chung Chi Chou, Dr Chou Technologies, Inc, South Huntington, NY and Wen Hong Gao, South China University of Technology, China, Guangzhou, China

Recent research has demonstrated relationship between the aging process and the damaging effects of free radicals on tissue cells, and the beneficial impact on blood plasma antioxidant capacity of the increased daily intake of antioxidant-rich foods. Two Japanese studies, published in 2001 and 2002 Sugar Industries Technologists Technical proceedings, have presented the physiological effects of
sugar cane extracts, viz. promotion of resistance against viral and bacterial infections, stimulation of immune response, protection against liver injuries and growth promotion in chickens.

The Oxygen Radical Absorbance Capacity (ORAC) method to quantify the antioxidant property, as promulgated by USDA scientists, has been used to rank (ORAC units/100 g) common foods: Prunes (5,770), and blueberries (2,400) top the list, trailed by such health food industry favourites as kale (1,770), spinach (1,260). ORAC values of various sugarcane products, as reported by Dr. Saska (Saska and Chou, 2002) of Louisiana State University, range from some 5000 (ORAC units/100g dried solid) to over 35,000, and antioxidants in concentrated sugarcane extracts obtained from cane juice was found to contain over one million ORAC unit (ìmole TE/100 g dry solids).

According to USDA research (Bank, 2005), ORAC value of an average serving of vegetables equals approximately 900 imoles TE, and that of fruit is approximately 3400 imoles TE. The estimated ORAC intake of the daily recommended nine servings of fruits and vegetables equals about 20,000 imoles TE.

This paper presents the physical chemical aspect of the antioxidants extraction methods from sugarcane products in a pilot plant operation.

412. The “WOW” Factor Secret behind Retail Cosmetics
John Gormley, Grant Industries Inc., Elmwood Park, NJ

How can a one ounce prestige-branded skin care product sell for a staggering retail amount and still retain incredible loyalty and repeat sales? The answer is ensuring a customers expectations were completely met or exceeded after using the product they were sold, otherwise, they would never buy it again. This is no small feat considering the high product price and the intensive or suggestive marketing involved behind the sale of product. All cosmetics are materials which involve chemistry, so the question becomes what “top-secret” chemistry is in the products that deliver such consistent value to the consumer? To be truthful, one “secret” ingredient class is silicone chemistry. But within the cosmetics industry, the secret is out since the majority of high-end cosmetics contain silicone chemistry in one form or another. The broad class of organo-silicone chemistry is in large part responsible for maintaining a profitable connection between actual product performance (eg. sensory) and the marketing expectations underpinning modern cosmetic products.

The aim of this presentation is to introduce the major areas of silicone chemistry used in the cosmetic and hair care fields, while providing a hands-on experience of touching the ingredients and products containing these ingredients. This presentation is based on the one given annually by the author at Fairleigh Dickinson University to chemists training for a masters degree in chemistry and science related to cosmetics and the greater personal care industries.

413. Creating Controlled and Sustainable Innovation for the Cosmetic Industry
Laurence Dryer, BASF Beauty Care Solutions, Stony Brook, NY

Novelty in the Beauty industry can be achieved in three ways: Doing it faster (e.g., melting cellulite in one week), doing it better (e.g., 90% improvement over placebo), or doing it differently (with a different technology that targets a new biological endpoints or uses a new plant or compound). Maximizing compound diversity is always a challenge, but it is one of the prevalent ways of our industry at this time.

Marine algae are a very popular source of biological activities and are used in numerous formulations targeting everything from anti-aging to slimming. However, sustainability and sourcing are often in question. Aquaculture has provided very reliable sources of marine organisms, but can often not go any further than Mother Nature has already invented. In order to add diversity to a natural source, we sought to marry a macroalgae with the yeast ferment of a microalgae and test the resulting brew
for biological activity. Such marriage, has in our hands, shown solid anti-aging capabilities, and we are only now beginning to uncover the diversity of activities and compounds we are putting to the service of Skin Care with this technology.

414. Application of Rheology and in-Vitro SPF Testing to Optimize Sunscreen Emulsion Formulation
Laura A. Spaulding and A. Christopher Pattillo, Energizer Personal Care, Allendale, NJ

Results from a formulation case study are presented to show how information from rheological studies can be utilized to help characterize a complex emulsion system. Viscoelastic rheological behaviors in conjunction with In Vitro SPF testing are studied to optimize a multi-component sunscreen emulsion formulation. Data from amplitude sweeps, flow curves, and dynamic frequency tests from an Anton Par Physica 301 Rheometer are discussed with corresponding SPF results generated from a Labsphere UV Transmittance Analyzer. Microscope pictures are presented to verify findings and provide a visual understanding of the results.

More specifically, the data generated was used to characterize the effects of a polymeric substance that varied in molecular weight and degree of ethoxylation. Examination of concentration dependence and comparison to appropriate controls in the experimental design enabled selection of the appropriate polymeric substance to be incorporated into a sunscreen emulsion composition that provided the highest SPF value. The ethoxylated polymeric materials had no inherent UV absorbing capability and had no affect on particle size at the low concentration levels in this investigation. Yet, not only did these ethoxylated polymeric substances increase the efficiency of the sunscreen filter system, one of the polymeric substances behaved in a synergistic manner causing a significant increase in the In-Vitro SPF.

415. Adventure in Product Development - Water-Based Primer for Coatings
T. Page McAndrew, Arkema Inc., King of Prussia, PA

A major aspect of industrial chemistry is product development. This comprises issues not usually part of academic chemistry: scale-up, manufacturing, and customer introduction. Primgreen(tm) 2 is a water-based primer for polyamide-11 powder coatings (Rilsan(tm) Fine Powder). Presented is the story of its development – from idea conception through commercialization. Emphasized are factors that led to success, in particular, relying on established chemistries, and good understanding of customers' needs.

416. Forensic Chemistry in the Investigation of Product Tampering
Jason E. Schaff, FBI Laboratory, Quantico, VA

Allegations of product tampering can be among the most complex and challenging cases handled in forensic laboratories. The vast majority of reported product tampering is, in fact, nothing of the sort, leaving the analyst in the unenviable position of trying to prove a negative. Yet, in instances of real tampering, the adulteration can take an almost infinite variety of forms. Tampering is usually thought of as the addition of some deleterious material to a product, but can also be the removal of a desired material from the product, or substitution of an ingredient of inferior quality for a specified component. Any of these forms of tampering has the potential to cause injury or death, even if that is not the intent of the perpetrator. Furthermore, when tampering does happen, an added or substituted agent can be almost any chemical entity imaginable, meaning that a thorough and conscientious investigation may require the application of an incredible variety of analytical techniques, from basic wet chemical color tests to analysis using top of the line instrumentation. This talk will provide an overview of key issues and considerations in the chemical analysis of alleged product tampering incidents, and will illustrate those points with examples drawn from real casework submissions at the FBI Laboratory.
417. Consultancy: A Prospective Career for Scientists and Engineers
Jennifer Vondran, PA Consulting Group, Princeton, NJ

Do you envision having a career that offers you a diversity of project experiences, traveling and networking opportunities, and the ability to provide insights into industry and global best practices? How about a profession that thrives on innovative thinking and creativity? Then technology consulting may be the answer for you!

Jennifer's presentation highlights the ins and outs of the technology consulting world (explaining what a technology consultant actually does), giving examples of client projects (emphasizing science and engineering applications), and how recent graduates can navigate and direct their own career paths. Technical, professional, and personal benefits of the consulting career will also be covered. Additionally, the presentation will provide insight and tips for how to succeed in any consulting environment.

Jason O. Clevenger, Exponent, Inc., Natick, MA

Analytical and physical chemistry play increasingly important roles in the field of failure analysis consulting. The global nature and growing technological sophistication of consumer and medical product development are two important drivers for the future growth of the area. Examples from recent Exponent work in the pharmaceutical, medical device, and portable power/battery sectors will be discussed, with an emphasis on showing that chemists can make significant contributions in a discipline traditionally dominated by mechanical and materials engineers. An overview of the opportunities as well as strategies for prospective chemists interested in entering the dynamic field of technical consulting will also be presented.

Photochemistry, I
Sponsor: Boston Electronics Corporation; Edinburgh Instruments Ltd.; HORIBA Jobin Yvon Inc.; Coherent Inc.
Organizer: Steffen Jockusch Columbia University, New York, NY

Session Overview: Photochemistry is an interdisciplinary research area, which includes aspects of organic and inorganic chemistry, material sciences, biochemistry, spectroscopy, physics and chemical engineering. The involvement of light brings these diverse fields together. The morning session of this photochemistry symposium focuses on environmental topics, luminescence sensors, and biological systems.

419. Photophysical and Photochemical Investigations of CO₂-Soluble Catalysts for the Reduction of CO₂ to CO in Supercritical CO₂
David C. Grills, Mark D. Doherty and Etsuko Fujita, Brookhaven National Laboratory, Upton, NY

The reduction of CO₂ into useful fuels and chemicals (e.g. CO, CH₃OH etc.) is an increasingly important field of research, particularly due to the twin problems of global warming and the world's rapidly depleting fossil fuel reserves. Our goal is to harness the Sun's unlimited supply of solar energy by using efficient photocatalysts to perform these reactions. We are developing homogeneous catalysts based on the general formula, [Re(CO)₃(4,4'-X₂-2,2'-bipyridine)L]¹⁺ (X = polyfluorinated substituents;
L = Cl⁻ (n=0), and various neutral ligands (n=1)) for the photoreduction of CO₂ to CO in supercritical CO₂. These compounds have been designed to exhibit a high solubility in supercritical CO₂, and thus they allow us to carry out the photoinduced reduction of CO₂ in the absence of conventional solvents, which have been shown to significantly hinder the catalytic cycle.

In this talk we will present the results of photophysical and photochemical studies on some of these catalysts, in both conventional solvents and supercritical CO₂. This includes nanosecond UV-vis transient absorption and time-resolved infrared spectroscopy to characterize the metal-to-ligand charge transfer excited state and the one-electron reduced species, which is formed by quenching of the MLCT state by an electron donor. The photocatalytic activities of the catalysts will also be compared to previously studied catalysts in this family.

This research was supported under contract DE-AC02-98CH10886 with the US Department of Energy.

420. Photocatalytic Reduction of Organic and Inorganic Compounds
Miguel Valenzuela, Sergio Flores and Omar Rios, Instituto Politécnico Nacional, Mexico City, Mexico

Organic synthesis through semiconductor photocatalysis has become an important research area in photochemistry in the last two decades. Significant examples of organic transformations employed for synthetic purposes are oxidation and reduction reactions, isomerization reactions, C-H bond activations and C-C and C-N bond forming reactions. The photocatalytic oxidation of organic compounds have been studied largely because the most common metal oxides and metal chalcogenide semiconductors have valence band edges that lie positive of the oxidation potentials of most organic functional groups. In contrast, photocatalytic reductions are less frequently found, because the reducing power of a conduction band electron is significantly lower than the oxidizing power of a valence band hole and because most reducible substrates do not compete kinetically with oxygen in trapping photogenerated conduction band electrons. The most significant and studied photocatalytic reductions have been water photoreductive hydrogen production, carbon dioxide reduction in presence of water to obtain methane and oxygen and nitrogen reduction with water to obtain ammonia and oxygen. In the present work we report three study cases for benzaldehyde, nitrobenzene and chromates carrying out the photocatalytic reduction in the presence of pure and modified titanium dioxide.

421. Optical Switches for Affinity-Switchable Molecular Interaction and Fluorescence Tracking
Jochen Mattay, Bielefeld University, Bielefeld, Germany

Photoswitches based on anthracene, diarylethenes and spiropyrans were synthesized and attached to supramolecular host molecules as calixarenes (1) as well as fluorescence dyes (2). Photoaffinity switching of 1 were studied in solution and on surface by means of AFM. Photochemical and photophysical investigations of 2 show that these compounds efficiently interact with the attached fluorescence dyes in order to achieve photoswitchable fluorescence.

422. An Exploration into the Structure and Photophysics of Hemilabile Coordination Complexes
Anthony Tomcykoski and Wayne E. Jones, State University of New York at Binghamton, Binghamton, NY

Luminescence chemosensors are a powerful tool for providing selective and sensitive detection of a variety of chemical stimulus. Hemilabile coordination complexes have recently been used as a new type of sensor that exhibits reversible binding in the presence of small molecule analytes. It has also been demonstrated that phosphine-ether hemilabile ligands coordinated to ruthenium (II) bipyridyl
systems produce luminescent signals dependent upon analyte-coordination. The inner-sphere coordination detection mechanism of the complex produces a multitude of ligand field states which in turn allow for a tunable ligand field. In the presence of H₂O, phosphine-ether hemilabile ruthenium complexes have shown spectral shifts in the MLCT band of [Ru(bpy)₂POMe]⁺² of 8nm to the red when titrated against H₂O 5% (v/v). The results suggest many sensing applications for these hemilabile complexes, for example as humidity and carbon monoxide sensors. This talk is to focus on the synthesis, structure, and photophysics of hemilabile complexes. An exploration into the structure and chemistry of hemilabile coordination complexes provides insight for potential applications of this novel sensor technology.

423. Use of Luminescence Resonance Energy Transfer to Identify Locations of Site-Bound Metal Ions in the Spliceosomal U2–U6 snRNA Complex

Nancy L. Greenbaum, Hunter College, City University of New York, New York, NY and Faqing Yuan, Florida State University, Tallahassee, FL

U2 and U6 snRNAs pair to form a phylogenetically conserved complex at the catalytic core of the spliceosome. Interactions with divalent metal ions, particularly Mg(II), at specific sites are essential for its structural stability, folding and catalytic activity. We used a new Förster Resonance Energy Transfer (FRET) method between site-bound luminescent lanthanide ions and a covalently attached fluorescent dye, as well as supporting stoichiometric and mutational studies, to determine the locations of site-bound Tb(III) on the U2-U6 complex. At pH 7.2, we detected three metal ion binding sites situated in: 1) the consensus ACACAGA sequence, which forms the internal loop between helices I and III; 2) the four-way-junction, which contains the conserved AGC triad, and; 3) the internal loop of the U6 intra-molecular stem loop (ISL). Binding at each of these sites is supported by previous phosphorothioate substitution studies and, in the case of the ISL site, by NMR-based structural studies. Binding of Tb(III) at the four-way junction and the ISL sites was found to be pH-dependent, with no ion binding observed below pH 6 and 7, respectively. This pH-dependence of metal ion binding suggests that the local environment may play a role in the binding of metal ions, which, in turn, regulates splicing activity.

424. New Chromophore Systems and Photoactive Compounds Arising from Chlorophyll Breakdown in Plants

Bernhard Kraeutler, University of Innsbruck, Innsbruck, Austria

The chlorophylls (Chls), the highly visible and photoactive “green pigments” of plants, are magnesium complexes of a unique macro-cyclic tetra-pyrrole ligand. Breakdown of these green “pigments of life” has attracted profound interest recently. As is established meanwhile, breakdown of chlorophyll in higher plants opens up the macrocycle and rapidly leads to colourless linear tetapyrroles called “non-fluorescent” catabolites (NCCs). Red and “fluorescent” (slightly yellow) tetapyrrolic intermediates are proposed to precede the NCCs in the common biochemical pathway, observed in senescent leaves and ripening fruit. However, during chlorophyll breakdown in most plants, photo-chemically interesting coloured or luminescent catabolic intermediates either are elusive or fleetingly existent only.

The lecture will mainly deal with the structures of the new chromophores contained in the Chl catabolites and with the result of preliminary studies of their photochemical properties.

Further reading


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**Spectroscopy of Biological Systems**

**Organizer:** Ruel Desamero York College, Jamaica, NY  
**Organizer:** Emmanuel Chang York College, Jamaica, NY

**Session Overview:** Advances in instrumental techniques are pushing the analytical boundaries for the spectroscopic study of biological macromolecules. Both the structure and dynamics of biomacromolecular assemblies are being probed with unprecedented detail using optical, NMR and mass spectroscopies. This symposium highlights some recent developments in the application of these cutting edge technologies to important problems in basic and disease-related biochemistry. The session will be headlined by Dr. David Cowburn of the NY Structural Biology consortium, and Dr. Bob Callender of Albert Einstein College of Medicine, and will include other leading speakers from industry and academia.

**425. Mass Spectrometry and the Bioprocessing of Vaccines and Therapeutic Proteins**

**Steven L. Cohen**, Merck Research Laboratories, West Point, PA

Advances in molecular biology and the many -omics fields promises to continually deliver new targets for drug development. Bringing these breakthroughs to the general public as useful drugs, however, entails an intricate path. This is particularly true for vaccine and therapeutic products which, unlike small drug molecules, can involve complex systems and very large biomolecules. Bioprocessing plays a key role along the path of developing these products by providing high-quality candidates for safety assessment, preclinical and formulation studies and for the clinical trials as well as developing production processes scalable for manufacturing of a licensed product. Analytical capabilities such as mass spectrometry must be at hand to ensure a well characterized and consistent product. Here, examples will be shown highlighting some of the key contributions made by mass spectrometry in the development and bioprocessing of Merck vaccines and therapeutic protein products.

**426. Dynamic Processes**

**David Cowburn**, New York Structural Biology Center, New York, NY, Taiwan

This proposal will extend the knowledge of the structure, in solution, of the protein kinases, Csk, and Abelson (Abl), and their complexes in intracellular signal transduction using contemporary NMR and molecular biology approaches, and new technologies. The last will extend segmental labeling using expressed protein ligation, and direct determination of segmental motion of multidomain proteins from relaxation studies and from residual dipolar couplings. The kinases to be studied and their close homologs are key targets for increased understanding of signal transduction in processes associated with human health - immune system signaling, the DNA damage response, osteoclast differentiation, and general cellular growth and differentiation control. These kinases are prototypical of many signaling molecules in that it consists of multiple functional modules, some of which are independently folded structural domains, and these interact both among themselves, and with other ligands, in complex ways which are not readily characterized by conventional structure determination methods. In this proposal, the focus will be on the medium resolution interaction of domains, understanding their role in modification reactions of phosphorylation, and dephosphorylation, the interaction of kinase control with ligands, substrates, adaptors, and the adjacent domains, and examination at high resolution in solution of those which are found amenable in solubility and complexity for complete structural and dynamic characterization.
427. EPR Measurements of Distances and Electronic Couplings in Biological Macromolecules

Dr. Donald J. Hirsh, Ryan Biczo, Xi Jun Chen and Steven Wisniewski, The College of New Jersey, Ewing, NJ

We report on a DNA-based model system for studying weak dipole-dipole and exchange interactions between a paramagnetic metal ion and a stable radical. The goal is to use the information gained from studying the electron spin-spin interactions in this model system to measure distances and electronic couplings in large protein complexes. Molecular modeling studies, spectroscopic measurements of the thermodynamic stability of the DNA duplex, and electron paramagnetic resonance (EPR) measurements of the spin-label dynamics are used to generate a picture of the model system's structure when dysprosium (III) is the paramagnetic metal ion. Electron spin-spin interactions are observed by both continuous wave and pulsed EPR over distances as large as 5 nm. Pulsed EPR experiments suggest that the exchange interaction makes a significant contribution to the spin-lattice relaxation of the spin-label at low temperatures (T < 77 K).

428. The Dynamical Nature of Proteins: Understanding the Physics of Enzymes

Robert Callender, Albert Einstein College of Medicine, Yeshiva University, Bronx, NY

It is widely recognized that the static structures of proteins yield substantial insights into how they function. It is also widely understood that considerable atomic motion takes place in proteins. A protein is not the single structure suggested by the static pictures, but rather consists of multiple structures interconverting on various time scales. This rich dynamical nature is crucial to understanding protein function but very little is really understood quantitatively about protein dynamics. The reason for this is that motions on a broad time scale, from femtoseconds to minutes, can be important, but there are both experimental and theoretical challenges in characterizing motion on such a broad time scale. It will first be discussed how the development of new experimental approaches in our lab and our collaborators, (1) initiating structural transformation in chemical systems (like laser induced temperature jumps and fast mixing devices) and (2) spectroscopic probes of structure (like time-resolved isotope-edited IR spectroscopy), permit the experimental characterization of atomic motion within proteins from 10 ps to minutes with considerable structural specificity. Then some specific studies on enzyme systems, focusing on lactate dehydrogenase, will be discussed relating dynamics to function.

429. Q-Space NMR Imaging Studies of Water in Elastin

Gregory Boutis, York College of CUNY, Jamaica, NY

Q-space Nuclear Magnetic Resonance imaging is a well-known non-invasive experimental technique allowing for structural investigations of a variety of complex systems relevant to problems in industry, material science and biology. The technique allows one to accurately measure the morphology of a confining pore and molecular diffusion rate of mobile molecules within interstices of a structurally complex system. In our laboratory we have recently designed a variable temperature NMR microscope capable of delivering gradient pulses on the order of 50,000 G/cm allowing for high resolution (less than 1 micrometer) scattering studies. Elastin is an insoluble and highly cross-linked protein in the extra cellular matrix responsible for the elastic properties of vertebrate tissues. This work focuses on probing the dynamics of waters of hydration in elastin, via q-space NMR imaging, to better the understanding its functional properties.
430. Fourier Transform Mass Spectrometry Identification of Disease Biomarker Proteins

P. Pevsner, G. Kruppa, T. Remsen, F. Naftolin, P. Kessler and A. Stern, New York University School of Medicine, New York, NY

The 'top-down' proteomics approach utilizes molecular and fragment ion mass data obtained by ionizing and dissociating a protein in the mass spectrometer for the characterization of protein sequences and post-translational modifications. The topdown data are far more specific than the more widely used 'bottom-up' approach. False-positive rates for the identification of proteins are lower with the top-down approach, and quantitation of multiply modified isomers is more efficient.

This report is concerned with the structural characterization of a protein, e.g., identifying and locating post-translational modifications or errors in the predicted sequence. The 'top-down' methodology can directly subject a mixture of proteins, even of >10 components to yield a spectrum of their molecular ions that indicates the molecular mass values of individual proteins. MS MS of the mass-selected ions of a protein then provides fragment mass values for its structural characterization.

The top-down approach may be the method of choice for quantitation of position isomers of proteins containing multiple modifications.

In previous communications we reported MALDI, 'bottom-up' approach yielding biomarkers of colorectal carcinoma, competent embryos, proteomic changes in acute stroke and retinoic acid treated breast cancer cells. This report details and compares those results with data obtained from a 12 T Brucker Fourier Transform mass spectrometer (FTMS) with the same samples, and additional samples from placentas of smokers and non-smokers and breast cancers treated with caffeic acid and caffeic phenethyl ester. Sample preparation is by high pressure extraction (Barocycler) from tissue with ammonium bicarbonate buffer, and HPLC electrospray loading of the FTMS.

Analytical Chemistry, General Session II
Organizer: Rosario LoBrutto Novartis Pharmaceutical Corporation
Organizer: Richard Thompson Novartis Pharmaceutical Corporation

431. Use of the Quartz Crystal Microbalance to Monitor Deposition from Organic Solvent

Hyun-Su Lee and Lynn S. Penn, Drexel University, Philadelphia, PA

The quartz crystal microbalance (QCM) is mainly used to monitor deposition from aqueous media and has been used only rarely to monitor deposition from organic media. We report the use of a QCM to monitor the formation of a self-assembled monolayer of 11-mercapto-1-undecanol on the surface of gold. This process was selected because it has been well studied by ex situ methods, such as ellipsometry and contact angle measurement. Because the layer deposited is thin and behaves fairly elastically, the change in frequency could be converted validly to mass deposited on the gold surface, thereby providing an average value for packing density. The value of 3.74 ± 0.47 chains/nm² determined in our laboratory compares reasonably well with the few existing experimental values determined from diffraction data and from electrochemical data. In addition, the QCM studies verified the two-stage kinetics found by those using ex situ methods: fast deposition of most of the mass followed by a very slow consolidation to form a stable monolayer.
432. Silver Coated Barium Titanate Beads as Surface-Enhanced Raman Scattering (SERS) Substrates for the Detection of Aromatic Thols
Jonathan Onuegbu¹, Charles Hosten¹, Angie Fu², Orest Glembocki² and Sharka Prokes², (1)Howard University, Washington, DC, (2)Naval Research Laboratory, Washington, DC

SERS-active surfaces were prepared by depositing a silver film using Tollon's reaction on to barium titanate beads. SERS activity of the surface was probed using three thiols (benzene thiol, 1,2 benzene dithiol, and 1,4 benzene dithiol) and rhodamine 6-G. The sensitivity of the SERS substrate was probed as a function of silver deposition time. The SERS signal was found to increase as the thickness of the silver film increased until maximum signal intensity was achieved. Additional silver deposition resulted in a decrease in the SERS intensity for all of the studied molecules. SEM measurement of the barium titanate surface as a function of silver deposition time indicate that maximum SERS intensity corresponded with the formation of large atomic scale islands of silver nanoparticles. Complete silver coverage of the beads resulted in a decreased SERS signal. The largest SERS intensity was observed at a deposition time of 30 minutes for the thiols and 20 minutes for rhodamine 6G.

433. Impedance Behavior of Conducting Polymer Electrodes in Vivo and in Vitro
Yohani Kayinamura and J. Faye Rubinson, Georgetown University, Washington, DC

A semiconductor|electrolyte interface is normally characterized by double layer capacitance leading to reactive impedance. This characteristic is undesirable for bioelectrode design. Since uncompensated charge exists only at the surface in steady-state for conductors, sensing is detrimentally affected, as the reactive impedance creates a high-pass filter intrinsic to series reactances. For this reason, the achievement of an Ohmic interface would be highly desirable. In our laboratory, we have achieved near Ohmic behavior for electrodes in vitro within a broad frequency range when modified with PEDOT film. We have suggested that ohmic behavior is primarily due to the identity of counterion, homogeneity and low porosity of the film. Using Electrochemical Impedance Spectroscopy and Raman Spectroscopy, we have conducted a comparative study of PEDOT and PEDOP based on their chemical identity and we found that the heteroatom may be playing a role in observed ohmic behavior for PEDOT by contributing to the formation of specific chemical states that affect the uncompensated charge at the surface. Results will be reported and discussed for PEDOT and PEDOP.

434. POLY(2,2’-BITIOPHENE)– Modified Electrodes for Detection of Neurotransmitters in the Presence of Interferents
Justyna Widera and Natana Podlubnaya, Adelphi University, Garden City, NY

Catecholamines are a class of neurotransmitters (1, 2-dihydroxybenzenes) secreted in the brain and their detection in the human body has been of great interest to neuroscientist. Altered levels of catechol and catecholamines are associated with mental and behavioral disorders. Catecholamines undergo oxidation within the usable potential range for aqueous electrochemistry and they can be detected by applications of electrodes modified with conducting polymers. These types of novel electrodes have shown many advantages over the conventional electrodes.

We will present the studies of optimization of preparation of poly(2,2’-bithiophene) modified electrode and their application in the detection of various neurotransmitters in the presence of common interferents such as: ascorbic acid, uric acid and acetaminophen. The stability and reproducibility of the polymer were studied by comparison of cyclic voltammograms of poly(2,2’-bithiophene) deposited on conventional size Pt and GC electrodes at various potentials ranging from 1.3 - 1.8V. The sensor selectivity will be demonstrated by showcasing the ability of the polymer to detect catechol, dopamine and various neurotransmitters in the presence of common interferents such as: ascorbic acid, uric acid or acetaminophen that are of industrial and medicinal interest. The
results of studies in concert with structural IR and SEM morphological studies suggest that poly(2,2'-bithiophene) obtained at 1.8V show most efficient catalytic behavior towards redox of catechol in presence of interferents.

The comparison of performances of poly(2,2'-bithiophene) and polythiophene derivatives based sensors for detection of catechol in the presence of various biological molecules of medicinal and industrial interest will be also demonstrated.

435. Enhancement in Teaching and Learning IR, UV-Visible and Fluorescence Spectroscopy through Animation and Virtual Experiments

Savitri Chandrasekhar, Michael Murphy Boyer, Julia Bronfenbrener and Amanda Peruzza, University of Toronto Scarborough, Toronto, ON, Canada

Computer technology allows us to mimic laboratory experiments and to provide video images of laboratory procedures in an easily accessible manner. The goal of the present study is to maximize student learning experience by developing virtual experiments in order to allow students to visualize and gain confidence prior to performing them in the laboratory. More specifically, the aim of this study is to develop multimedia courseware at the undergraduate level for Analytical Chemistry and Organic Chemistry. This method of introducing virtual experience through the use of technology is innovative and it is hoped that the lessons learned in this study will be applied in a variety of programs so that students can benefit more broadly across the curriculum. The virtual exercises, being self-paced, will provide students with an understanding of the principles of instrumentation and technique. To support the lecture component, video clips, animations and virtual demonstrations have been developed and these will be presented.

Although there have been several animations on Infrared spectroscopy, very few interactive exercises have been developed that directly address problem solving techniques. In addition, there have not been many studies made in the area of virtual experiments in UV-visible and fluorescence spectroscopy. In this project, virtual quizzes and experiments have been created to understand infrared, UV-visible and fluorescence spectroscopy as taught in an undergraduate curriculum. The details of these virtual experiments will be presented. Student comments in using multimedia tools will also be discussed.

436. The Next Generation Raman Microscope – Putting the Emphasis on Microscopy

Andrew Whitley, Eunah Lee, Fran Adar, Emmanuel Leroy and Emmanuel Froigneux, Horiba Jobin Yvon, Edison, NJ

The recent growth in popularity of Raman microscopy has been nothing short of spectacular. This growth is still accelerating due to the continued increase in performance coupled with significant reductions in cost. And now the size of the spectroscopic part of the system has been further reduced so that the entire system mounts on top of a microscope; the final result is a substantial increase in the performance/price ratio over the last few years, dramatically reducing the barrier to entry for the acquisition of a Raman system. A large proportion of analytical chemistry laboratories now own at least one Raman microscope or are about to purchase a one due to the quick return on investment this technique brings. We briefly revisit the advantages of the Raman technique highlighting applications from the pharmaceutical products, biomedical research, forensic analysis, contaminant identification and materials analysis including polymers, oxides and nanomaterials. These developments include rapid imaging using fast scanning and detector technologies that allow full Raman chemical images to be obtained in times two orders of magnitude faster than just a few years ago. We will also review the critical components that make up a typical Raman microscope and how, with the use of new state of the art components, Raman microscopes have shrunk in cost and size while offering much easier use and improved performance. The components reviewed will include CCD and EMCCD detectors, filters, lasers, fast scanning devices and rapid imaging software.
**Arthur C. Cope Scholar Symposium**

**Sponsor:** ACS Division of Organic Chemistry  
**Organizer:** Christian Rojas Barnard College, New York, NY

**Session Overview:** This symposium honors Cope Scholar Awardee Colin Nuckolls of Columbia University for fundamental studies toward molecular-scale electronic components and devices. Achievements from the Nuckolls group include self-assembled columnar structures having supramolecular dipoles and methodology for oxidatively cutting nanotubes and bridging the gaps with conducting organic fragments.

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**437. Glycal Metallanitrenes for 2-Amino Sugar Synthesis**

**Christian Rojas**, Barnard College, New York, NY

Various glycal 3-carbamates undergo rhodium(II)-catalyzed oxidative cyclization with incorporation of an alcohol nucleophile at the anomeric site. The overall process--amidoglycosylation--likely proceeds via a rhodium-complexed nitrene and provides 2-amino sugars having a 1,2-trans-2,3-cis stereoarray. Anomeric stereoselectivity and partitioning between amidoglycosylation and an undesired C3-H oxidation pathway depend on the relative stereochemistry within the starting glycal 3-carbamate and on the 4O and 6O protecting groups. Our studies have led us to a mechanistic paradigm for stereo- and chemoselectivity in these metallanitrene-mediated amidoglycosylations.

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**438. Through-Bond Interactions "beyond the Molecule"**

Ling Yuan¹, Yan Li¹, Andrew J. Lampkins¹, Jennifer K. Mattler¹, Khalil A. Abboud¹, Bobby G. Sumpter² and Ronald K. Castellano¹, (1)University of Florida, Gainesville, FL, (2)Oak Ridge National Laboratory, Oak Ridge, TN

We have developed a program to show how well-defined stereoelectronic interactions within molecules can be used to control self-assembly and emergent macromolecular behavior. Our latest results establish, through X-ray crystallography and high-level computation, that cyclic beta-aminoketones are useful molecular constructs for these studies. In the solid state, through-bond communication between donor and acceptor orbitals is reflected by understandable but dramatic changes in bond lengths, bond angles, and conformational preferences. When the right functional groups are then introduced to such "donor-sigma-acceptor" scaffolds, the molecules can form infinite and ordered networks in solution and the solid state. While the behavior is complex, it does respond to changes in molecular structure in ways that draw relationships between through-bond interactions and bulk properties. 1-Aza-adamantanetrones bearing naphthylamide groups have recently been prepared and are illustrative; the molecules aggregate in organic solvents at exceedingly low concentrations, and form gels at ~ 1 mM in toluene and benzene. The assemblies can be monitored for the first time by fluorescence spectroscopy and dynamic light scattering. The latest synthetic approaches for preparing the first differentially functionalized and even chiral molecules for ongoing studies will be reported.

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**439. Stretching the Limits of Chemical Reactivity through Mechanochemistry**

**Stephen L. Craig**, Duke University, Durham, NC

It has been known for decades that breaking high molecular weight polymeric materials often involves the scission of carbon-carbon bonds. To an organic chemist, this reaction outcome is pretty remarkable, and it underscores the fact that the macroscopic forces typical of daily life are many orders of magnitude greater than the interatomic forces that hold molecules together. This talk will
describe efforts to channel mechanical force into molecules and probe its influence on the rates of reactions involving those molecules.

**440. Reaction Chemistry Meets Lithography**

Colin Nuckolls, Columbia University, New York, NY

This talk will focus on using reaction chemistry and self-assembly as a means to construct nanoscale electrical devices. Through these studies we are developing molecular-based materials that forge a connection (both literally and figuratively) between the ultra-fine lithographic tools of the semiconductor industry and reaction chemistry that has largely driven the chemical and pharmaceutical industries. The meeting of these seemingly disparate fields is the nanometer length-scale, which holds the future for molecular electronics.

**Computational Chemistry for the Health of Humanity and the Planet, II - Energetics, Structure, and Functionality**

**Sponsor:** Healthcare & Life Sciences Department, Dell, Inc.; Chemistry Department, Brookhaven National Laboratory  
**Organizer:** Daqing Gao Queensborough Community College, Bayside, NY  
**Organizer:** Seogjoo Jang Queens College of the City University of New York, Flushing, NY

**Session Overview:** Computational chemistry has become an essential tool for biomedical research (health of humanity) and renewable energy research (health of the planet). This session discusses recent advances in understanding how the energetics and the structure are related to the functionality of important systems in these research areas.

**441. Computational Studies of Artificial Photosynthesis**

James T. Muckerman and Etsuko Fujita, Brookhaven National Laboratory, Upton, NY

Artificial photosynthesis is an area of research that seeks to replicate the natural process of photosynthesis that coverts sunlight, water and carbon dioxide into carbohydrates and oxygen. The visible-light driven splitting of water into hydrogen and oxygen and even the targeting of methanol as the product of CO2 reduction are sometimes included in the definition. There are two distinct approaches to realizing the goal of artificial photosynthesis: structural models vs. functional models of the natural systems. We are pursuing theoretical and experimental studies of functional models as exemplified in recent work on hydrogenase-inspired catalysts for H2 oxidation and proton reduction. But this is only one aspect of the complicated set of processes that replicate natural photosynthesis. We will present examples from our recent work in a number of aspects of artificial photosynthesis. We will discuss how the function of the chlorophyll arrays in plants might be replaced with a suitable band-gap-narrowed semiconductor photoanode in a photoelectrochemical cell, possibly with the aid of a molecular multi-electron water oxidation catalyst. We will also describe how the role of a reduced nicotinamide adenine dinucleotide phosphate (NADPH) co-factor as the carrier and donor of two electrons and a proton might be replaced by a photogenerated hydride donor to carry out the function of Photosystem I.
442. Solvent Structure on Surfaces and Its Relation to Protein-Ligand Binding

Tom Young¹, Robert Abel², Richard A. Friesner² and Bruce Berne², (1)Yeshiva University, New York, NY, (2)Columbia University, New York, NY

We explore the relationship between the complex electrostatic and van der Waals surfaces of proteins and the structure and thermodynamics of the water solvating these surfaces. We present a method for estimating the entropy and enthalpy of solvating these surfaces and demonstrate how this can be used to predict difference in binding affinities between congeneric pairs of ligands. This methodology gives a great deal of physical insight into the interplay of protein surface structure and the thermodynamics of solvation which plays an essential role in molecular recognition.

443. Characterization of the Solvation Dynamics of Ionic Liquids

Mark N. Kobrak, Brooklyn College -- CUNY, Brooklyn, NY

Ionic liquids represent a novel and intriguing class of liquids, yet little is known about their dynamic response to polarization. We present the results of molecular dynamics simulations that characterize the response of ionic liquids with respect to collective motion and translational vs. rotational dynamics. The approach represents an extension of the Steele analysis to binary liquids, and is comparative across a set of three ionic liquids of different character.

444. An Electrostatic/Geometric Mechanism for Compact Chromatin Stabilization

Tamar Schlick, New York University, New York, NY and Gaurav Arya, University of California, San Diego, La Jolla, CA

Eukaryotic chromatin is the fundamental protein/nucleic acid unit that stores the genetic material. Understanding how chromatin fibers fold and unfold in physiological conditions (divalent ions, with linker histones) is important for interpreting fundamental biological processes like DNA replication and transcription regulation. Using a mesoscopic model of oligonucleosome chains and tailored sampling protocols, we elucidate the energetics of oligonucleosome folding/unfolding and the role of each histone tail, linker histones, and divalent ions in regulating chromatin structure. The geometric/electrostatic mechanism by which linker histones, histone tails, and divalent ions consort to form chromatin higher-order structure involves: a rigid DNA `stem'' formed by linker histones to reduce nucleosome triplet angles and change the internucleosomal arrangement from a loose to tight two-start zigzag with straight linker DNA dominated by interactions between alternate nucleosomes; bends by divalent ions in some linker DNAs to accommodate linker DNA crossings at the fiber axis; and mediation of internucleosomal interactions by the H3 and H4 histone tails to shield electrostatic repulsion at the fiber core. The overall compact topologies reconcile features of the zigzag model with straight linker DNAs with the solenoid model with bent linker DNAs for optimal fiber organization and reveal a dynamic synergism of internal and external factors in chromatin compaction.

References
T Schlick, Molecular Modeling: An Interdisciplinary Guide, Springer-Verlag, New York, 2002;
445. Characterizing Drug Resistance Using All-Atom Molecular Dynamics Simulations

Robert C. Rizzo, Trent E. Balius, Rashi Goyal, Brian E. McGillick and Sudipto Mukherjee, Stony Brook University, Stonybrook, NY

Characterizing origins of drug resistance will ultimately enable the design and optimization of improved compounds. We are using computational simulation methods, followed by energetic and structural analysis, to probe the binding interfaces of protein-ligand complexes to determine which features are most important for molecular recognition and/or change upon point mutation. All-atom molecular dynamics, MM-GBSA binding energy estimation, and per-residue molecular footprinting are used to delineate which residues loose Coulombic energies, van der Waals energies, or H-bonds interactions at specific sites. Results will be presented for small molecule inhibitors which target the viral enzyme neuraminidase, the antic-cancer target EGFR, and for peptide inhibitors of the HIV glycoprotein gp41. Progress towards development of a docking test-set aimed at improving virtual screening will also be presented.

446. Quantum Calculations as a Tool in Structural Biology: Protons and Water in Biological Molecules

Michael E. Green, City College of the City University of New York, New York, NY

Quantum mechanical calculations are now sufficiently advanced that they can be used in a practical way to answer certain structural questions in biology. These calculations are particularly valuable for the positioning of protons, and the orientation of water. Water can be found in X-ray structures as a blob of electron density, but the length and strength of hydrogen bonds is not known, and the orientation of the hydrogens can at best be inferred from neighboring groups. However, these uncertain properties can be critical in understanding the behavior of a protein. Cooperative effects in hydrogen bonding are important; hydrogen bonds are modified as to length and strength by neighboring hydrogen bonds. We have found this effect to be equivalent to more than ± 2 k_BT, compared to the TIP3P potential, at room temperature. This has implications for the accuracy of molecular dynamics simulations of water in protein clefts, where the hydration cannot be assumed to be ergodic on the time scale of the simulation. Water wires are similarly not easily found in X-ray or NMR structures, but can be seen in quantum calculations. Water can also play a role in certain complexes, such as those between phosphate and arginine, as well as in modifying salt bridges in proteins. Examples of the use of QM calculations to understand structure, including water wires near a peptide, and the gating of an ion channel, will be discussed. Possible future extensions, to allow other functional calculations, including pK values, will also be briefly considered.

447. The Role of Modeling and Simulation in Bringing Drugs to Market

August Calhoun and Stefan Unger, Dell, Inc., Round Rock, TX

Computational techniques have long played a role in drug discovery by providing chemical and biological insight into complex problems. With the advent of experimental techniques that create vast amounts of data through discovery and into clinical trials, computation has been playing a larger role in interpreting and reacting to this data. The end goal of targeted treatments based on an individual phenotypic and genotypic profile drives further need for integrated techniques where multiple simulation and data interpretation methods can address medically relevant questions. This is currently the leading edge of innovation of not only developing, but delivering drugs to the market. Modeling and simulation pervade virtually all aspects of drug discovery, development, manufacturing and distribution.
448. Occurrence and Fate of Pharmaceutically Active Contaminants in the Hudson Basin
Bruce Brownawell, Xiaolin Li, Mark Benotti and Joseph Ruggieri, Stony Brook University, Stony Brook, NY

There has been growing concern about the detection and potential toxicological significance of pharmaceutically active compounds in sewage impacted surface waters and sediments. The concentrations of municipal wastewater-derived chemicals in the highly urbanized NY/NJ Harbor Complex are among the highest reported. In this paper we review some of the progress we have made in LC-MS-based detection of many classes of pharmaceutically active compounds, as well as work on understanding their fate in estuarine waters and sediments. Those studies have allowed us to assess the potential uses of wastewater contaminants as tracers of contaminant sources and transport in seawater (e.g., persistent and soluble pharmaceuticals) and in sediments (persistent and strongly sorbed quaternary amine disinfectants). These tracers have allowed us to further assess the sources and in-situ transformations of a wider range of contaminants, including natural estrogens and estrogenic detergent metabolites.

449. Biomagnetic Microcapsules for Environmental Applications
Silvana Andreescu, Matthew T. Ravalli and Cristina R. Ispas, Clarkson University, Potsdam, NY

Techniques of microencapsulation and fabrication of core-shell structures are widely used in drug delivery and in the pharmaceutical and cosmetic industry for the encapsulation of aromas and solvents. Their use for environmental purposes has been less exploited. In this presentation, we report the use of natural polymers in conjunction with magnetic nanoparticles for the development of multifunctional core-shell structures with immobilized enzymes for environmental applications including remediation and sensing of phenolics, pesticides and certain endocrine disrupting chemicals. The method is based on the combined use of enzymatic oxidation of the substrate and subsequent adsorption of the reaction product onto a specifically tailored core material. Thus, both enzymatic and chemical reactions are performed in the interior of a core/shell structure with multifunctional properties including biocatalytic and magnetic capabilities for easy removal and handling. These multifunctional structures are stable to ambient conditions and are environmentally benign. We will discuss the fabrication, optimization, and analytical performance of these systems for the sensing and remediation of environmental pollutants.

450. Sub-Lethal Effects of Anthropogenic Chemicals on Behavior of Winter Flounder (Pseudopleuronectes americanus) in New Jersey, New York and Virginia Estuaries
Daniel Wieczorek, Andrew F. J. Draxler, Ashok Deshpande and Thomas H. Cleary, NOAA-Fisheries, NEFSC, Howard Marine Sciences Laboratory, Highlands, NJ

Sediments in estuaries near industrialized areas along the east coast of the United States, such as Chesapeake, Raritan, and Newark Bays, are contaminated with an array of anthropogenic compounds including PCBs, PAHs and pesticides. Young-of-the-year winter flounder (Pseudopleuronectes americanus) that settle on contaminated sediments risk both sub-lethal and lethal effects. Accumulation of these compounds through respiration, ingestion, and transdermal uptake has the potential to alter behavior and reduce the ability of fish to perform essential
ecological functions. In controlled experiments using both wild-caught and laboratory-reared fish, we examined survival, behavioral responses, and contaminant accumulation by winter flounder (20-30 mm SL) that were exposed to sediments for 7 to 14 days. Fish held on sediment from Elizabeth River, Virginia displayed significantly higher mortality and higher predation by common or sand shrimp (Crangon crangon) than fish held on (relatively) uncontaminated York River, Virginia sediment. Fish held on Newark Bay, New Jersey sediment had a decreased ability to exploit an available food resource (Artemia sp. nauplii). Alteration of such essential behaviors is expected to reduce growth, increase susceptibility to predation, and limit long-term viability of a local population. Ongoing work seeks to determine variation among life history stages.

451. Temporal Trend of Perchlorate in Arctic Snow

Vasile Furdui and Frank Tomassini, Ontario Ministry of the Environment, Toronto, ON, Canada

Perchlorate is a known contaminant in both drinking water and groundwater, with natural and manufacturing sources. A strong oxidizer, perchlorate has been used in solid rocket fuels, airbags and fireworks. It was identified in low concentrations in the Chilean fertilizers, extensively used in the 19th century in the United States. Perchlorate has atmospheric sources, being reported previously in precipitations. As an anion, it is not expected to travel free for long distances in the atmosphere.

This study, designed to assess natural sources of perchlorate, considered collecting samples from a remote area, with no exposure to manufactured perchlorate. High Arctic ice caps receive contaminants solely from atmospheric sources, which allow determining the annual flux of perchlorate received through precipitation. Depth samples, dating between 1996 and 2005, were collected from Devon Island, Nunavut, Canada, in the spring of 2006. A direct injection, optimized ion chromatography-tandem mass spectrometry (IC-MSMS) method allowed detection of perchlorate in all samples. Concentrations were in low ng/L range and showed seasonality. This represents the first temporal trend reported for perchlorate in precipitation. The same samples were previously analyzed for perfluorinated acids, evidencing their atmospheric formation [1].


452. Surge in NOx Emissions on High Ozone, High Electric Demand Days

Thomas F. McNevin, New Jersey Department of Environmental Protection, Trenton, NJ

Elevated tropospheric ozone is a photochemical product of natural and anthropogenic volatile organic chemical emissions, and nitrogen oxides, which are mainly the product of fuel combustion. Examination of fossil-fueled electrical generating unit (EGU) operations before and during eastern seaboard heat wave events, which also tend to produce violations of the 8-hour ozone standard, reveals substantial daily as well as hourly variations in NOx emission profiles.

In general, baseload coal-fired units, many of which lack adequate NOx control technology are ramped up as load increases. Also as load increases, intermittently used residual oil-burning load-following boilers are deployed. As electric supply must always equal demand, intraday hourly peaks are generally met by generation from high NOx-emitting quick starting combustion turbines.

These phenomena are illustrated through comparison of operating profiles on an average day in June 2005 and the then record demand day of July 26, 2005, which also saw numerous ozone standard violations throughout the region. While peak hourly generation on the PJM power grid mid-Atlantic sector on the two days was 31,162 MW and 58,509 MW, respectively, NOx emissions from "peaking" EGUs in the 6-state Maryland-Connecticut region increased 145% from 492 to 1,202 tons, with a rate increase of 41% from 1.50 lbs NOx / MWh to 2.11 NOx / MWh.
Many of these high-emitting units have been in service since the 1970’s and even earlier. While lower emitting units of more modern vintage also are deployed in response to rising demand, their contributions to elevated NOx emissions are miniscule.

453. Hydroperoxide Measurements in Mexico City

Judith Weinstein-Lloyd1, Barbara Hillery2, Linda Nunnermacker3, Lawrence Kleinman3 and Brian Giebel4, (1) State University of New York, Old Westbury, NY, (2) State University of New York / Old Westbury, Old Westbury, NY, (3) Brookhaven National Laboratory, (4) Rosenstiel School of Marine and Atmospheric Sciences

Ozone is formed in the troposphere through a complex series of photochemical reactions involving oxides of nitrogen (NOx) and volatile organic compounds (VOCs). Atmospheric scientists conduct field measurements of these and other trace gases to validate and improve air quality models, which can then be used to test various mitigation strategies. One such field campaign occurred during March 2006 in Mexico City, one of the world’s largest cities. During the campaign, we determined concentrations of hydrogen peroxide, a photochemical termination product, aboard the U.S. Department of Energy research aircraft, and at a surface site northwest of the city. We observed surprisingly low peroxide mixing ratios near the source region, and decreasing abundance downwind of the city. However, relatively high values of peroxide were observed at takeoff and landing near Veracruz, a site with much higher humidity and lower concentrations of NOx. Our observations are consistent with the accepted mechanism of peroxide formation in a high-NOx, low humidity environment.

454. Spatial Distribution of Mercury Vapor in Homes in Brooklyn, New York

Clyde Johnson, Ramapo College of New Jersey, Mahwah, NJ

Elemental mercury is an important Persistent, Bioaccumulative and Toxic indoor pollutant. Measurements of ambient and indoor mercury vapor concentrations were made in 23 homes in Brooklyn, New York. For dwellings, measurements were performed at the breathing zone of infants, toddlers and adults (6”, 2’, and 5’, respectively). Measured mercury vapor levels ranged from 4 - 112 ng/m3 (mean: 25 ng/m3) for indoor air and N.D. (none detect) - 11 ng/m3 (mean: 5 ng/m3) for ambient air. On average, the indoor level was five times the amount found in ambient air. Little variation in mercury concentration with respect to height from the floor was observed.

455. Oil Sector Complex at An Old Salt-Chlorine Industrial Site

Abdul Rehman Khan1, Layla Al-Awadi1, Mohammad Al-Ramadhan2, Awadh Saeed2, Abdulraheem Al-Rashidi2 and Fatimah Al-Shatti2, (1) Environment and Urban Development Division, Kuwait, Kuwait, (2) Kuwait Petroleum Corporation, Kuwait

There is already large flux of population from rural areas towards cities based on economics, education and employment rendering high demand onto limited resources already urban communities are facing. To meet this highly increasing housing demand, multistory building complex are emerging in all mega cities in the world adversely effecting the supply of utilities (fresh water, clean air, electricity, waste disposal etc.). Kuwait is located in the northeastern corner of Arabian peninsula and weather is very hostile that forces people to spend 90% of their time in indoor environment and the design of buildings are highly energy intensive due to air conditioning load. There is new approach to seek renewable energy resources and optimizing the use of energy in residential and office buildings.

Kuwait Petroleum Corporation, KPC has financed a project to construct new headquarters, Oil Sector Complex, (OSC) that has been completed recently at an old salt-chlorine industrial location. This site has reminiscence history of Salt-Chlorine Plant using large number of mercury cells for electrolysis of brine to produce caustic soda and chlorine gas resulted into mercury pollution in marine waters and
silt sediment. The present study focuses on mercury measurements in air, water and sediments around this building and assessment of air quality and comfort levels in KPC building consisting of 22 floors, and adjacent building, Ministry of Oil of 14 floors facing Kuwait Bay.

**Frontiers in Nanoscience and Nanotechnology - Fabrication**

**Sponsor:** Momentive Performance Materials  
**Organizer:** Bhanu P. S. Chauhan William Paterson University  
**Organizer:** Kenrick Lewis Momentive Performance Materials, Tarrytown, NY  
**Presider:** Geraud Dubois IBM, San Jose, CA  
**Presider:** Gilbert K. Min Agilent Technologies, Inc., Philadelphia, PA  
**Presider:** Vinod M. Menon Queens College of CUNY, Flushing, NY

456. Welcome Remarks  
Geraud Dubois, IBM, San Jose, CA  

Welcome Remarks

457. Device Fabrication and Materials Synthesis in Bionanotechnology Approach; Biomimetic Assemblies of Peptide Nanowires and Nanoparticles and Their Controlled Mineralization at Room Temperature  

Hiroshi Matsui, City University of New York, Hunter College, New York, NY

Non-lithographic fabrications of devices such as electronics and sensor have been studied extensively by assembling nanometer-sized building blocks into the device configurations. While various nanowires and nanoparticles with superior physical properties have been synthesized as the building blocks, more reproducible methods to assemble them onto precise positions are desirable to construct nanodevices. We developed triple helix peptide nanowires to incorporate biomolecular recognition components (antibody), and our strategy is to use those functionalized peptide nanowires, which can recognize and selectively bind a well-defined region on antigen-patterned substrates, as building blocks to assemble nanoscale architectures at uniquely defined positions. In order for the application in electric device fabrications, after configuring device geometries with these nanotubes by the biomolecular recognition, we turned on the biomineralization function of peptides on the nanotube sidewall to develop various material coatings such as metals and semiconductors for electronics and sensor applications. It should be noted that the coating morphology such as particle-domain size and inter-particle distance on the nanotubes could be tuned by peptide sequences and conformations. Due to these peptides' catalytic function, some semiconductor coatings could be developed at room temperature on the nanotube. We also produced various nanoparticles by using ring-shaped peptide assemblies as enzymatic templates. These nano-rings mimic the nature to grow crystals inside the cavities at room temperature, which normally require high temperature to grow by other synthetic methods. This approach was demonstrated to grow various nanocrystals such as BaTiO3 and β-Ga2O3 at room temperature.

458. Biocompatibility Testing of a Novel Nanoporous Hemodialysis Membrane  
Loyd D. Bastin, Mark Schneider and Robert Morris, Widener University, Chester, PA

The vast and continual improvements in hemodialysis therapies since the 1940s have saved many patients struggling with end stage renal disease. Although the membranes currently used in industry, synthetic membranes such as polysulfone, perform well they still have several disadvantages. These performance disadvantages include intrinsic hydrophobicity (poor interaction
with blood) and asymmetric pore diameter (inconsistent mechanical performance) and shape. Huang et al. have developed a novel nanoporous alumina hemodialysis membrane that will optimize the effectiveness of dialysis therapy and improve the removal of middle and larger molecular weight substances. Before implementation, the biocompatibility of the nanoporous membrane must be evaluated. Here we report on our studies to determine the feasibility of the membranes use in kidney dialysis treatment. The biocompatibility tests performed to date are the testing for: the loss of serum proteins during the dialysis process, specifically testing the loss of albumin to the membrane; leaching of the alumina from the dialysis membrane into the blood; the loss of cholesterol and calcium during the dialysis process; membrane hemocompatibility (hemolysis), and the viability of the leukocyte population. To date, all tests indicate that the membrane is biocompatible through six hours of dialysis.

459. Carbon Nanostructures Made by Focused Ion Beams
Alexander Zaitsev, College of Staten Island, Staten Island, NY

Ion irradiation with doses exceeding the amorphization threshold converts carbonaceous materials into amorphous carbon, which may possess high electrical conductivity and considerably different chemical activity. This effect is especially pronounced in diamond, which is an insulating and chemically inert material. Because of very sharp threshold of the ion-induced diamond-carbon conversion, the interface between the amorphized carbon and the intact substrate may be as narrow as a few nanometers. Thus using controlled scanning of the ion beams focused at nanoscale, one can reproducibly fabricate complex carbon nanostructures of predetermined 2D geometry. It has been shown that the focused ion beam-written carbon nanostructures possess novel electronic properties: non-linear behavior, electronic switching, anomalously high conductivity, Coulomb blockade at elevated temperatures. These structures can also form regular hydrophobic-hydrophilic nanopatterns or functionalized nanoarrays, which may be used for 2D self-assembly of macromolecules and polymers. The FIB-written carbon nanostructures are discussed as novel devices for carbon-based nanoelectronics and sensorics.

460. Hybrid Photonic Devices Based on Colloidal Quantum Dot Composites
Vinod M. Menon, Queens College of CUNY, Flushing, NY

In this talk we will discuss our work on organic-inorganic hybrid photonic devices that allow us to exploit the properties of the two different material systems. Specifically we will report our recent work on photonic emitters and circuits that utilize colloidal quantum dot composites comprising of the inorganic quantum dots in an organic host matrix as the active medium. Some of the prototype devices that will be discussed include flexible microcavity laser, active micro-resonators integrated with passive waveguides, and quasi-periodic photonic structures. All of the above devices are fabricated using simple spin coating or soft-lithography. In addition to their specific functionalities, these novel device demonstrations and their development present a low cost alternative to the traditional photonic device fabrication techniques.

461. Synthesis and Self-Assembly of Smart Hydrogel Nanoparticles into Soft Opals
Xihua Lu, Northwestern University, Evanston, IL and Gao Qiu, Donghua University, Shanghai, China

Hydrogels have been extensively studied because of their abilities to simulate biological tissues and to swell or collapse reversibly in response to external stimuli. Without adding a coloring agent, the hydrogels exhibit optical transparency when they fully swell in water.

In this talk, I'll first present design and synthesis of novel hydrogel crystals with nanoscale lattice spacings, also known as “Hydrogel Opals”. Hydrogel opals were created by first making monodisperse N-isopropylacrylamide (NIPA) /2-hydroxyethylacrylate (HEAC) hydrogel nanoparticles and then covalently inter-connect the self-assembling nanoparticles in aqueous medium at room
temperature using crosslinker divinylsulfone (DVS). The inter-nanoparticle covalent bondings contribute to the stability of crystal structure, while self-assembly provides the crystal structure that diffract light, resulting in different colors of the hydrogel opals. As a result, the novel hydrogel crystals, which contain up to 97 wt% water, display a striking iridescence like precious opals but soft and flexible like “Jello”. The novel nanostructured hydrogels demonstrated the good mechanical strength and reversibly thermo- and compressive-induced stabilities of the hydrogel crystal structures.

Another interesting subtopic is about aqueous synthesis and self-assembly of monodisperse, interpenetrating (IPN) poly(NIPA-co-HEAC)/poly(acrylic acid) (PAA) nanogels in water. Novel IPN nanogels dispersions formed thermo-induced sol-gel transition above the phase transition temperature (Tp), 33°C, of poly(NIPA-co-HEAC) nanogels. More importantly, IPN nanogels self-assembled into giant colloidal crystals (up to 6 mm). Controlled growth of such large crystals will be of significant importance in fundamental studies and practical applications.

462. Solvent and Concentration Effects on the Two-Dimensional Network Formation of Benzene Carboxylic Acids

Gina M. Florio, Kimberly A. Stiso and Joseph S. Campanelli, St. John’s University, Jamaica, NY

The molecular self-assembly of a series of benzene carboxylic acid derivatives has been investigated at the liquid-graphite interface using scanning tunneling microscopy (STM) and computational chemistry methods. The two-dimensional self-assembled networks are stabilized through the formation of multiple, cooperatively strengthened hydrogen bonds. The structure of the monolayers formed on graphite by three different molecules – trimesic acid (1,3,5-benzenetricarboxylic acid), trimellitic acid (1,2,4-benzenetricarboxylic acid), and pyromellitic acid (1,2,4,5-benzenetetracarboxylic acid) – in a series of alkanoic acid and alcohol solvents and solvent mixtures will be described. In conjunction with STM imaging, Density Functional Theory calculations are used to shed light on the structural preferences of isolated analogue molecules and the energetics of conformational change. Solvent induced pseudo-polymorphism is observed in the assembly structures of trimesic acid and pyromellitic acid. Furthermore, the deterministic role played by the solution concentration on network formation will be discussed in light of these and recent literature results.

463. AFM-Based Nanofabrication Techniques: Non-Conventional Nanolithography


The precise creation of nanoscale structures is a fundamental requirement of research in nanotechnology. Most current nanolithography techniques can be grouped into three general approaches – optical-, electrical-, and mechanical-based nanofabrication. Surface probe microscopy, atomic force microscopy (AFM) in particular, offers the high resolution and control necessary for nanolithography applications by using electrical and mechanical approaches to create nanopatterns of material. While there have been many advances in one of the earliest AFM techniques, dip-pen nanolithography, other nanofabrication methods such as nanografting and tip-induced anodic-oxidation have proven to be useful for depositing a wide range of materials onto diverse surfaces in a controlled manner. We will present different strategies and examples of AFM-based nanofabrication that demonstrate the importance of various factors (such as controlled atmosphere, humidity, applied tip force, and write speed) and their limitations.
Session Overview: A panel discussion to allow conference attendees to find out everything they wanted to know about life in industry, but were too afraid to ask.

464. John Gormley’s Bio

John Gormley, Grant Industries Inc., Elmwood Park, NJ

John is Director of Regulatory Affairs for Grant Industries, Inc. He is a prolific technical writer and contributes to the company’s patent writing, marketing and advertising projects. Gormley is the webmaster for Grant’s web site (www.grantinc.com) and enjoys developing new products for Grant’s Hair Care business unit. His main scientific interests are polymer chemistry and vitamin biochemistry. John enjoys teaching the silicone chemistry module at Fairleigh Dickenson University for their cosmetics program. He has contributed to six issued US patents and six pending patents. John is a member of the SCC has supported various technical poster sessions and given a podium presentation at the IFSCC in Edinbrough Scotland on computational calculations for surfactant mildness.

He has a broad corporate background having previously held new technology positions at Uniqema, Mona Industries, National Starch, Unilever, and Abex Corp. He has contributed to a number of successful commercial projects, some replacing older materials with safer and greener options as well as being a proponent of businesses working closely with regulatory agencies to develop realistic solutions to on-going issues.

465. Jennifer Vondran’s Bio

Jennifer Vondran, PA Consulting Group, Princeton, NJ

Jennifer is an Analyst with PA Consulting’s Global Technology Group. Currently, she is working with an international pharmaceutical company in two areas: parametric evaluation of a powder nanomilling process and optimizing particle deagglomeration. She has co-authored articles about medical devices, automation, and sustainability, and will be writing her own pieces about risk assessment and new product ideas for the cosmetics industry later this year. Jennifer recently completed a dual BS/MS degree in Biomedical and Materials Science and Engineering from Drexel University in Philadelphia. Her masters research is featured in the Journal of Applied Polymer Science.

466. Page McAndrew's Bio

T. Page McAndrew, Arkema Inc., King of Prussia, PA

Page McAndrew is a Senior Research Scientist in the Corporate & External Research Group of Arkema Inc., in King of Prussia, Pennsylvania. His current assignment is development of applications for Graphistrength multi-wall carbon nanotube products. His prior positions include research positions at Air Products and Chemicals and IBM. He received his B.S. in Chemistry from King's College and Ph.D. in Chemistry from the University of Pennsylvania, under the direction of 2000 Nobel Laureate Alan MacDiarmid.
467. Jason Schaff's Bio

Jason E. Schaff, FBI Laboratory, Quantico, VA

Dr. Schaff has, since 1999, worked as a forensic chemist in the Chemistry Unit of the Federal Bureau of Investigation Laboratory Division. There he conducts a wide variety of chemical analyses supporting toxicological investigations of matters that come before the FBI. These cases include suspicious deaths on federal lands and of U.S. citizens overseas, public corruption allegations, support of coroners' inquests in U.S. possessions and territories, and support of local law enforcement criminal inquiries, including drug-facilitated sexual assaults, poisonings, and allegations of product tampering. Prior to joining the FBI, Dr. Schaff worked for two years at an International Olympic Committee accredited drug testing lab associated with the Indiana University Medical Center. There he conducted fundamental research on mass spectrometry of anabolic-androgenic steroids and worked on development and validation of new analytical methods for exogenous steroid identification in urine.

468. Jason Clevenger's Bio

Jason O. Clevenger, Exponent, Inc., Natick, MA

Jason O. Clevenger is a Managing Scientist in the Mechanics and Materials Practice of Exponent Failure Analysis Associates. Dr. Clevenger earned his Ph.D. in Physical Chemistry from the Massachusetts Institute of Technology, and has worked extensively in the field of materials characterization, particularly for thin films and surfaces, with applications to the semiconductor, pharmaceutical, and medical device sectors. Prior to joining Exponent, he worked at Applied Materials, Inc, where he assisted the development of a plasma-based etching system for latest generation photomasks, as well as an amorphous carbon CVD film for sub-wavelength photolithography applications.

Inorganic Chemistry, General Session

Organizer: Roberto A. Sanchez-Delgado Brooklyn College and The Graduate Center, CUNY
Organizer: William H. Hersh Queens College of the City University of New York, Flushing, NY
Organizer: Zhaohua Dai Pace University

469. Further Study of Dr. Frankenstein's Reaction

Stephen A. Koch, State University of New York at Stony Brook, Stony Brook, NY

The reaction of Fe(II) with CN⁻ has been studied for more than three hundred years, making it the oldest reaction in synthetic chemistry. The case can be made that Dr. Frankenstein was the first chemist to study this reaction. Work in the author's laboratory has been directed toward the synthesis of analogs for the active sites in hydrogenase enzymes using the Frankenstein reaction.

470. Effect of Solvent Environment on the CO Band Position in the Infrared Spectrum of [Fe(CN)₄(CO)₂]²⁻

R. Viswanathan, A.M. Etra and J. Jiang, Yeshiva University, New York, NY

We present recent results on the effect of solvent environment on the IR spectrum of trans-[Fe(CN)₄(CO)₂]²⁻ using ab initio methods. Gas-phase calculations have been carried out on the metal complex with explicit solvent molecules ranging from a few to a number that is representative of a primary solvation shell. Using a Natural Bond Analysis (NBO) method, we find that the presence of
solvent molecules capable of hydrogen bonding to the cyano ligand of trans-[Fe(CN)₄(CO)₂]²⁻ results in an enhancement of the lone orbital electron density on the metal atom and a decrease in metal-ligand back bonding. Decrease in metal-ligand back bonding results in decreased population of the anti-bonding orbitals of the C-O bond. This leads to the strengthening of the C-O bond, the decreasing of the C-O bond length, and a blue shift in the CO band position. We show that the observed shift in the carbonyl peak position could be used to predict the number of nearest neighbor solvent molecules interacting with the metal complex.

471. Chemistry of Ruthenium and Osmium Cyanide Compounds

Daniel Amarante, Stony Brook University, Stony Brook, NY

The chemistry of [Ru(CN)ₓL(6-x)]ⁿ and [Os(CN)ₓL(6-x)]ⁿ complexes has not been well studied where L is a monodentate ligand and x is less than five, with a few exceptions. Recent progress has been made in developing the chemistry of iron cyanide complexes. These compounds have now been extended to ruthenium and osmium. Among the new compounds which have been synthesized and structurally characterized are: [PPN]₃[RuII(CN)₅(CO)], trans-[PPN]₂[RuII(CN)₄(CO)₂], trans-[PPN]₂[RuII(CN)₄(CO)(py)], trans-[PPN]₂[RuII(CN)₄(CO)(Im)] and [PPN]₃[OsII(CN)₅(CO)].

472. Tailoring Tripodal Ligands for Zinc Sensing

Zhaohua Dai, Pace University, New York, NY and James W. Canary, New York University, New York, NY

Zinc plays important role in biological processes. It is implicated in many diseases including brain diseases. Imaging zinc is becoming crucial to the elucidation of zinc concentration, distribution, kinetics and functions in cells and tissues. This presentation highlights recent advances in the development of picolylamine-based tripodal compounds as zinc sensors, especially our work in the field of sensing the invisible Zn(II) using steady-state fluorescence and chiroptical spectroscopy. Our approach has emphasized creative ligand design and detection schemes. Utilizing tris(2-pyridymethyl)amine -based N₄ tripodal ligands has provided a flexible system for engineering zinc sensors with improved sensitivity, selectivity and contrast.

473. Kinetic and Equilibrium Studies of Small Molecule Binding to (PCP)Rh¹ Pincer Complexes

Mark D. Doherty¹, David C. Grills¹, Kuo-Wei Huang², Dmitry Polyansky¹ and Etsuko Fujita¹, (1)Brookhaven National Laboratory, Upton, NY, (2)National University of Singapore, Singapore, Singapore

The binding of small molecules such as N₂, H₂, C₂H₄, etc., to coordinatively unsaturated transition metal centers is an important first step in their activation and conversion to useful chemicals. Thermodynamic and kinetic parameters governing this process in (PCP)Rh¹ pincer complexes have been examined using a variety of techniques including UV-vis flash photolysis, time resolved infrared (TRIR) spectroscopy and NMR spectroscopy. Results will be discussed in the context of a proposed mechanism for small molecule coordination to transition metal complexes.

The research carried out at Brookhaven National Laboratory was supported under contract DE-AC02-98CH10886 with the U.S. Department of Energy.

474. Reactions of Inorganic Tin (IV) and Lead (II) Compounds with Mono- and Bi-Dentate Ligands Having Nitrogen and Oxygen Donors

Burl C. Yearwood, Emily Bouret and Ronke Alo, LaGuardia Community College (CUNY), Long Island City, NY

It is proposed that Tin(IV) Chloride pentahydrate and Lead(II) Chloride will react with ortho and para aminophenol, p-toluidine (4-aminotoluene), and 2-tert-butyl-4-methylphenol either via an elimination
reaction or by adduct formation. The inorganic tin and lead compounds were reacted with the ligands in an alcoholic medium under aerobic conditions. The effect of temperature, differing mole ratios of metal to ligand, and reaction times were examined. The products of the metal-ligand reactions were characterized by melting points and Fourier Transform Infra-Red (FT-IR) spectroscopy. Solubility tests were also carried out. Melting point tests confirmed that the final products were different from the starting materials. Melting point tests, at various times after the reaction, showed that the products were relatively air-stable. Infra-red spectroscopy revealed that there was oxygen bonding to the Tin(IV) or Lead(II) moiety after replacement of the phenolic hydrogen, and that there was nitrogen bonding to the Tin(IV) or Lead(II) moiety after replacement of the aromatic amino hydrogen. The FT-IR spectra showed the disappearance of absorption bands corresponding to the phenolic OH group and/or aromatic amino group in the starting material. The FT-IR spectra also showed the appearance of tin-oxygen and tin-nitrogen absorptions. These results demonstrate that Tin(IV) Chloride pentahydrate and Lead(II) Chloride react with the mono and bi-dentate ligands used in this study to produce complexes via an elimination reaction, rather than adduct formation.

**Photochemistry, II**

**Sponsor:** Boston Electronics Corporation; Edinburgh Instruments Ltd.; HORIBA Jobin Yvon Inc.; Coherent Inc.

**Organizer:** Steffen Jockusch Columbia University, New York, NY

**Session Overview:** Photochemistry is an interdisciplinary research area, which includes aspects of organic and inorganic chemistry, material sciences, biochemistry, spectroscopy, physics and chemical engineering. The involvement of light brings these diverse fields together. The afternoon session of this photochemistry symposium focusses on supramolecular photochemistry.

**475. Supramolecular Photochirogenesis with Biomolecules**

**Yoshihisa Inoue**, Osaka University, Suita, Japan

Supramolecular approach to chiral photochemistry becomes more popular in recent years. Supramolecular photochirogenesis utilizes the noncovalent interactions both in the ground and excited states to photochemically transfer the supramolecular chirality to molecular chirality through the photoreaction occurring in chiral supramolecular environment. Supramolecular photochirogenesis with biomolecules is particularly attractive in view of their inherently chiral and well-defined 3D structures.

Serum albumins (SA) possess inherently chiral binding sites for endogenous and exogenous organic compounds, which can be exploited for supramolecular photochirogenesis. In this study, we chose 2-anthracencarboxylate (AC) as guest substrate, and first examined spectroscopically the binding behavior of AC toward various mammalian SA in aqueous buffer solution at pH 7 to characterize the available binding sites for AC. Then, the enantiodifferentiating photocyclodimerization of AC was performed in the presence of SA to give four stereoisomeric [4+4]-cyclodimers. We found that (1) mammalian SA possess 3-5 binding sites for AC of different affinities, stoichiometries, and chiral environment for the photoreaction, (2) the head-to-tail/head-to-head ratio critically depends on the SA used, and (3) SA-mediated photodimerization of AC affords optically active cyclodimers in excellent ee's.

In conclusion, the supramolecular photochirogenesis with SA is a promising strategy for asymmetric synthesis that is not only an attractive alternative to the thermal counterpart but also a unique methodology for obtaining chiral compounds through the electronically excited state in chiral low-entropy environment.
476. Singlet Oxygen Generation at the Porous Glass-Water Interface

Alexander Greer, City University of New York, Brooklyn College, Brooklyn, NY

I will describe our study of singlet oxygen photochemically generated at a water-solid interface, and how \(^1\)O\(_2\) then diffuses into the aqueous medium. Collaborations with Ruomei Gao and Harry Gafney revealed that singlet oxygen is generated cleanly in aqueous solution upon irradiation of a heterogeneous complex, \(meso\)-tetra(N-methyl-4-pyridyl)porphine adsorbed onto porous Vycor glass (PVG). Despite the effectiveness of this and other heterogeneous systems to generate \(^1\)O\(_2\), little is known about the dynamics of \(O_2\) quenching at water-solid interfaces. For example, how does the oxygen encounter the excited heterogeneous sensitizer? What mechanism (static or dynamic) converts ground-state oxygen into singlet oxygen, which then escapes into the surrounding aqueous solution? Our recent work with Jovan Giaimuccio and Jerry Meyer led us to conclude that \(O_2\) quenching at the glass-water interface differs from \(O_2\) quenching at the glass-gas interface. Sensitizer binding and distribution, and excitation intensity distribution within the porous glass are examined in the hopes of optimizing \(^1\)O\(_2\) formation and diffusion into the surrounding aqueous environment.

477. Photo-Fries Rearrangements of O-Cresyl Acetates in Isotropic Solutions and in Polyethylene Films. the Role of Reaction Cavities

Yuzhe Chen and Richard G. Weiss, Georgetown University, Washington, DC

The photo-Fries rearrangements of \(o\)-cresyl acetate (\(1\)) and 2-benzylphenyl acetate (\(2\)) have been investigated in two unstretched and stretched polyethylene (PE) films and in isotropic solutions. For example, irradiation of \(1\) yields principally \(o\)-cresol, \(o\)-xylene, 3-methyl-2-hydroxyacetophenone (\(2\)-PF) and 3-methyl-4-hydroxyacetophenone (\(4\)-PF) in isotropic solvents, but \(2\)-PF dominates in PE films, especially in stretched PE films. The influence of variables, such as the degree of film crystallinity, film free volume, and the unstretched/stretched state of the films, on the rearrangements has been explored. The selectivity of the photo-Fries rearrangements of \(1\) is higher in PE films than in isotropic solutions, and increases with degree of crystallinity of the films and upon film stretching. \(o\)-Cresol, a product from cage-escape of the initially generated aryloxy and acyl radical pairs, and \(o\)-xylene, a product from concerted decarboxylation, are formed in yields that depend upon the nature of the films. These and other results will be discussed.

We thank the U.S. National Science Foundation and the China Scholarship Council for their support of the research.

478. Controlling Photochemistry with Weak Non-Covalent Forces and Confined Spaces

Vaidhyanathan Ramamurthy, University of Miami, Coral Gables, FL

Life sustaining highly specific chemical reactions occur in the confined and organized medium of protein. Our projects aimed at achieving similar selectivity in photochemical reactions explore the use of readily available hosts that bear similarity to biological environment. In our laboratory, spatially confined cavities provided by crystals, zeolites, and water-soluble cyclodextrins (natural and functionalized), organic hosts such as cucurbiturils, cavitands, cholic acid micelles, and dendrimers are currently being explored as reaction media.
In this talk selectivities obtained in photoreactions conducted in aqueous medium using a water soluble deep cavity cavitand (octa acid) as host (shown below) will be presented. Photochemistry and photophysics of aromatics, alkenes and carbonyl compounds included in the above host system are distinctly different from that in isotropic solvent medium. Photofragmentation of dibenzyl ketones, geometric isomerization of stilbenes, singlet oxygen mediated oxidation of cyclic olefins would be used as examples to illustrate the power of a confined space and weak C–H---π interaction in controlling chemistry.

479. Controlling Photoreactivity of Coumarins in Water Soluble Nano-Cavities

Sivaguru Jayaraman and Nilotpal Barooah, North Dakota State University, Fargo, ND

This presentation will focus on ways of controlling photoreactivity of coumarin derivatives within cucurbit[8]uril (CB[8]) nano-cavitie s. Substituted coumarin derivatives that are either neutral (7-alkyl, 6-alkyl, 7-hydroxy or 6-hydroxy) or cationic (7-ammonium or 6-ammonium) form 1:2 host-guest complex with CB[8], that are completely soluble in water and are characterized by NMR spectroscopy. Direct irradiation of these coumarin-CB [8] complexes in water gives anti-head-to-tail (anti-HT) adduct as the major product, which is again characterized by NMR spectroscopy. Preferential formation of anti-HT adduct within cucurbiturils, not generally observed upon direct irradiation in isotropic media, highlights the role of CBs in altering photoreactivity of coumarin derivatives. Selective formation of coumarin adducts (4-different adducts are possible) in different organized assemblies is generally unpredictable. Based on reported crystal structure parameters and optimized structures for various coumarin adducts, it is speculated that the available free space within CB[8] nanocavity facilitates formation of the anti-HT 5. Employing CBs as a template is a powerful tool to control photoreactivity of various substituted coumarin derivatives leading to selective formation of anti-HT adduct, which is not generally observed in other isotropic media.

480. From Molecular to Supramolecular to Superdupermolecular Organic Photochemistry

Nicholas Turro, Columbia University, New York, NY

The reactions of carbon centered radical pairs often involve diffusion controlled combination and/or disproportion reaction which are non-selective. A geminate triplet geminate pair of radicals is produced by the photolysis of suitable ketones. The reactions of such geminate pairs can be controlled though the application of supramolecular concepts which emphasize non-covalent interaction to "steer" the geminate pair toward a selected pathway. In addition, "superdupermolecular" concepts, which emphasize the control of radical pair reactions and spectroscopy through the orientation of electron spins, can be employed to further control the course of geminate pair reactions. Examples of control of a range of the selectivity of geminate radical combinations, which form strong covalent bonds, through supramolecular and superdupermolecular effects will be presented for the photolysis of ketones adsorbed in the supercages of zeolites.
481. Polycarbosilanes as Ceramic Precursors and Low-K Dielectric Materials

Leonard V. Interrante, Rensselaer Polytechnic Institute, Troy, NY

Our efforts over the past 20+ years on the synthesis and study of polycarbosilanes has led to the development of a precursor for SiC that is now being produced and used commercially to fabricate ceramic composites for a variety of applications, on earth, such as friction materials (brakes) for motorcycles and other land vehicles, and in space, in an emergency repair kit on the U.S. space shuttle. The basic research that led to the discovery of this precursor (a hyperbranched polycarbosilane), as well as the applications that have resulted, will be described, along with the results of our more recent efforts to employ a novel series of cyclolinear polycarbosilanes as a source of low-k materials for integrated circuits.

482. Organic Electronics for Early Detection/Diagnostics

Kalle M. Levon, Polytechnic University, Brooklyn, NY

Electrically conducting polymer based electrodes in potentiometric detection of macromolecular binding processes are important novel electronic components for early diagnostics of diseases or biological warfare agents.

Biological molecules like proteins, DNA and lipids have strong ionic components in their molecular structures and electrostatic interactions between such biological molecules play important roles in functional binding processes. Immunosensors have been developed based on monitoring pH changes during the metabolic activities. Such potentiometric measurements follow potential changes evolved from ion activity during the binding with no electric current applied. The selectivity for the specific ion detection can be optimized using special membranes on electrode surfaces for the ion differentiation. We've developed another option for selectivity with surface imprinting; the analyte is “molded” on the electrode surface, washed out and the empty cavity of molecular parameters provides the antibody mimicking selective binding.

Antibody-antigen binding or in general protein-protein interactions cannot be diagnosed with metaloxides/electrodes as the electric double layer of less than 1nm allows protein adsorption studies but not interactions on protein surfaces. Organic electronics, electrically conducting polymers, are organic material with 3D composition of ions and electrons, and do have the electric double layer to limit the binding dimensions. We present how polyaniline electrodes can be used for the monitoring protein-protein interactions and also DNA hybridization. Protein studies include determination of the binding conditions for antibody-antigen reactions, and binding studies using lectins and heptapeptides selective for exosporium protein binding. DNA hybridization studies present our efforts on SNP detection, and hybridization with genomic target.

483. Metal Ion Affinity of Polymer-Supported Phosphoryl Oxygen in Nitric Acid Solution

Xiaoping Zhu and Spiro D. Alexandratos, Hunter College, New York, NY

The necessity in heavy metal ion reduction to meet stricter environmental requirements in wastewater treatment, nuclear fuel recycle and their selective recoveries has led to the increasingly attractive development of selective reagents. Knowledge about complexation mechanism of metal ions is essential to design new functional polymer with much higher adsorption efficiency and
specificity. Traditional ligand design mostly relies on the HASB principle, but the presence of non-ion-binding moieties might also greatly promote or disrupt the resulting metal bond strengths. Our work shows that introduction of additional hydroxyl group next to the neutral phosphate ligand (P=O) changes its polarizability, leads to significantly different metal ion affinity. Little Pb(II), Cu(II), Cd(II) are adsorbed on neutral phosphonate resin at pH 2, while their complexation is greatly enhanced with pentaerythritol resin phosphorylated with diethylchlorophosphate. Uranium(VI) adsorption at low acid solution proceeds through a coordination process and changes to ion exchange at high acid concentration. The unphosphorylated polyol resins have little metal ion affinity. It is clear that the metal ion complexation is dependent on both ion binding ligands (phosphoryl oxygen) and non-binding ligands (hydroxyl).

484. Ultrathin Responsive Polymer Films and Capsules

Svetlana Sukhishvili, Stevens Institute of Technology, Hoboken, NJ

We report on stimuli-responsive ultrathin polymer films and capsules with controlled pH-response properties and well defined mesh size, which have been fabricated via chemical crosslinking of hydrogen bonded layer-by-layer films. As surface-attached films, such hydrogels reversibly absorb and release large amounts of proteins in response to pH variations. As free-standing 3D structures (hollow capsules), they can encapsulate and controllably release a wide range of materials of various molecular weights, and show a distinct pH-dependent molecular sieving behavior. By varying the acidity and the chemistry of weak polyelectrolytes and/or neutral polymers, as well as the type of crosslinking, a high control of pH swelling including (1) the critical swelling pH, (2) the swelling amplitude; and (3) a complete switching swelling profiles in the pH scale can be achieved. The fine control over the response properties of such coatings enables their use in biomedical applications.

485. Polymer-Supported Reagents and Their Application to Environmental Remediation

Spiro D. Alexandratos, Hunter College, New York, NY

Polymer-supported reagents as crosslinked beads can be modified with ion-selective ligands and used to remove toxic metal ions from water in the environment. A series of three polystyrene-based reagents will thus be described with different immobilized ligands: N-methyl-D-glucamine for arsenic recovery, trihexylammonium for pertechnetate and perchlorate recovery, and phosphorylated pentaerythritol for uranium recovery.

486. Controlling Porphyrin Affinity in Designed Proteins

Ronald L. Koder, Christopher Negron and Andrew C. Mutter, The City College of New York, New York, NY

Active site design coupled with binary patterning is a simple, robust method for creating self-assembling functional proteins. Cofactor binding can be guided computationally, biomimetically, or using simple metal-ligand interactions. A new bioinformatic analysis of natural heme cofactor binding sites is introduced, and its application in the creation of high affinity heme, porphyrin and porphyrin-like macrocycles is presented. Application of this analysis toward the creation of artificial hemoglobins, oxygen-activating enzymes and solar energy conversion will be discussed.

487. Organoborane Functionalized Conjugated Polymers as Optoelectronic Materials

Frieder Jäkle, Haiyan Li and Anand Sundararaman, Rutgers University, Newark, NJ

Organoboron materials are known for their interesting electronic and photophysical properties, which have been exploited, for example, in the development of new linear and non-linear optical materials, emission and electron conduction layers in organic light emitting devices (OLEDs), and new probes
and sensors for anions. Interaction of the empty p orbital on boron with an organic pi-system has been shown to be at the origin of these unusual properties.

We have developed different modular routes for incorporation of electron-deficient boron centers into the main chain and side chain of thiophene-based polymers. The direct attachment of boron to the thiophene moieties provides for strong electronic coupling of the boryl groups and the organic polymer main chain. The photophysical properties, relative Lewis acidity, and environmental stability can all be fine-tuned by introducing suitable pendant aryl groups to the boron centers. The new polymers will be discussed in the context of potential applications as optoelectronic materials and as sensors for nucleophiles.

488. Guided Self-Assembly of Block Copolymer Thin Films
Alamgir Karim, National Institute of Standards and Technology, Gaithersburg, MD

A primary limitation of block copolymer films as templates for next generation electronic or data storage devices is the prohibitively long times required for thermally driven self-assembly and defect annihilation and long range order development. We demonstrate a rapid approach involving temporal zone (cold-hot-cold) annealing of block copolymer films well below their order-disorder transition temperature (T HOT << T ODT) that produces low defect concentrations, large grain size and a preferential alignment of the block microphase relatively rapidly [1]. Towards understanding some of the concepts involved in zone annealing under ideal conditions, we implement a time- and space-dependent mobility field in the relaxation of a diblock copolymer self-consistent field theory [2]. Promising results have been obtained by combining zone annealing with directed assembly on topographically patterned substrates. This combination results in the rapid development of long-range order which persists over the entire patterned area. The evolution of order in these templates is quantified using neutron reflection in conjunction with tomographic small angle scattering (T-SANS), and compared to scattering from model simulations to obtain a 3-D description of ordering within channel templates. The ability to rapidly achieve quantifiable long-range order in block copolymers (with inaccessible order-disorder transition temperatures) using non-destructive methods within templates suggests zone annealing as a robust nanomanufacturing method for guided self-assembly.


Poster Session III
Organizer: Irina Rutenburg Queensborough Community College, Bayside, NY
Organizer: Marie Thomas Queens College, CUNY, Flushing, NY

489. Determination of the Ionization Constant of Carboxylic Acids Using Microscale Freezing Point Depression Measurements
Junior Gonzales¹, Gopal Subramaniam², Paris Svoronos¹, David M. Sarno¹ and Pedro Irigoyen¹,
(1)Queensborough Community College - CUNY, Bayside, NY, (2)Queens College, Flushing, NY

Freezing depression measurements are generally used to determine the molecular weight of an unknown solute. This project involves the use of microscale probes to determine the ionization constant of four carboxylic acids using the experimentally obtained value of the van't Hoff factor of their aqueous solutions. The quantities used are as low as 0.1g of the carboxylic acid and 4mL of water. The carboxylic acids used in this study are dichloroacetic, trichloroacetic, maleic and malonic acids.
490. Influence of Cation Size and Charge in Ion-Pair Formation

Thomas Kim¹, Paris Svoronos¹, Gopal Subramaniam², David M. Sarno¹ and Pedro Irigoyen¹,
(1)Queensborough Community College - CUNY, Bayside, NY, (2)City University of New York, Queens
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The van't Hoff factor, which can be calculated from freezing depression measurements, can be used
to study the effect of ion-pair formation in inorganic salts. We studied the effect of ion-pair
formation in a systematic way by varying the size of the cation from lithium to potassium as well as
the change of the ion charge from +1 to +3 using various metal ions. Increasing the charge and
reducing the size of the ion results in a lower degree of dissociation in accordance to the theory. The
basic theory behind these experiments is covered in the General Chemistry I courses while the
experimental setup costs are very low and the data collection and time spent are minimal. Both the
results and challenges in adopting this experiment in an undergraduate laboratory are presented.

491. Studies on the Anion Size, Charge and Nature in the Dissociation of Salts in
Aqueous Solutions

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NY

Freezing point depression measurement has served as a routine experiment to measure the molar
mass of organic compounds in the freshman chemistry laboratory. Using this principle we carried out
a systematic study of the effect of anion size, charge, and nature in the salt dissociation in aqueous
medium. No significant difference in the dissociation of chloride, bromide and iodide salts was
observed. A similar study in determining the effect of hydrogen bonding and anion shape, using
nitrate, sulfate and carbonate salts was also conducted. These experiments require multiple freezing
point measurements in a short three-hour laboratory period. Modern temperature probes and digital
devices to record temperature changes allow the completion of these experiments during a first
semester undergraduate laboratory as a group activity learning exercise.

492. Thermal Intramolecular H-Atom Transfer across Hydrogen Bonds in Radicals

Theodore S. Dibble¹, Keith T. Kuwata², Emily Sliz² and Erin B. Petersen², (1)SUNY-ESF, Syracuse,
NY, (2)Macalester College, Saint Paul, MN

The HOCH2CH2OO• and HOCH2CH2O• radicals are prototypes of species that possess intramolecular
hydrogen bonds which enable intramolecular hydrogen shift reactions across those hydrogen bonds:

\[
\text{HOCH}_2\text{CH}_2\text{OO}• \rightarrow \cdot\text{OCH}_2\text{CH}_2\text{OOH} \ (1)
\]

\[
\text{HOCHRCH}_2\text{O}• \rightarrow \cdot\text{OCHRCH}_2\text{OH} \ (2)
\]

These types of reactions may play an important role in both the atmosphere and in combustion
systems. We have used density functional theory and composite electronic structure methods
determine that Reaction (1) has a barrier of 23.6 kcal/mol, and that Reaction (2) has a barrier of
22.7 kcal/mol. We used RRKM/master equation simulations to model the kinetics of chemically
activated HOCH2CH2OO• formed in the reaction HOCH2CH2• + O2; our calculations suggest that a
majority of chemically activated HOCH2CH2OO• undergoes a prompt hydrogen shift reaction across
the at pressures up to 10 Torr. This low pressure is relevant to many experiments.

Variational transition state theory (TST) calculations were carried out using the POLYRATE program.
For Reaction 1 at 298 K, the variational TST rate constant is \(~30\%\) lower than the conventional TST
result, and the \(\mu\)OMT method predicts that tunneling accelerates the reaction by a factor of 3. TST
calculations on Reaction (2) reveal no variational effect. Tunneling is very important in Reaction (2);
the 298 K \(\mu\)OMT transmission coefficient is \(10^3\).
493. Synthesis and Characterization of the Asymmetric Bimetallic Complexes\([(\text{tpy})\text{RuCl(dpp)Ru(bpy)}_2]^{3+}\) and \([(\text{tpy})\text{RuCl(bpm)Ru(bpy)}_2]^{3+}\)

Rustam Vachhani and Matthew T. Mongelli, Kean University, Union, NJ

Asymmetric bimetallic ruthenium (II) complexes of the form \([(\text{tpy})\text{RuCl(BL)Ru(bpy)}_2]^{3+}\), where tpy = 2,2':6',2''-terpyridine, bpy = 2,2'-bipyridine, and BL = the bridging ligand dpp (2,3-bis(2-pyridyl)pyrazine) or bpm (2,2'-bypyrimidine), have been synthesized. These complexes show low energy visible MLCT electronic absorbance and well separated oxidation potentials due to the metals being in different ligand environments. The synthesis, purification and characterization of these complexes will be presented.

494. An EPR and NMR Study of Supramolecular Effects on Spin-Spin Coupling Between a Nitroxide Incarcerated within a Nanocapsule with a Nitroxide in Bulk Aqueous Media

Judy Y. -C. Chen\(^1\), Nicholas Turro\(^1\), Steffen Jockusch\(^1\), Vaidhyanathan Ramamurthy\(^2\), Francesca Ottaviani\(^3\) and Jayaraj Nithyanandhan\(^2\), (1)Columbia University, New York, NY, (2)University of Miami, Coral Gables, FL, (3)University of Urbino, Urbino, Italy

A \(^{15}\text{N}\) labeled nitroxide derivative containing a benzophenone chromophore was incarcerated into an octaacid nanocapsule, which was confirmed by \(^1\text{H}\) NMR and EPR spectroscopy. Electron spin-spin superexchange between the \(^{15}\text{N}\) labeled incarcerated nitroxide and a \(^{14}\text{N}\) labeled free nitroxide in the external aqueous solution was observed by EPR spectroscopy. The observation of spin-spin coupling, through the walls of the carcerand is reflected in the simultaneous line-broadening of both the \(^{15}\text{N}\) labeled and \(^{14}\text{N}\) labeled nitroxides. The computer-assisted analysis of the EPR data further provides direct information on the motion and the polarity of both the incarcerated paramagnetic nitroxide and the nitroxides in the external bulk aqueous phase. We also show how communication between an incarcerated guest and molecules in the bulk solvent can be enhanced or inhibited by supramolecular factors such as Coulombic attraction or repulsion between a charged guest@host complex (incarcerated \(^{15}\text{N}\) nitroxide) and charged molecules in the aqueous phase. In addition, time resolved EPR experiments were performed, where incarcerated \(^{15}\text{N}\) nitroxide labeled benzophenone was excited by laser pulses to generate spin polarized \(^{15}\text{N}\) nitroxides. The spin polarization of the incarcerated \(^{15}\text{N}\) nitroxide was transferred to a \(^{14}\text{N}\) labeled free nitroxide in the external solution.

495. Investigation of Mono- and Bimetallic Ruthenium Complexes with the Facial Terminal Ligand Tris(1-pyrazolyl)Methane

Theresa Yi and Matthew T. Mongelli, Kean University, Union, NJ

Ruthenium (II) complexes of the form \([(\text{tpm})\text{RuCl(BL)}]^+\) and \([(\text{tpm})\text{RuCl}_2(BL)]^{2+}\), where tpm = tris(1-pyrazolyl)methane and BL = the bridging ligand dpp (2,3-bis(2-pyridyl)pyrazine) or bpm (2,2'-bypyrimidine), have been synthesized. The terminal ligand tpm has a facial arrangement which should change the properties of the complexes over the more common meridional arrangement seen with the tpy (2,2':2'',6''-terpyridine) terminal ligand. The synthesis, purification and characterization of these complexes will be presented. Comparison of previously known tpy complexes and the newly synthesized tpm complexes will be investigated.
496. ANALYSIS of the Alternation of Vibration Modes on the Ring STRUCTURE of Mono-Substituted and Di-Substituted Benzene

Sharmaine Lewis, Yi Da and Ruel Desamero, City University of New York - York College, Jamaica, NY

The central aim of this study is to analyze the effect of peak shifts and intensity changes on the IR and Raman spectrum caused by mono- and di-substituted benzene ring structures. The presence of benzene plays a pivotal role in both biochemical and biological systems. Benzene provides the framework by which amino acids can be analyzed both structurally and functionally to detail the behavior of vibrations on substituted aromatic rings. This analysis will provide detailed information that will further expand the study of aromatic amino acids. Examination of aromatic functional groups in amino acids is essential because benzene is a core constituent of several essential amino acids such as tyrosine, phenylamine, and tryptophan. Analysis is achieved by examining the vibrational modes evident by IR and Raman simulations using the Gaussian software under DFT Restricted, BLYP 6-31G (d) conditions. The results of mono-substituted IR spectroscopic analysis to date have yielded significant splitting signals at 1650 cm\(^{-1}\) compared to the aromatic ring at the same absorption. The data will be analyzed in terms of its significance to the study of aromatic amino acids.

497. Synthesis and Characterization of the Asymmetric Bimetallic Complexes [(tpy)RuCl(dpp)Ru(phen)\(_2\)]\(^{3+}\) and [(tpy)RuCl(bpm)Ru(phen)\(_2\)]\(^{3+}\)

Julio Calixto and Matthew T. Mongelli, Kean University, Union, NJ

Asymmetric bimetallic ruthenium (II) complexes of the form [(tpy)RuCl(BL)Ru(phen)\(_2\)]\(^{3+}\), where tpy = 2,2':6',2\(^{\prime}\)-terpyridine, phen = 1,10-phenanthroline, and BL = the bridging ligand dpp (2,3-bis(2-pyridyl)pyrazine) or bpm (2,2\(^{\prime}\)-bipyridylpyrimidine), have been synthesized. The complexes have the potential to interact with biomolecules such as DNA. The phen ligand should increase the light absorbing ability over terminal ligands such as 2,2\(^{\prime}\)-bipyrimidine. The synthesis, purification and characterization of these complexes will be presented.

498. Computational Study of Structural Modifications to a Novel Class of Paramagnetic Chemical Exchange Saturation Transfer Agents

Whelton A. Miller III, Zhiwei Liu and Vojislava Pophristic, University of the Sciences in Philadelphia, Philadelphia, PA

MRI is a non-invasive tool used by the medical community to diagnose disease. Imaging agents, usually chelates, are used to enhance MRI signals. Our study focuses on the physical basis of MRI signal enhancement induced by structural modifications of a novel class of Paramagnetic Chemical Exchange Saturation Transfer (PARACEST) agents. With these agents, the MR image is modified by magnetization transfer between the H\(_2\)O molecule bound to the EuIII(DOTA) chelate and bulk water, which is inversely proportional to the rate of H\(_2\)O exchange between the bound and bulk H\(_2\)O. The water exchange rate depends on the size, the coordination geometry of the lanthanide ion and the electronic properties of the groups attached to the coordinating pendant arm. We present here a computational study of the effect of attaching two pendant arms in either a diagonal or adjacent fashion, rather than having a single pendant arm as well as the effect of chemical modifications of the para-substituents in the coordinating pendant arms on the CEST signal. The effect of simple electron-withdrawing (e.g. nitro) and electron-donating (e.g. methyl) substituents chemically attached to the chelate arms is quantified by correlating the experimental CEST signal with charge transfer interactions in the coordinated water-chelate system computed from quantum mechanics. This study reveals the origin of the substituent effect on the CEST signal and the electronic structure of the complex.
499. Building Aromatic Oligoamide Foldamers

Jessica Amber Geer¹, Zhiwei Liu¹, Jhenny Galan², Jayme Wildin¹, Guillermo Moyna¹ and Vojislava Pophristic¹, (1)University of the Sciences in Philadelphia, Philadelphia, PA, (2)University of the Sciences in Philadelphia, Phila, PA

Over the past ten years, synthetic oligomers and the way that they fold in solution have been of great interest. We investigate synthetic oligomers comprising of benzene rings connected by peptide bonds, which can be designed to have medical functions. The torsions that occur around the backbone of these molecules control their shape, which in turn controls their biological function. Therefore, our current focus is on the torsions related to the backbone bonds and how the nature of benzene substituents influences these internal motions.

Presented here is a computational study of ortho-methoxy benzamide derivatives with side chains on the amide nitrogen systematically grown. The torsional profiles related to the backbone dihedral angles are obtained using ab initio calculations and subsequently applied in force field parameterization. In addition, we discuss the conformational distribution obtained from molecular dynamics simulations based on modified force field, for both the model compounds and related oligomers in aqueous solution. This approach helps us study the effects of side chain lengths and charge on the flexibility of the backbone, therefore on the conformational distribution of related synthetic oligomers.

500. Reactivity of Tris(trimethylsilyl) Phosphite (TMSP): Reactions with Halo-Chloroformates

Jeong-hoon Ham and Luis Vargas, Queensborough Community College, Bayside, NY

Tris(trimethylsilyl)phosphite (TMSP) was reacted with 1- and 2-Chloroethylchloroformate followed by hydrolysis. The purpose of the work was to determine the reactivity of TMSP with compounds having two different reactive functional groups: acyl and halide. Arbuzov and Perkow types of the reactions were expected; however, only the identification of the product(s) could explain the final outcomes of the reactions. Preliminary results will be discussed.

501. Reactivity of Tris(TrimethylSilyl)Phosphite (TMSP): Reactions with Halo-Acetyl Chlorides

Jazmin Garduno and Luis Vargas, Queensborough Community College, Bayside, NY

TMSP was treated with 2-chloro-2,2-diphenylacetyl chloride and the reaction then hydrolyzed. ARBUZOV and PERKOW types of reactions are expected; the outcome of our reaction will be deduced from IR and NMR spectra.

502. Reactivity of Tris(trimethylsilyl)Phosphite (TMSP): Reactions with Chloroformates

Joseph Mammano and Luis Vargas, Queensborough Community College, Bayside, NY

Previously, we demonstrated that TMSP reacts with (I) p-tolyl and (II)benzyl chloroformates, followed by hydrolysis, forming the corresponding acyl phosphonates. Now, in a similar reaction performed with (III)p-nitro and (IV)p-fluoro chloroformates, we have identified the products as the corresponding bis-phosphonates derivatives. The effect of electron-withdrawing groups on the formation of the products will be discussed.

Qingmei Ye, Zhongmin Xu, George Crull, Vera Leshcninskaya, Yande Huang and V Palaniswamy, Bristol-Myers Squibb, New Brunswick, NJ

Brivanib is an oral dual inhibitor of VEGFR and FGFR tyrosine kinases. Brivanib inhibits FGF-stimulated and FGF-dependent cell lines. During the synthesis of its penultimate, an impurity at 0.18% level with MW 517 Da was observed in HPLC profiles. In order to control the formation and prevent its possible conversion to the corresponding impurity in the next step of the synthesis to form the API, its structure information was needed. In this presentation, we report the isolation and comprehensive spectral characterization of this impurity using HPLC, LC/MS and one and two-dimensional NMR techniques such as 1H, 13C, DEPT, 2D-COSY, 1H-13C HMQC and 1H-13C HMBC, and 1H-15N HMQC and 1H-15N HMBC. Rationale for the formation of this impurity and how to control its formation are also presented.

504. Synthesis of Ligands for Iron–Based Blood–Pool MRI Contrast Agents

Maryam T. Siddiqui, Staten Island Technical High School, Staten Island, NY

Blood–pool or intravascular contrast agents (BPCAs) for magnetic resonance imaging (MRI) are specifically designed to stay in the vascular system for a prolonged time. Human serum albumin (HSA), produced by the liver, is the most abundant protein found in blood. Employing current knowledge about which molecules are capable of binding to HSA, synthesis was directed in order to create an iron(III) complex able to bind to this protein and make an effective blood–pool contrast agent. Two ligands were synthesized based upon the molecule maltol: one with beta-alanine inserted into the maltol ring and another with ethylene diamine (or diethylamine) inserted into the ring. Beta-alanine contains a carboxyl group, while ethylene diamine contains an amine group. Each ligand was then used to create a complex with iron(III). Using Bruker minispec, the T1 spin-lattice relaxation rate was measured for each sample by plotting 1/T1 verses concentration (the slope is the relaxivity, R1) in both water and HSA solutions. The steeper the slope was interpreted as a more effective contrast agent, and the comparison between the contrast agent in water and the protein solution indicates if any significant binding takes place. The T1 values for each iron compound were measured at concentrations of 2.5mM, 5.0mM, 7.5mM, and 10.0mM. The iron(III) complex of beta-alaninemaltol derivative had a significantly higher relaxivity in HSA solution than in water, while the relaxivity decreased for the diethylaminemaltol derivative. Thus compounds with a carboxyl group are more suitable for BPCA contrast agents.

505. Progress on Determining the Active Site of Cytochrome P450 BMP

Jaclyn I. Catalano, Michael J. Harris and Ann E. McDermott, Columbia University, New York, NY

Cytochromes P450 are heme monooxygenases that play critical roles in the biosynthesis of lipids, steroids, antibiotics, and drugs metabolism. Understanding the active site structure and dynamics is important for drug discovery and providing insight on biological processes. Crystal structures of numerous P450 isoforms show the substrate positioned too far away from the heme to be the catalytically relevant binding mode. One proposed reason for the distant substrate is a temperature dependence on the ligand confirmation. This hypothesis is supported by molecular dynamic and deuterium NMR studies by Levy, Friesner, Jovanovic and coworkers. In this study we use solid state NMR to collect structural information at a variety of temperatures of N-palmitoylglycine (NPG) bound to cytochrome P450 BMP. Cytochrome P450 BMP is the heme domain of cytochrome P450 BM-3 from Bacillus megaterium, which is widely used as a model for human P450s. Since cytochrome P450 is paramagnetic it may be difficult to observe magnetization transfer from the ligand to the protein close to the heme. As a control we labeled an isoleucine and glycine pair approximately 5 Å away from the heme in order to find the best methods of detection close to the paramagnetic

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center. In addition, we have assigned peaks for the methyl group of NPG, for the "gatekeeper" phenylalanine 87, and for alanine 82, which is close to the substrate in the low temperature form. Ongoing efforts focus on observing transfer of magnetization from the protein to substrate and identifying markers for the high temperature form.

506. Elastic Network Molecular Dynamics Simulations of Coarse-Grained Molecular Systems
Marco Cavalli, Yi He and Marco Ceruso, The City College of New York, New York, NY

Most biological processes in the cell occur at time-scales and involve macromolecular assembly sizes that are often beyond the current limits of classical all-atom computational simulation approaches. One possible solution to overcome these time- and size-related limitations is to move from all-atom to coarse-grained representations of molecules. A successful example of such an approach is the MARTINI force field developed by Marrink and co-workers. This force field was originally developed for the simulations of lipid assemblies. The thermodynamics and physical properties computed using the MARTINI have shown remarkable agreement with experimental behavior. Taking advantage of the fact that the MARTINI force field has been recently extended to include coarse-grained representations of amino acids, we have undertaken the development of structural representations that can enable an accurate description of the conformational dynamics and known structural transitions of protein macromolecules. The long-term objective is to be able to elucidate in a realistic environment that includes both lipids and whole transmembrane protein receptor assemblies the molecular mechanisms underlying receptor-mediated transmembrane signaling events. We report here a systematic investigation of the dynamical properties computed using a structural representation of proteins that combines a coarse-grained representation of amino-acid with an elastic network framework to represent the protein structure. The results show that the conformational dynamics properties computed using this combined representations can be as accurate as those obtained from more costly computational simulations such as all-atom normal mode analysis.

507. Coarse-Grain Molecular Dynamics of Tetrapeptides
Kenny Nguyen¹, Russell DeVane², Zhiwei Liu¹ and Preston B. Moore¹, (1)University of the Sciences in Philadelphia, Philadelphia, PA, (2)University of Pennsylvania, Philadelphia, PA

Coarse-grain molecular dynamics (CGMD) is a reduced model approach that expands existing all-atom (AA) MD techniques. Temporal and spatial scales can be extended by a factor of 1000 at the expense of atomistic details. CGMD simulations have been extensively used on lipid bilayers and have been extended to complex protein systems. A new CG model is presented, which has been parameterized from AAMD simulations of tetrapeptides GXYG in which G represents glycine and XY represents any two amino acid residues (400 combinations). Physicochemical information from AAMD simulations, such as bond lengths, bond angles, and torsions, is used to derive CG parameters. CGMD simulations of tetrapeptides using the derived parameters, as well as parameters derived from PDB structures of proteins are carried out where comparisons are made.

508. Undergraduate Research at PSU Abington: IR Prediction of Methylarsine and Methylstibine Using HF Method
Mitalben K. Patel and Hae-Won Kim, Abington College Penn State, Abington, PA

We use the computer program Gaussian 03 to predict the IR spectra of ground state CH3AsH2 and CH3SbH2. The calculations are performed at HF level of theory. The 6-311G** basis set is used for methylarsine and the CEP-121G basis set is used for methylstibine. Normal mode assignments of the IR frequencies of methylarsine and methylstibine and their deuterated isotopomers are determined based on calculated potential energy distributions. The PED for each frequency is found using Kim's Correspondence Rules of unified group theory and the program MOLVIB. The predominant motion of
each PED is used to name the corresponding vibrational frequency. We compare our results with literature values. Our IR frequency assignments show generally good agreement with experiment.

**509. Fourier-Transform Infrared Analysis of Some Amino Acids and Peptides That Are Precursors of a Bivalent Src Kinase Inhibitor**

**Justina Chinwong**, Adam Profit and Ruel Z. B. Desamero, York College of CUNY, Jamaica, NY

Protein kinases have the ability to phosphorylate tyrosine residues of other proteins and play prominent roles in the regulation of normal cell growth, as well as tumor growth. In this experiment, we identified marker bands that would be used as indicators of protein kinase-inhibitor binding. Good candidates are the phosphate group modes on phosphotyrosine and the ring modes of pentafluorophenylalanine. Fourier-Transform infrared (FTIR) marker bands for pentafluorophenylalanine are at 960, 1527 and 1510 cm\(^{-1}\). To help us analysis our results we did some Gaussian 03 ab initio calculations, we verified that the bands correspond to the C-F modes on the aromatic ring. The FTIR marker band found for phosphotyrosine was at 930 cm\(^{-1}\). Again using Gaussian simulations, we verified that this band belongs to the phosphate functional group. Solvent dependence studies of these amino acids were also performed. Our results indicate that when dissolved in different solvents, the marker bands determined for pentafluorophenylalanine and phosphotyrosine are still visible and are slightly shifted. Data were discussed in terms of the viability of these modes as marker for studying Src Kinase-Inhibitor interactions.

**510. Conformational Dynamics of Ionotropic Glutamate Receptors: Apo Vs Holo, Monomers Vs. Dimers**

**Rodney Versace and Marco Ceruso**, The City College of New York, New York, NY

Ionotropic glutamate receptors (iGluR), classified as NMDA, AMPA or kainite receptors on the basis of their pharmacological properties, are ligand-gated ion channels that mediate the major excitatory synaptic signals in the central nervous system. Seminal X-ray crystallographic studies have established that the two lobes of the extra-cellular ligand-binding domain of these receptors move as rigid-domains as they close in around the ligand in a Venus fly trap like mechanism. The degree of closure has been correlated with the efficacy of the ligand. But the structure of some functional states of these receptors, such as the desensitized state (a state in which the receptor no longer is active although the ligand is still bound), remain unknown. With the long-term objective of obtaining a structural context for the desensitized state of non-NMDA ionotropic glutamate receptors, we have undertaken a systematic study of the conformational dynamics of the AMPA receptor iGluR2 and the kainate receptor iGluR6. We report the results of Molecular Dynamics simulations of the apo and holo-forms (glutamate bound) for the iGluR2 and iGluR6 receptors in their isolated state and in their dimer state (iGluR receptors are dimers of dimers). The results of these computational studies indicate the existence of several rigid-domain motions that modify the interface between the two lobes of the ligand-binding domain. The functional significance of these motions is addressed by combining bioinformatics approaches with in-silico mutational analyses that can serve as the basis for an experimental validation of the identified molecular mechanisms for these motions.

**511. Structural and Chemical Effects of Alkylation in Nickel Thiolate Dimers**

**Gerard Davidson\(^1\), Michael J. Maroney\(^2\) and Seleena Rashid\(^1\), (1)St. Francis College, Brooklyn, NY, (2)University of Massachusetts, Amherst, MA

Dimeric nickel thiolate complexes have been used to model the structural aspects of the Ni-Fe active site of hydrogenases. Previous studies of monoprotonated and monoalkylated nickel thiolate dimers indicated that alkylation of terminal thiolates caused minimal structural changes, but significant changes in electrochemical behavior, similar to that observed in the Ni-Fe active site of hydrogenase. The current study extends the structural and electrochemical effects upon alkylation to
include the dialkylated nickel thiolate dimer. The results of x-ray absorption spectroscopy (XAS), crystallographic, and electrochemical analyses are reported.

512. Success Rates by Protein Family in Small Molecule Docking

Sudipto Mukherjee and Robert C. Rizzo, Stony Brook University, Stony Brook, NY

Structure-based computational design techniques can significantly reduce the time and expenditure required for new drug discovery. However, origins of ligand binding which drive molecular recognition are difficult to predict and remain a challenging problem. Docking and virtual screening have proven to be very useful computational methods but further development, testing, and algorithmic improvements are needed to make such techniques more robust, reproducible, and ultimately more fruitful. In this study, we have developed a testset consisting of ~600 hand-curated x-ray small molecule ligand-receptor complexes, constructed from the Protein Databank, for use in redocking experiments. The goal is to evaluate different protocols for recovery of the bound ligand pose, using the program DOCK, and examine causes for failure. Results will be presented for redocking the entire set as well as an examination of docking successes for individual protein families including carbonic anhydrase, alpha and beta trypsin, neuraminidase, thrombin, T4 lysozyme and coagulation factor Xa. The correlation between binding energies estimated with DOCK and available experimental activities will also be reported.

513. Synthesis and Characterization of Bis-(Diimine)Carbonylalkylosmium(II) Complexes

Vennesa O. Williams, Sarswati Ramoutar, Viet Tran and Elise G. Megehee, St. John's University, Queens, NY

Osmium metal complexes are of interest as they exhibit visible luminescence upon excitation with visible or ultraviolet light and as such are possible models of photosynthetic reaction center, possible energy and electron transfer agents, and possible photochemical or electrochemical reaction catalysts. Recently we have synthesized a series of bis-(diimine)carbonylalkylosmium(II) complexes using 2,2-bipyridine and 1,10-phenanthroline and alkyl ligands such as methyl, ethyl, butyl and isopropyl. We will discuss the synthesis of these complexes which yield both cis- and trans- isomers that are isolated and have their own individual electrochemical and photochemical properties. The characterization of the electronic states of these compounds by UV-visible absorbance and $^1$H NMR spectroscopies will also be discussed. We will discuss our conclusions about the effect of these ligand variations on the electronic properties of these compounds.

514. Synthesis and Characterization of Bis-(Diimine)Carbonylpyridineosmium(II) Complexes

Carina Hernandez, Ryan Mahabir, Carmen Leung and Elise G. Megehee, St. John's University, Queens, NY

As a part of an ongoing project on the synthesis and spectroscopic studies of osmium compounds with interesting electrochemical and photochemical properties, we have synthesized a series of bis-(diimine)carbonylpyridineosmium(II) complexes where diimine = various substituted 2,2'-bipyridines and 1,10-phenanthrolines; pyridine = pyridine, 4-phenylpyridine and 5-pyridyl-10,15,20-triphenylporphyrin. We will discuss the synthesis and initial characterization of these compounds by $^1$H NMR, and UV-visible absorbance spectroscopies. These compounds are of interest as possible models of the photosynthetic reaction center, as energy transfer agents, as photochemical electron transfer agents, and as potential DNA, molecular oxygen and anion sensors.
515. Computational Analysis of Intramolecular Interactions in Serine and Threonine, at Their Isoelectric Points
Elizabeth Cipriana, Alexandru Pestesi and Mihaela D. Bojin, Queensborough Community College, CUNY, Bayside, NY

In the past twenty years, with the development of efficient computational methods, amino acids have been a permanent research target for theoretical chemists, not only because of their remarkable role in our lives (as components of proteins), but also because of their relatively small sizes, which render them suitable for an extensive range of theoretical investigations. We carried out computations on serine (Ser) and threonine (Thr) to understand the predominant intermolecular associations at their corresponding isoelectronic points (pI), using the hybrid method Hartree-Fock (HF) and density functional theory (DFT), B3LYP/6-31+G(d,p), as implemented in the Gaussian 03 program. In addition, we calculated Ser and Thr’s chemical shifts, and compare our theoretical results to those acquired experimentally.

516. The Nature and Distribution of Tungsten Oxide Photocatalysts
Edward G. Look and Harry D. Gafney, Queens College, City University of New York, Flushing, NY

WO₃ photocatalyzes the conversion of CO₂ to CH₄, but the conversion requires light of ≤ 312 nm. Particle growth, quantum size effects, offers the potential of shifting the photoaction spectrum to longer wavelengths. Tungsten hexacarbonyl adsorbed on porous Vycor glass, photoactivated by ultraviolet light, was heated in air to produce WO₃ nanoparticles in the surface layers of glass substrate. SIMS depth profiling shows that tungsten species are uniform to a depth of 800 nm. No measurable particles could be detected after photolysis. However, heating of the samples resulted initially in the appearance of WO₃ absorption bands and prolonged heating leads to a small but noticeable redshift of the initial 460-nm band of the WO₃ particles. X-ray diffraction indicates the particles are both monoclinic and orthorhombic structures, the latter more apparent with longer heating times. Analysis of the XRD linewidth via the Scherrer equation indicates a particle size ≤ 10 nm. The calculation is consistent with TEM imaging of the doped glasses which indicate a WO₃ particle size of ≤ 0.3 nm.

517. Energetic and Structural Analysis of EGFR Inhibition Using Molecular Dynamics Simulations
Trent E. Balius and Robert C. Rizzo, Stony Brook University, Stonybrook, NY

The overexpression of epidermal growth factor receptor (EGFR) is observed in several types of cancers including non-small cell lung cancer, head and neck, bladder, breast, and ovarian carcinomas. We are using computational techniques (molecular dynamics) to simulate the kinase domain of EGFR in complex with ATP competitive-inhibitors in an effort to determine origins of resistance to cancer causing and drug resistant mutations. Several analyses are used to evaluate the EGFR-ligand complexes including MM-GBSA post-processing to estimate the free energies of binding and molecular footprinting to examine per-residue interactions. The goal is to elucidate which
energetic and structural features change for any given mutation in an effort to explain the experimentally observed differences in affinity.

518. Excited State Coordination Chemistry: Synthesis, Characterization and Acid-Base and Coordination Chemistry of a Ruthenium (II) Diimine – [Ru (bpy)2(ppz)] 2+ (ppz- 4’7’-phenanthrolino-5’,6’:5,6-pyrazine)

Anthony Perri and Harry D. Gafney, Queens College, City University of New York, Flushing, NY

[Ru(bpy)2(ppz)] 2+ (ppz- 4’7’-phenanthrolino-5’,6’:5,6-pyrazine) is one of a group of compounds that exhibit enhanced reactivity upon exitation with visible light. In contrast to thermal reactivity, optical excitation enhances both acid-base and redox activity. This research focuses on characterizing the excited state acid-base properties of [Ru(bpy)2(ppz)] 2+ and whether the enhanced basicity translates into excited state coordination chemistry. Quenching of this excited complex by different metal ions capable of only coordination will be compared to that of metals capable of both coordination and electron transfer.

519. Theoretical Studies of Basic and Acidic Serine and Threonine – An Exploration of Hydrogen Bonding Patterns

Alexandru Pestesi, Elizabeth Cipriana and Mihaela D. Bojin, Queensborough Community College, CUNY, Bayside, NY

One of the greatest challenges posed to chemists by amino acids is determining their preferred conformations, due to their intrinsic flexibility that gives rise to various intra- and intermolecular hydrogen bonding interactions. Most of these conformers are close in energy, within less than 5 kcal/mol. The specific hydrogen-bonding pattern controls the structure of these amino acids in an enzyme, and can significantly affect its activity. Mutation studies demonstrated that altering a single amino acid could reduce or even eliminate the activity of that particular enzyme. By employing theoretical tools, such as, the hybrid Hartree-Fock (HF) and density functional theory (DFT), B3LYP/6-31+G(d,p) method implemented in the Gaussian 03 program, we determined the major conformers of serine (Ser) and threonine (Thr) in acidic and basic pHs. The acidity of the medium greatly influences hydrogen bonding patterns, and thus the stability of the resulting conformers. We will also discuss the theoretical chemical shifts of these molecules, and compare them to available experimental data.

520. Using Computation to Elicit the Structure of HIVgp41 in Lipid Membranes

Brian E. McGillick and Robert C. Rizzo, Stony Brook University, Stonybrook, NY

The virus/host fusion event of HIV is believed to be predominantly mediated by the viral envelope glycoprotein gp41. The N-terminal fusion peptide of gp41 penetrates the host cell membrane which is required for fusion, however, many details of this event are poorly understood including the secondary structure of the fusion peptide when inserted into the membrane. We are using molecular modeling tools to simulate how fusion peptides interact with lipid membranes and test several proposed models for secondary structure in this region. Specifically, models of gp41 in an explicit POPC lipid bilayer are being constructed and all-atom molecular dynamics simulations are being used
to test the stability of various structures including a coiled-coil alpha helix, different β-sheet arrangements, and a β-barrel. Simulations will be used to predict the most likely fusion peptide structure(s) as well as potentially eliminate certain structures as implausible.

521. Targeted Drug Design for Pandemic Influenza Strain H5N1
Rashi Goyal and Robert C. Rizzo, Stony Brook University, Stony Brook, NY

The highly pathogenic avian influenza strain H5N1 has resulted in 372 confirmed cases of human infection since 2003 with a fatality rate of more than 60%. Although the H5N1 strain is sensitive to currently approved drugs oseltamivir and zanamivir, which target the viral enzyme neuraminidase (NA), single point mutations have been identified in some NA strains of subtype N1 which confer resistance to both drugs. In this study, crystallographic structures are being used to construct protein-ligand complexes with various N1 mutations for computational modeling. Specifically, all-atom molecular dynamics simulations are being used in an effort to understand the basis of resistance due to H274Y and N294S point mutations. The goal is to determine which interactions are most crucial in the binding site for wildtype N1 and then lost as a result of either mutation. Future goals include virtual screening against N1, specifically targeting the recently reported novel 150-loop cavity, in an effort to discover new drug leads. In light of the potential for a future H5N1 pandemic the need for additional antivirals is paramount.

522. Assessment of a Service-Learning Chemistry Course for Widener Students
Louise M. Liable-Sands, Mark G. Bradley, Nadine McHenry, Steven Menden, Stephanie Nilan, Heaven Pokorny, Jillian Filewicz, Carly Graffeo and Jennifer Pinel, Widener University, Chester, PA

An inquiry-based laboratory course to accompany a general chemistry course for elementary education majors was developed to enhance their science experience and help Widener students (teacher candidates) understand and apply state academic content standards. Teacher candidates experienced a chemistry activity three times, by performing the activity, by writing a lesson plan related to state standards, and by teaching the activity in a middle school classroom. The first offering as a service-learning course involved teacher candidates and a middle school science teacher in the fall 2006 semester. The overall impact on middle school students was positive since the course provided exposure to hands-on, guided-inquiry chemistry activities. The middle school students became engaged in problem solving and were empowered by the active learning process. The middle school teacher was equipped with inquiry-based chemistry activities tied to state content standards. Teacher candidates experienced the benefits of employing inquiry-based activities in engaging middle school students to learn-by-doing. They also learned how to adapt their lesson plans based on limitations presented in the classroom. The current offering of this course in the spring 2008 semester is facilitated by an after school program run by Crozier Wellness Center, Chester, PA. The middle school students attend a six-week program at Widener University's Science Teaching Center. The teacher candidates learn how to assess the middle school students' achievement of content standards by examining and rating laboratory notebooks and worksheets in an ongoing, formative way. The teacher candidates develop rubrics to use as a means of student achievement.

523. Tetraphenylporphyrin Photosensitizer Covalently-Bonded by a Urea Linkage Onto Porous Vycor Glass
Matibur Zamadar1, David Aebisher1, Steven Greenbaum2 and Alexander Greer3, (1)City University of New York, Brooklyn College, Brooklyn, NY, (2)City University of New York, Hunter College, New York, NY

A porous Vycor glass (PVG)-attached porphyrin photosensitizer has been synthesized. A phenyl-urea linkage at the 5-position covalently bonds 10,15,20-triphenylporphyrin onto PVG. Investigations are underway to determine whether singlet oxygen is generated in aqueous solution upon irradiation of this PVG-based complex.
524. Computations of Singlet Oxygen Release from 1,4-Polymethylene Linked Naphthalene Endoperoxides

Alvaro Castillo and Alexander Greer, City University of New York, Brooklyn College, Brooklyn, NY

We describe an effort to understand how singlet oxygen dissociates from several 1,4-polymethylene-naphthalene endoperoxides from a computational study. The number of methylene groups was varied from 20-30. An obvious problem is size, since large compounds cannot be computed at CCSD or QCISD levels. However, B3LYP/6-31+G(d)//AM1 and ONIOM(B3LYP/6-31+G(d):AM1) calculations seem to permit us to disentangle the energetics of \(^1\text{O}_2\) release from the rope skipping action of the polymethylene group. The challenges of computing and understanding \(^1\text{O}_2\) movement across an environment bearing a rotating chain will be discussed.

525. Spin-Forbidden Resonance Energy Transfer Probes for DNA Detection

Angel Martí, Columbia University, New York, NY

We describe the design of new fluorescent binary probe sensors for DNA detection based on spin-forbidden resonance energy transfer (SF-RET). Binary probes consist of a donor and acceptor fluorophores that are attached to two different oligonucleotides and serve as resonance energy transfer (RET) donor-acceptor pair when hybridized to adjacent sites of a target sequence. In the absence of target, excitation of the donor results in fluorescence only from the donor, but when the probes hybridize to target, the fluorophores are brought into close proximity favoring RET, yielding fluorescence mainly from the acceptor fluorophore. These new binary probes use the metal complex Ru(bpy')2(DIP)22+ as the energy donor and an organic fluorophore (Cy5) as the energy acceptor. Energy transfer from the MLCT state of the Ru complex to singlet Cy5 is spin forbidden and produces a delayed fluorescence of Cy5. This paper demonstrates that fluorescence delay of Cy5 can be used to time resolve the emission of the probe from the intense fluorescence background of a model system for cellular background; this provides the reported system to overcome intense autofluorescence, an important and general advantage over “classical” spin-allowed steady-state probes.

526. Tin-Free and Catalytic Radical Cyclizations

Mary E. Pulling, Deborah M. Smith, Jong Wook Choi and Jack Norton, Columbia University, New York, NY

Radical cyclization reactions are important and versatile tools in organic synthesis. Most of these reactions include the use of toxic tin hydrides and a heavy element (typically iodine, bromine, selenium, or sulfur) to form the initial organic radical. The replacement of stoichiometric tin hydride reactions with catalytic reactions involving non-toxic reagents would render radical cyclizations more useful for pharmaceutical applications. We have developed radical cyclization reactions that use transition-metal hydrides to donate hydrogen atoms to substituted dienes, forming organic radicals that can then cyclize. In addition, performing the reaction in a hydrogen atmosphere regenerates the transition-metal hydride from the resulting metal radical, making the reaction catalytic. A model compound study was used to determine the rates of hydrogen atom transfer to variously substituted olefins. This newly developed method for radical cyclization reactions is not only tin-free but catalytic.

527. Mechanism of Insertion of Unsaturated Electrophiles into a “Constrained Geometry” Zirconaaziridine

Kathleen E. Kristian, Sarah A. Cummings, Masanori Iimura and Jack R. Norton, Columbia University, New York, NY

The “constrained geometry” zirconaaziridines \(\text{Me}_4\text{C}_5\text{SiMe}_2\text{N(tBu)}\text{Zr-}\langle\text{eta}-2\rangle-[\text{N(Ph)}\text{CH(Ph)}]\text{(PMe}_2\text{R})\) have been synthesized and the \(\text{R = Ph}\) derivative has been structurally characterized by X-ray
crystallography. Treatment of these compounds with carbodiimides results in insertion into the Zr-C and Zr-N bonds, while treatment with diphenylacetylene results in insertion into the Zr-C bond only. Kinetic data for these irreversible reactions indicate that phosphine dissociation must occur prior to carbodiimide or alkyne insertion. Insertion of these electrophiles into the analogous bis(cyclopentadienyl)zirconaaziridine proceeds several orders of magnitude more slowly than insertion into the “constrained geometry” complex. Comparison of kinetic data for the bis(cyclopentadienyl) vs. “constrained geometry” complexes allows quantitative descriptions of ligand binding in these systems.

528. Enantioselective Carboalumination of Olefins

James M. Camara, Robby A. Petros and Jack R. Norton, Columbia University, New York, NY

The enantioselective carboalumination of alkenes leads to asymmetric carbon-carbon bond formation. Upon oxidation of the resulting aluminum alkyls, chiral primary alcohols may be obtained. The rate constants for dissociation of the relevant heterobimetallic species, \([L_2Zr(\mu-R)AlR_2]^+\), were measured by magnetization transfer. Based on the magnitude of the dissociation rate constant, promising catalysts were identified for use in the asymmetric carboalumination of olefins. The ability of various enantiopure zirconocenes to catalyze the asymmetric methylalumination and ethylalumination of allylbenezene has been tested. The observed enantioselectivity in methylalumination using an ethylenebis(indenyl)zirconium dichloride/MAO ((EBI)ZrCl₂/MAO) system is the same as that of the authentic methyl cation generated with trityl cation from (EBI)ZrMe₂, thus confirming that the methyl cation is the active catalyst from the (EBI)ZrCl₂/MAO system.

529. LCMS Analysis of Drug Molecules in Serum by Restricted Access Material Column

Ken Tseng¹, Junji Sasuga², Kei Oide², Eiji Kagawa² and Hideyuki Kondo², (1)Shodex, New York, NY, (2)Showa Denko, K.K., Kawasaki, Japan

We have developed a novel polymer-based restricted access material (RAM) column for small molecule analysis. This column operates as a reversed-phase column, but it has size-exclusion and normal-phase properties. It retains very well both polar and non-polar molecules under MW 1,000 even in the presence of proteins. It is especially useful in minimizing sample preparation for small molecule analysis in biological fluids, e.g., serum, plasma, urine, etc. This column is operational in pH range of 3 – 12, temperature range of 20 – 60 deg.C, and pressure of up to 150 bar. The column generates sharp peaks even with low salt concentration and without ion pairing reagent.

We applied ODP2 HP column for drug molecule analysis in BSA and control serum by column-switching experiment in a LCMS system. We obtained good recovery rate of 88 to 112% with a wide variety of small molecules.

530. Electron Exchange Involving a Sulfur-Stabilized Ruthenium Radical Cation

Anthony P. Shaw, Bradford L. Ryland, Jack R. Norton, Daniela Buccella and Alberto Moscatelli, Columbia University, New York, NY

Half-sandwich Ru(II) amine, thiol, and thiolate complexes \([CpRu(dppe)L][BPh_4]\) (\(L = H_2NCH(CH_3)Ph, HSC(H(CH_3))Ph\) and \(CpRu(dppe)SCH(CH_3)Ph\) were prepared and characterized by X-ray crystallography. The thiol and amine complexes react slowly with acetonitrile to give free thiol or amine and the acetonitrile complex. With the thiol complex, the reaction is dissociative. The thiolate complex has been oxidized to its Ru(III) radical cation and the solution EPR spectrum of that radical cation recorded. Cobaltocene reduces the thiol complex to the thiolate complex. The \(^1\)H and \(^{31}\)P NMR signals of the thiolate complex in acetonitrile become very broad whenever the thiolate and thiol complexes are present simultaneously. The line broadening is primarily due to electron exchange between the thiolate complex and its radical cation; the latter is generated by an unfavorable redox equilibrium between the thiol and thiolate complexes. Pyramidal inversion of sulfur in the thiol
complex is fast at room temperature but slow at lower temperatures; major and minor conformers of the thiol complex were observed by $^{31}$P NMR at $-98 \degree$ C in CD$_2$Cl$_2$.

**531. Complexation Behavior, Photoluminescence Properties and Supramolecular Structures of Pentafluorophenylcopper**

Ami Doshi$^1$, Krishnan Venkatasubbaiah$^1$, Anand Sundararaman$^1$, Lev N. Zakharov$^2$, Arnold L. Rheingold$^2$ and Frieder Jäkle$^1$, (1)Rutgers University, Newark, NJ, (2)University of California - San Diego, La Jolla, CA

Treatment of arylcopper species with strongly coordinating ligands is known to lead to break-down of the aggregated structures. We found that the 1:1 complex of pentafluorophenylcopper with pyridine displays interesting cuprophilic and π-stacking interactions that result in the formation of extended supramolecular structures. This complex was also found to display strong blue luminescence in the solid state. To further examine the structural and photophysical properties of this new class of complexes, the pentafluorophenylcopper tetramer was treated with different substituted pyridine ligands. The coordination of these ligands to copper was confirmed by $^1$H, $^{19}$F, $^{13}$C, NMR spectroscopy and x-ray crystallography. All these complexes show interesting luminescence properties in the solid state at low temperature. The relation between structural properties and photophysical properties was further studied.

**532. Ruthenium Complexes with Non-Innocent O-Quinonoid Ligands**

Jonathan Rochford and Etsuko Fujita, Brookhaven National Laboratory, Upton, NY

Transition-metal complexes with redox-active, or “non-innocent”, ligands have generated much interest in recent years. Ru-dioxolene complexes possess strong dπ-pπ metal-ligand interactions resulting in extensive delocalization of electron density which is very sensitive to the energies of the pπ dioxolene orbitals. The charge distribution between the metal center and the ligand in these systems can be modulated depending on the nature of the ligand substituents. This charge distribution is often expressed in terms of resonance structures as dioxolene ligands can exist in quinone (Q), semiquinone (SQ) or catecholato (Cat) forms.$^1$ A number of Ru(OAc)(o-Iminosemiquinone)(tpy) complexes will be presented and their spectroscopic and electrochemical properties discussed (tpy = 2,2′:6′,2″-terpyridyl).

The research carried out at Brookhaven National Laboratory was supported under contract DE-AC02-98CH10886 with the U.S. Department of Energy.


**533. Non-Radiative Deactivation of Singlet Oxygen ($^1$O$_2$) by Cubane and Its Derivatives**

Jeffrey R. Lancaster$^1$, Angel A. Marti$^1$, Juan Lopez-Gejo$^2$, Steffen Jockusch$^1$, Naphtali O’Connor$^1$, Philip E. Eaton$^3$ and Nicholas J. Turro$^1$, (1)Columbia University, New York, NY, (2)Universidad Complutense de Madrid, Madrid, Spain, (3)University of Chicago, Chicago, IL

The quenching rate constants of singlet oxygen ($^1$O$_2$) by cubane and cubane derivatives were determined. Two methods were used for the generation of singlet oxygen: decomposition of endoperoxide (shown) and photosensitization (tetraphenylporphyrin, TPP, exc. = 532 nm). Both methods gave similar quenching rate constants for cubane and its derivatives. The bimolecular quenching rate constant was unexpectedly higher (10$^4$-10$^5$ M$^{-1}$s$^{-1}$) than what is expected for aliphatic alkanes. This can be explained by the combination of two different deactivation mechanisms: energy transfer to cubane C-H vibrational modes and the formation of a charge-transfer complex between $^1$O$_2$ and cubane ($^1$O$_2$--•••cubane•••).
534. The Synthesis of Diaryl Sulfones Via Rearrangement of Sulfonanilides
Lisa Marie Neuls Meseroll, James R. McKee and Murray Zanger, University of the Sciences in Philadelphia, Philadelphia, PA

Previous work in this laboratory revealed that tetrahydroquinoline sulfones (in particular, NSC 667952) are effective NNRTIs. When administered with popular nucleoside reverse transcriptase inhibitors commonly used to treat HIV patients a synergistic inhibition of HIV-1 was observed. Many of these drugs remain in use today and are highly toxic with unfavorable pharmacokinetics. Therefore, synthesizing NNRTIs which allow for enhanced reverse transcriptase (RT) inhibition with decreased side effects is highly desired.

In this laboratory, rearrangement of the cyclic aryl aminesulfonanilides to diaryl sulfones with heating in the presence of concentrated acid (sulfuric or phosphoric) provided a convenient one-step route to the sulfones. The tetrahydroquinoline and tetrahydrobenzazepine diaryl sulfones showed anti-viral activity, while the trihydroindoline derivatives are awaiting testing.

Microwave synthesis, when compared to conventional heating methods, often results in increased reaction rates, improved yields, cleaner products and less solvent use. Currently, rearrangement conditions are being optimized for the familiar tetrahydroquinoline sulfonanilides. Our primary goal is to demonstrate advantages and allow for comparison of microwave energy versus conventional heating methods to induce rearrangements to diaryl sulfones.

In hopes of further expanding our knowledge of these rearrangements, we will use the microwave parameters established in the tetrahydroquinoline studies as preliminary conditions for rearrangement studies using pyrrole and phenothiazine sulfonanilides. Conventional rearrangements of pyrrole and phenothiazine derivatives are currently underway for comparison with optimized microwave studies. Our secondary goal is to successfully synthesize biologically valuable diaryl sulfones to obtain a new series of potential NNRTIs.

535. Novel Chiral Biphenol-Based Monodentate Phosphoramidite Ligands and Their Application to Asymmetric Allylic Substitution Reactions
Stephen J. Chaterpaul1, Ce Shi1 and Iwao Ojima2, (1)State University of New York at Stony Brook, Stony Brook, NY, (2)Institute of Chemical Biology and Drug Discovery, State University of New York, Stony Brook, NY

A new class of monodentate phosphorus ligands based on the axially chiral biphenol have been designed and synthesized in our lab. These ligands possess fine-tuning capabilities through systematic modifications not only on the amine, alcohol or alkyl moieties, but also at the 3,3'-positions of the biphenol moiety. In this work, we have investigated applications of these ligands to allylic substitution reactions. The key step in the synthesis of Huperzine-A is a Pd-catalyzed bicycloannulation reaction. With excellent potential pharmaceutical applications of Huperzine A, we have chosen this double allylic alkylation reaction to test the efficacy our chiral ligand system. We have also chosen a Pd-catalyzed intramolecular asymmetric allylic amination reaction, which leads to the formation of chiral C1-substituted tetrahydroisoquinoline skeleton. We wil present our newly designed library of phosphoramidite ligands and their successful applications to these reactions

(See Figure on Next Page)
536. Conformational Equilibria of Simple Organic Molecules in the Gas Phase and Solution

Ermir Pjetri, Yinjuan Cui, Eza Chikashvili and Daqing Gao, Queensborough Community College, Bayside, NY

The free energy differences between the E and Z conformers of formic acid and methyl formate, and the keto-enol tautomerization of 2,4-pentanedione in the gas phase and in organic solution, acetonitrile, are studied by ab initio molecular orbital calculations at the HF/6-31G(d), B3LYP/6-31G(d), and MP2/6-31+G(d) levels. The solvation free energies are calculated by using the continuum CPCM model. In addition, treating the solute with one and two explicit water molecules in the continuum model is pursued. Solvent effects on the conformational preference of the conformers will be discussed.

537. Molecular Interactions of Amino Acids and Water

Athanasia Pavlou, Yinjuan Cui, Anibal Davalos and Daqing Gao, Queensborough Community College, Bayside, NY

The structures and the binding free energies between the protonated amino acids, glycine and alanine, with one, two, and three water molecules were extensively studied by ab initio molecular orbital and density functional theory calculations, at the HF/6-31G(d), B3LYP/6-311++G(d,p), and MP2/6-311++G(d,p) levels, respectively. Higher level calculations such as CCSD(T) and newly developed DFT methods with BSSE corrections were also explored in the evaluation of these non-covalent interactions. All the optimized conformers were confirmed as local minimum structures from frequency calculations. The computed binding enthalpies, entropies and free energies were compared to the latest experimental values from electrospray ionization high pressure mass spectrometry obtained by the scientists of the National Institutes of Health.

538. Ab Initio Computation of the Pka Values of Neutral Molecules and Anions in Water

Yinjuan Cui, Athanasia Pavlou, Anibal Davalos and Daqing Gao, Queensborough Community College, Bayside, NY

In this paper, we present our progress and results on the computation of the pKa values of some neutral molecules and anions, including the organic carbon acids acetonitrile, methyl acetate, acetamide, N,N-dimethylacetamide, as well as acetate, bicarbonate, and dihydrogenphosphate, in aqueous solution by using a variety of solvation models such as the CPCM in Gaussian 03 and SM6 in Smxgauss along with high level gas phase ab initio MO calculations. In particular, we treated the solute molecule with one, two and three water molecules in the continuum model. This work provides important information on the use of explicit water molecules with the continuum models in the study of pKa values.
**539. Phase II Stormwater Management**

*Lorraine J. Kuhn*, Village of Ardsley, Ardsley, NY

Phase II Stormwater Management is a federally-mandated EPA program, administered in New York State by NYSDEC. The aim of the program is to clean up all the waters of the United States to swimmable and fishable quality. In 1990, Phase I program encompassed municipalities with population >100,000. In 1999, Phase II included all the rest of the municipalities regardless of size. Phase II specifies five Minimum Measures (MM’s) to accomplish the clean-up: Public Outreach, Public Participation, Illicit Discharge Detection, Pre-, Post-Construction Runoff Control and Municipal Good Housekeeping. MM3, Discharge Detection, requires mapping and testing of outfalls, all water courses leading to significant water bodies in the municipality. Using rudimentary chemical analyses and simple equipment and supplies, test kits for small municipalities can be assembled for under $200. Personnel with basic scientific training are needed by these small municipalities to conduct the testing. Phase II presents an excellent employment opportunity for science student interns and other scientists seeking part-time work. Of greater significance, Phase II is an important environmental outreach program to educate the public regarding safeguarding our potable water supply. Details for each MM outline an actual method whereby water quality can be improved and maintained.

**540. Optical Study of Src Kinase Inhibitors**

*Jeonghee Kang*, Adam A. Profit, Jong I. Lee and Ruel Z. B. Desamero, York College- City University of New York, New York, the Graduate Center and the Institute of Macromolecular Assembly of CUNY, Jamaica, NY

Src kinase is an enzyme of a family of tyrosine kinases proteins that is consisted of 451 amino acids and 4 domains. In biological processes, Src-family tyrosine kinases are important for cell signaling, proliferation, and survival. Their main function is to catalyze the phosphorylation of a tyrosine residue in targeted proteins. The activity of Src-family tyrosine kinases is conducted by the intramolecular interactions involving SH2 and SH3 domains. Activated Src-family tyrosine kinases allow the SH2 and SH3 domains to participate in intermolecular interactions that target Src-family tyrosine kinases to their substrates. Hence, to understand mechanism of Src kinase, peptide inhibitors that bind to the active site and the SH2 domain of the Src kinase were synthesized. The modified peptide inhibitors with phosphotyrosine on one end and pentafluorophenylalanine on the other end are believed to be involved in the binding process. In the course of gaining better insights into the mechanism for regulation of Src kinase enzyme, the photophysical properties of phosphotyrosine and pentafluorophenylalanine peptides were studied.

**541. Studies into the Gas Phase Chemistry of Phosphorylated Peptide Ions Using Mass Spectrometry**

*Teresa Allen-Michaud*, York College/Queens College, the City University of New York, Jamaica, NY and Emmanuel Chang, York College, Jamaica, NY

Mass spectrometry (MS) is a broadly applicable analytical method that is gaining wide use in protein biochemistry and cell biology. Tandem MS (MS2) fragmentation of analyte ions can be utilized for structural elucidation of proteins and peptides, often determining their partial or completed amino acid sequence and identification of post-translational modifications. Presented here is a study to investigate the behavior of gas phase peptide ions generated mass spectrometrically, focusing specifically on how modification of peptides by phosphorylation on serine/threonine amino acid residues affects their fragmentation chemistry under tandem MS conditions, utilizing a representative library of di-, tri, and tetrapeptides phosphorylated either on a serine or tyrosine residue, and des-phospho counterparts.
Some general traits of mass spectrometric phosphopeptide ion behavior are already characterized, but this investigation aims for a more detailed and sequence-specific understanding of these behaviors. For example, it is known that serine/threonine-phosphorylated, and some tyrosine-phosphorylated) peptide ions often undergo the neutral loss of the elements H3PO4 upon collisionally induced dissociation (CID) MS2. While this neutral loss can be diagnostic of the presence of a phosphorylated species, it can (if it dominates the spectrum) result in the absence of other structural data. The degree to which neutral loss occurs likely depends on chemistry that occurs proximal to the phosphate group. Results have been obtained thus far on a series of serine-phosphorylated tripeptides with the N-terminal residue varied. Differences in energy required for fragmentation are correlated with the chemical nature of the side chain of the N-terminal amino acid.

542. Synthesis and Photolysis of Phenylethynyl Dendron

Jong I. Lee, Jeonghee Kang, Kisha Ali and Azhad Chowdhury, York College- City University of New York, Jamaica, NY

Phenylethynyl (PE) dendron framework has been synthesized to serve as a drug carrier. The periphery of the carrier is equipped with phenacyl groups, a well studied phototrigger, to deliver drugs in the response of light signals with control of the spatial and temporal release. The dendron is known to have multiphoton absorptivity that might render release of drugs using IR light.

Upon photolysis under UV, PE dendron showed a potentially useful photoinduced Bergman cyclization along with the competing phototriggering phenomenon. The photorelease products and photoinduced Bergman cyclization products are being isolated and characterized. The mechanistic study and quantum efficiency will be further investigated.


Jacopo Samson1, Charles Michael Drain1 and Patrick Nahirney2, (1)Hunter College of City University of New York, New York, NY, (2)Rockefeller University, New York, NY

Attempts to image DNA via transmission electron microscopy (TEM) have been made since its discovery. Although numerous staining (positive as well as negative) techniques have been adopted to resolve the DNA strands, they do not show significant detail about its helical and periodical structure. A very common challenge has been to avoid the re-aggregation of DNA in aqueous solution caused by the drastic change of pH upon treatment with uranyl acetate or other compounds. Here we report a novel technique that exploits the electrostatic interaction between the negatively charged DNA phosphate backbone and the positively charged trimethyl phosphine gold (I) ion. This simple technique employs deionized water, plasmid DNA (3ug/mL) and a saturated aqueous solution of the gold phosphine salt. These characteristics make this technique very environmentally friendly and inexpensive. Potential applications of this technique may involve formation of nanowires used in creating microcircuits and other nanoscale conductive networks.


Julie C. Colis, Melissa D'Souza and Harry D. Gafney, City University of New York, Queens College, Flushing, NY

Porous Vycor glass (PVG) impregnated with WO3 photocatalyzes the conversion of CO2 to CH4, but requires ultraviolet light. Our investigations focus on the assembly of multicomponent sites in the glass matrix capable of carrying out this eight-electron reduction with visible light. To this end, we have begun to explore the synthesis of the bimetallic [(bpy)2RudppW(CO)4]2+, where dpp designates the bridging ligand 2,3-bis(2-pyridyl)pyrazine. Although dpp readily reacts with W(CO)6 thermally and photochemically to form W(CO)5dpp, the major obstacle to the synthesis of the bimetallic is the
difference in solubilities of the two reactants. This presentation will describe the use of \([\text{Ru(bpy)}_2\text{dpp}]^{2+}\)-doped-PVG in hydrocarbon solutions of \(\text{W(CO)}_6\) as a photochemical reaction system. Photolysis through the \(\text{W(CO)}_6\) solution leads to spectroscopic evidence of the formation of \([(\text{bpy})_2\text{RudppW(CO)}_4]^2+\) in the hydrocarbon solution.

545. Triggered Protein Derived Scaffold as Self-Assembled Materials
Susheel Kumar Gunasekar and Jin Montclare, Polytechnic University, Brooklyn, NY

Extensive progress has been made in the field of developing polymers based on DNA, proteins and other organic molecules as building blocks. Here we propose a novel approach of generating block co-polymers based on the self-assembly of α-helical peptides that can be induced. The coiled-coil region of cartilage oligomeric matrix protein (COMPcc) forms a homopentamer and consists of a 73 Å long hydrophobic pore with a diameter of 2-6 Å that is capable of binding of various hydrophobic molecules. ZE and ZR are two α-helical leucine zipper peptides that forms a heterodimer. Fusions of ZE and ZR to COMPcc results in the formation of pentameric COMPcc flanked by the zippers. We have designed block fusions of COMPcc-ZE-COMPcc and ZR-COMPcc that can be triggered to assemble upon mixing. Such bioinspired polymers possess great potential as artificial scaffolds in tissue engineering.

546. A Low-Cost Stable Metabolic Stable Isotope Labeling Method for Quantifying in Vivo Protein Phosphorylation
Emmanuel Chang, York College, Jamaica, NY

Because protein phosphorylation is a key means of initiating and propagating changes in cellular states, techniques to readily analyze and quantify the dynamics of protein phosphorylation can aid the study of cellular function. One such technique is stable isotope labeling with mass spectrometric readout.

For analysis of proteins, metabolic stable isotope labeling has the advantage over other isotope-incorporation techniques since label is introduced during cell growth and therefore, the labeled and unlabeled samples are mixed prior to cell lysis, ensuring that no artifactual differences are introduced during sample processing. Furthermore, metabolic labeling requires no derivatization steps that may lead to sample handling-related losses. However, growth of cells in labeled-medium to study proteins expressed at endogenous cellular levels, can be prohibitively expensive due to the cost of labeled medium.

We introduce an economically viable strategy using metabolic labeling for quantifying changes in phosphorylation at a two order-of-magnitude reduction in cost relative to typical metabolic labeling strategies. In our overexpression isotope-tag doping strategy, the phosphoprotein is purified from unlabeled cells under all conditions of interest. We then introduce a stable isotope labeled internal standard by doping them prior to cell lysis with small amounts of cells that overexpressed the same phosphoprotein while growing in stable isotope-labeled medium. After proteolytic cleavage, the labeled phosphopeptides from the overexpressing cells can be used for comparing phosphopeptide levels across all the samples of interest.

547. A Novel Photobioreactor for Algae Production
Arthur T. Poulos, Alex Angilella, Ester Byram, Andrew Flood, Joe Liu, Timothy McMichael, Spenser Reilly and Amanda Vangeli, SciCore Research Institute, Princeton Jct., NJ

Economically efficient farming of algae is of great interest due to the myriad of low to high value products derivable from algae, such bio-diesel fuel, thickening agents, lipids, pigments, fatty acids, amino acids, proteins, and pharmacologically active compounds. A bottleneck to cost-effective cultivation is the relatively low volumetric productivities obtainable from existing photobioreactor designs, generally less than 1 gram biomass per liter. Factors which limit biomass concentration and
volumetric productivity include low light penetration, photo-inhibition, dissolved oxygen accumulation, and CO2 availability. This project is an investigation of algae production using a novel photo-spray reactor which produces an optically thin substrate-light interface and high rate of gas exchange. The project involves the design and fabrication of a bench-scale photobioreactor and testing its productivity using representative green algae and cyanobacteria species. The performance of the photobioreactor is evaluated with respect to biomass volumetric productivity, quantum yield, and light saturation irradiance.

**548. Toward Photochemical CO2 Reduction by Rhenium Complexes**

Sean E. Hightower¹, David C. Grills¹, Jinzhu Chen¹, Koji Tanaka² and Etsuko Fujita¹,
(1)Brookhaven National Laboratory, Upton, NY, (2)Institute for Molecular Science and CREST, Okazaki, Japan

Rhenium complexes with NAD⁺ model ligands, Re(pbn)(CO)₃Cl and [Re(pbn)(CO)₃(PCy₃)]⁺ (pbn = 2-(2-pyridyl)-benzo[b]1,5-naphthyridine, Cy = cyclohexyl) were prepared. Our preliminary results indicate that the corresponding complexes with pbnHH (i.e., a bio-inspired NADH-like ligand) are formed upon irradiation in the presence of a sacrificial donor (e.g., Et₃N) through metal-to-ligand charge-transfer (MLCT) excited states. Herein we report the acid-base properties, electrochemical properties, and reactivity of these species toward CO₂ reduction.

The research carried out at Brookhaven National Laboratory was supported under contract DE-AC02-98CH10886 with the U.S. Department of Energy.

**549. Determination of Electron Transfer Rate Contant Between Congo Red and Selected Organic Fluorescence Quenchers**

Maurice Iwunze, Morgan State University, Baltimore, MD

Steady-state fluorescence was used to obtain a bimolecular rate constant for the reaction between congo red and the known fluorescence quenchers, H₂O₂, diethylamine, nitromethane and nitrobenzene. The observed bimolecular rate constant correlated quite well with the photo-induced electron transfer rate constant, kₚ, which was obtained through the Marcus dielectric continuum theory. The activation energy and the solvent reorganization energy associated with these reactants were also determined. The relation between the distance of sphere of reaction and the electron transfer rate constant will be discussed.

**550. Growth Inhibition of Retinoic Acid Treated MCF-7 Breast Cancer Cells- Identification of Sox 9 and Other Proteins**

Tiffany Remsen, P. Kessler, A. Stern, H. Samuels and P. Pevsner, New York University School of Medicine, New York, NY

Breast cancer is the second leading cause of cancer death in women. This study suggests a chemopreventive strategy. Retinoic acid can reduce expression of the inhibitor of apoptosis protein, survivin (induced three-fold by retinoic acid receptor (RARα)-selective agonist Am580 in T-47D breast cancer cells). In MCF-7 mammary carcinoma cells, growth inhibition by RA entails an early cell cycle arrest followed by induction of apoptosis. Expression array analyses revealed that RA induces the expression of several genes involved in cell cycle regulation, including the p53-controlled antiproliferative gene, B-cell translocation gene, member 2 (Btg2).

We measured histone H2A directly from breast cancer cells (MALDI). Protein extractions were obtained from RA treated MCF-7 breast cancer cells with organic solvent (ProteoSolve) and high pressure (Barocycler, Pressure BioSciences, West Bridgewater, MA), trypsinized, and the following proteins with LCMS (Hitachi NanoFrontier nLC, Dallas, TX): gi|938234 SOX-9 [Homo sapiens] Mass: 6448; gi|110591141 Chain A, Solution Structure Of The First Homeobox Domain Of At- Binding Transcription Factor 1 (Atbf1) Mass: 7974; gi|5454114 tissue factor pathway inhibitor isoform a
Mass: 124077; gi|119587536 ferredoxin 1 [Homo sapiens] Mass: 28101; and gi|3851261

High pressure extraction increased protein yield and helped to identify proteins not previously seen
and revealed marked differences between retinoic acid treated and non-treated cells. The
identification of additional proteins will allow characterization of the metabolic cascade induced by
RA and may lead to new therapeutic strategies in breast cancer.

551. IMAGING MALDI of Colorectal Carcinoma - Field Defects in Satellite Tissue

Tiffany Remsen¹, P. Kessler¹, F. Francois¹, A. Stern¹, S. Anand² and P. Pevsner¹, (1)New York
University School of Medicine, New York, NY, (2)Brooklyn Hospital Center, Brooklyn, NY

Colorectal cancer is the second-leading cause of cancer death in the USA, with more than 155,000
predicted new cases per year. Recently in specimens from consecutive patients, imaging MALDI
(IMS) demonstrated chemical evidence of two proteins, gi|119592539 hCG1787564 [Homo sapiens]
Mass: 57590, and gi|119592490 hCG2040674 [Homo sapiens] Mass: 108178 in colon adenocarcinoma and in histopathologically normal satellite tissue. This finding may represent a
potential marker for field carcinzeration or a field defect, e.g., age-related hypermethylation in
normal colonic mucosa. Such alterations result in microsatellite instability, and synchronous and
metachronous lesions which develop into cancers. Therefore, the use of histopathology alone may
significantly affect therapy by underestimating the extent of metaplastic or malignant disease. We
hypothesized that in comparison to conventional histopathology, using proteomic classification IMS
can better identify the extent of metaplastic disease beyond the recognized tumor.

The combination of high pressure protein extraction with organic solvent and LCMS increased the
yield of peptides obtained from the tissue digest and identification of heretofore unidentified
proteins. The protein mass numbers are used to reconstruct the IMS images, and localize the
proteins in tissue

The presence of variation in polyp proteins in the biopsy tissue strongly suggests genetic field
differences, which may be predictive of carcinoma not only developing in these polyps, but at other
sites in the colon as synchronous and metachronous lesions. These findings may alter the current
paradigm of histopathology tissue diagnosis for tumor and require examination of the biopsy tissue
with histopathology and mass spectrometry for complete diagnosis.

552. MALDI Mass Spectrometry Identification of Proteins in a Murine Transgenic
Model of Apert Syndrome

Gerson Rothschild, A. Mansukhani, C. Basilico and P. Pevsner, New York University School of
Medicine, New York, NY

The craniosynostoses are craniofacial skeletal disorders involving temporally inappropriate fusion of
the cranial sutures. The syndromes originate from mutations in the membrane-bound tyrosine
kinase receptor, fibroblast growth factor receptors (FGFR). Point mutations in the linker between Ig-
like domains 2 and 3 of human FGFR2 are known sources of five craniosynostoses syndromes:
Apert, Crouzon, Jackson-Weiss, Beare-Stevenson, and Pfeiffer. Apert syndrome is a rare autosomal-
dominant disorder characterized by premature fusion of the coronal suture, mental deficiency, and
brain malformations. The Apert etiological defect has been traced to one of two point mutations on
chromosome 10q in humans (7q in the mouse).

A transgenic mouse model of Apert syndrome was studied. MALDI mass spectrometry was used to
screen for transgene expression. Mass spectrometry provided the same data as the validated
Polymerase Chain Reaction (PCR) conventional approach, and provides a rapid throughput, high-
specificity method for determining construct expression.
The molecular weight of the endogenous FGFR2 protein was calculated at 81.3 kD and the addition of the myc-his tag (approximately 25 amino acids) increased the construct's mass to approximately 83.7 kD. Both proteins were identified with MALDI mass spectrometry from global protein extractions of murine tail tissue.

This study provides proof of principle for MALDI protein identification in transgenic mice. Thus, mass spectrometry may allow replacement of classical PCR in the study of protein expression in genetically engineered mice. This would provide large scale, rapid, robotic protein analysis in virtually any genetically engineered animal model.

553. LCMS Identification of in-Vitro Fertilization Growth Media Proteins

P. Pevsner, S. Talebian, T. Remsen, F. Naftolin, P. Kessler, A. Stern, F. Licciardi and J. Grifo, New York University School of Medicine, New York, NY

At the NYU Fertility Center 48% of cycles in women <35 years result in a live birth. Forty % of these births in women <35 years at the NYU Fertility Center are twin deliveries. A strong criticism of assisted reproductive technologies (ART) is the high incidence of multiple gestations that increase fetal and maternal morbidity and mortality.

Grifo et al recently described their clinic's progression to blastocyst transfer as a means to reduce the high-order multiple rate. The ART community has addressed the need for more single embryo transfers (SET) but also recognizes the lowered pregnancy rates that may ensue. The ability to identify additional markers associated with embryo viability and competence has been the greatest challenge towards promoting SET. In a recent study of 3 and 5 day growth media, we have identified gi|223976 haptoglobin Hp2, mass 41717. Two more proteins were identified in our latest report, gi|90108928 1 Chain H, Orally Available Factor7a Inhibitor, mass 28582, and gi|119573737 hCG1793647 [Homo sapiens] Mass: 6112. This study produced two new specific biomarkers unique to competent embryos: gamma-aminobutyric-acid receptor subunit and tetratricopeptide repeat protein 9.

The IVF growth media protein from 3 and 5 day embryos was extracted with organic solvent and high pressure using ProteoSolve© and the Barocycler© respectively (Pressure BioSciences, West Bridgewater, MA). The protein fraction was trypsinized, and the peptides studied with LCMS (Hitachi NanoFrontier nLC, Dallas, TX).

These new biomarkers of competent embryos should enhance embryo selection and effect more single embryo transfers.

554. Synthesis of Novel Tetrasubstituted Phthalocyanines with Dibenzazepine Frames as Potential PDT Agents

Matteo Parravicini, Stefano Tollari and Giovanni Palmisano, Universita` dell'Insubria, 22100 Como, Italy

The synthesis, photophysical and photochemical properties of tetrasubstituted phthalocyanines with a dibenzazepine frame are reported. The new compounds have been characterized by elemental analysis, IR, $^1$H and $^{13}$C NMR spectroscopy, electronic spectroscopy and mass spectra. General trends are described for photodegradation, singlet oxygen, fluorescence and triplet excited state quantum yields, and triplet state and fluorescence lifetimes of these compounds in dimethylsulfoxide (DMSO). The fluorescence of the complexes is quenched by benzoquinone (BQ). Photophysical and photochemical properties of phthalocyanine complexes are very useful for PhotoDynamic Therapy (PDT) applications. The substituted Zn(II) phthalocyanines show high triplet and singlet oxygen quantum yields. High singlet oxygen quantum yields are very important for a Type II photosensitization mechanism, so these complexes have potential for that application.
555. Validation of Analytical Procedures for the Determination of Some Pharmaceutical Products

Hilmi Ibar and Özlem Bayram Basdag, Trakya University, Edirne, Turkey

The Analytical methods for the determination of some pharmaceutical products have been developed and validated. The analytical methods used in the drug industry must be accurate, precise, reliable and repeatable. We investigated number of analytical procedures in order to ensure ones that would be suitable for application as a quality control procedure for studied drugs. For this purposes 3 different studies are performed:

1. Analytical method was developed for determination of Methylene Chloride film used for the coating of tablets which contains Sildenafil Citrate active material.
2. Analytical method for determination of products which contains Valaciclovire HCl active material.

Validation of the developed method is done according to the “European Agency for the Evaluation of Medical Products”, those includes: Accuracy of the Method, Precision, Specificity, Range and Linearity.

Evaluation of the procedures demonstrated that the procedures are reliable and are suitable for its intended purposes. From the data's obtained it was seen that amount of reagents used for performing analysis is 8-10 times lower, amount of sample used for analysis 6-12 times, and labor is 1-3 times lower than in used routine procedures.

556. Purification of Vitamin E from Waste Oil

H.R. Ferhat Karabulut, University of Trakya, Edirne, Turkey and Omar Zaim, University of Trakya, Edirne, Turkey

Vitamin E is a material which is essential in daily life. The importance of regaining of vitamin E which exists in the waste oil called the deodorization sludge has been the driving force for this research.

The sample were obtained from the plant of oil factory in Edirne. By examining four different methods we tried to find the most suitable one. To optimize the economy, speed, purity and yield were the criteria of importance.

In method I and method II by saponifying the fatty acids we tried to extract vitamin E from the soap. In method III and IV esterification. We found that method II is most suitable procedure for our purposes.

557. Extractive-Spectrophotometric Investigations on Ternary Ion-Associated Vanadium(V) Complexes

M. Türkyılmaz¹, O. Altun¹ and K. B. Gavazov², (1)University of Trakya, Edirne, Turkey, (2)University of Plovdiv, Plovdiv, Bulgaria

The formation and liquid-liquid extraction of ion-associated complexes between the vanadium(V) – 4-(2-pyridylazo)-resorcinol (PAR) anionic chelate and the cations of some methoxybis(tetrazolium) salts (MT²⁺), which contain different number of nitro groups {3,3’-(3,3’-dimethoxy-4,4’-biphenylene)bis[2,5-di(4-nitrophenyl)-2Htetrazolium] chloride (Tetranitrotetrazolium Blue chloride, TNBT), 3,3’-(3,3’-dimethoxy-4,4’-biphenylene)bis[2-(4-nitrophenyl)-5-phenyl-2H-tetrazolium] chloride (Nitro Blue Tetrazolium chloride, NBT) and 3,3’-(3,3’-dimethoxy-4,4’-biphenylene)-bis(2,5-diphenyl-2H-tetrazolium) chloride (Tetrazolium Blue chloride, BTC)} have been studied. The optimal conditions for extraction in chloroform (pH, concentrations of the reagents, extraction time) and the composition of the complexes (V:PAR:MT=2:4:3) have been found. The equilibrium constants (the
constants of extraction – KEx, the constants of distribution – KD, the constants of formation – â), and the recovery factors have been determined. The results show that a linear relationship exists between LogKEx and the number of nitro groups included in MT2+ (NNO2): the higher NNO2, the lower LogKEx. A similar relationship has been established between Logâ and NNO2. These relationships have been used to predict the values of LogKEx and Logâ for new (uninvestigated) methoxybis(tetrazolium) ion-associated complexes.

557A. Synthesis and Biological Activity of Multivalent Estradiol-Peptidomimetic Conjugates: A Novel Approach for Selectively Modulating Estrogen Receptors

Justin M. Holub, Kent Kirshenbaum, Department of Chemistry, New York University 100 Washington Square East.

N-substituted glycine (peptoid) oligomers can be used as substrates for Cu(I) catalyzed azide-alkyne [3+2] cycloaddition reactions. Using this approach, we synthesized a novel set of bioactive estradiol-peptidomimetic conjugates (EPCs) that multivalently display estrogen receptor (ER) ligands in a site-directed fashion. Radiometric competitive binding assays demonstrated that EPCs bind the ER with strong avidities (EC50 = 10.9 nM for hexavalent conjugate). Comparative live-cell imaging in ER(+) MCF-7 cells using fluorescent EPCs show enhanced vesicular concentrations of divalent EPCs over monovalent EPCs, indicating that molecular size affects the cell uptake efficiency of these constructs. Luciferase reporter assays demonstrated that EPCs are able to regulate ER-mediated transcription in a size-dependant manner. EPCs may be capable of selectively modulating ER signaling through non-genomic versus genomic pathways.
Computational Chemistry for the Health of Humanity and the Planet, III - Complexity and Accuracy

Sponsor: Healthcare & Life Sciences Department, Dell, Inc.; Chemistry Department Brookhaven National Laboratory
Organizer: Daqing Gao Queensborough Community College, Bayside, NY
Organizer: Seogjoo Jang Queens College of the City University of New York, Flushing, NY

Session Overview: Computational chemistry has become an essential tool for biomedical research (health of humanity) and renewable energy research (health of the planet). This session discusses recent advances in how the issues of complexity and accuracy can be overcome in these research areas.

558. Desulfurization Reactions on Metal Carbides and Phosphides: Complex Role of C and P Sites
Jose A. Rodriguez, Ping Liu and James T. Muckerman, Brookhaven National Laboratory, Upton, NY
Sulfur-containing molecules are common impurities in fuels and oil-derived chemical feedstocks. In our industrial society, these impurities have a negative impact in the petrochemical industry and degrade the quality of the air by forming sulfur oxides (SOx) during the burning of fuels and by poisoning the catalysts used in vehicle catalytic converters. Hydrodesulfurization (HDS) is one of the largest processes in petroleum refineries where sulfur is removed from the crude oil. The current HDS catalysts cannot provide fuels with the low content of sulfur required by new environmental regulations. Transition metal carbides and phosphides have shown a tremendous potential as highly active HDS catalysts. At a microscopic level, it is not well understood how these new catalysts work. Recently, density-functional calculations and synchrotron-based techniques (high-resolution photoemission, x-ray absorption spectroscopy, time-resolved x-ray diffraction) have been used to study the chemistry of S-containing molecules on single-crystal surfaces and nanoparticles of metal carbides and phosphides. These studies reveal that the C and P sites in the catalysts play a complex and important role in HDS reactions and cannot be considered as simple spectators. They moderate the reactivity of the metal centers (allowing the cleavage of C-S bonds, but preventing the formation of strong metal-sulfur bonds) and provide bonding sites for the H adatoms necessary for the hydrogenation of S and CxHy fragments.

559. Effect of Hydrogen-Bonding Strengths in Various Foldamer Building Blocks on the Conformational Distributions of Aromatic Oligomers
Jhenny F. Galan, Zhiwei Liu, Jodion Brown, Whelton A Miller and Vojislava Pophristic, University of the Sciences in Philadelphia, Philadelphia, PA
Hydrogen bonding is known to play an important role in biological secondary structures, such as alpha-helices and beta-sheets. In synthetic foldamers, which mimic naturally occurring polymers, the same principles that govern the conformations of biofoldamers are used. In this study, we investigate the intramolecular hydrogen-bonding ability of different model aromatic amides and its effect on the conformational distributions of the aromatic oligomers. We have developed a systematic scheme using a combination of quantum mechanics and molecular dynamics simulations to estimate the strengths of hydrogen bonds and their effect on the conformational distributions of the aromatic oligomers. In addition, we modified the GAFF (general AMBER force field) parameters for this class of compounds and applied them in the molecular dynamics simulations. This study is aimed to provide further insights in the design of aromatic foldamers.
560. **Ab-Initio Density Matrix Renormalization Group and Tensor Network Wavefunctions**

**Garnet K. Chan**, Cornell University, Ithaca, NY

The Density Matrix Renormalization Group is a new technique in quantum chemistry that is enabling the solution of many problems of electronic structure previously thought impossible. In my talk I will explain the basic idea behind the method and give many examples of classes of calculations, ranging from exact small molecule potential energy curves to excited states of conjugated polymers, that can now be performed using this theory. In addition, I will explain the connection between the Density Matrix Renormalization Group and the emerging paradigm of Tensor Network wavefunctions, which appear to underlie all computationally tractable strongly interacting systems.

561. **Towards Computational Simulation of Receptor-Mediated Transmembrane Signaling Events in Realistic Environments**

**Marco Ceruso**, The City College of New York, New York, NY

The regulation of many cellular functions involves receptor-mediated transmission of chemical or physical information across the extracellular membrane. These processes entail cooperative interactions and structural changes within and between multiple macromolecular entities that can range in size from a few hundred to several thousand amino acids. The size of these macromolecular systems as well as the complexity of the environment in which they evolve present formidable challenges for computational simulation approaches aimed at determining the molecular bases of the interactions and structural changes that underlie the transmission of the information across the membrane. Elucidating these mechanisms is key to understanding the normal function of transmembrane receptors but is also key to developing therapeutic strategies that can target effectively the dysfunctional and disease-related states of these receptors. To address these challenges we have undertaken a systematic approach for the development of coarse-grained representations of macromolecular entities. This approach keeps a residue-level description of macromolecules in order to maintain a direct link with experimental approaches that can probe the effects of single residue substitutions. Similarly, in order to maintain simulation conditions that describe as realistically as possible the environments in which these entities evolve, we keep explicit representations of aqueous and lipid molecules. Here, I present results which show that our approach can reliably reproduce the conformational dynamics and known structural transitions for a number of macromolecular systems, rivaling in accuracy all-atom computational approaches such as normal modes analysis and molecular dynamics simulations, but at less than 1/10th of the computational cost.

562. **Computational Design of Structured RNA Pools for in Vitro Selection of RNAs**

**Hin Hark Gan**, Namhee Kim, Shereef Elmetwaly and Tamar Schlick, New York University, New York, NY

In vitro selection is a versatile experimental technology for screening large random-sequence libraries of nucleic acid molecules for a specific function, such as binding or catalysis. It has enabled discovery of numerous nucleic acid molecules binding diverse targets (e.g., organic molecules, antibiotics, proteins), and novel ribozymes. Such synthetic RNAs are being used to develop RNA-based biosensors, inhibitors of protein function, and tools for exploring biological interactions. However, the probability of finding complex RNA molecules in random pools is low because simple motifs dominate such pools. To overcome this problem, we have developed methods for designing structured pools using concepts such as modeling and optimization of RNA pool synthesis, analysis of RNA structure space using molecular graphs, and screening of large sequence pools for active RNA species. These methods parallel advances in combinatorial chemistry for design, analysis and synthesis of compound libraries used in drug discovery. Specifically, we design structured RNA pools by optimizing the sequence/structure space to yield the target or user-defined structural...
characteristics. The target structured pool corresponds to an optimal combination of nucleotide transition matrices used for pool synthesis, starting sequences, and associated pool fractions. Our pool design method has been automated and made available through the webserver RAGPOOLS that offers a theoretical companion tool for RNA in vitro selection. Thus, our designed structured RNA pools can serve as a guide to researchers who aim to analyze and synthesize RNA pools with favorable properties for current biomolecular engineering applications.

563. Computational Design of Small Molecular Inhibitors to Promote Induction of Bone Growth by BMPs

Boojala Vijay B. Reddy¹, Sreedhara Sangadala², Raghu Prasad Rao Metpally¹, Shaila Ahmed³ and Pooja Makkar³, (1)Queens College of City University New York, New York, NY, (2)Atlanta VA Medical Center, Atlanta, GA, (3)Graduate Center, The City University New York, New York, NY

Many Americans are afflicted with low back pain, degenerative spinal disease or bone fractures. Orthopedic surgical treatment of these problems frequently requires bone grafting to promote healing. Over 500,000 bone grafting procedures are performed each year in the United States. Over 50% of these are related to some type of spine fusion. Using small molecular inhibitors of different interacting partners in the BMP mediated pathway have potential to promote osteoblast differentiation and there by quick healing surgical treatments. We present the three approaches we have adapted to design the small molecular antagonists to Noggin, Smurf1 and Ski proteins: (i) To design inhibitors that may block BMP2/Noggin interaction with the goal of lowering the dose of BMP-2 required in clinical applications. (ii) To design inhibitors that may block Smad-WW2/Smurf1 interaction with the goal to reduce the ubiquitination of Smads there by promoting BMP induced cascade of events. (iii) To design inhibitors to the Smad binding nuclear protein Ski to promote Smad mediated gene expression.

564. Network Approach for Analysis of Residue Packing in Helical Membrane Proteins and Its Application in Membrane Protein Structure Prediction

Vagmita Pabuwal and Zhijun Li, University of the Sciences in Philadelphia, Philadelphia, PA

Structure prediction of membrane proteins includes computational methods, mainly the de novo protein structure prediction and homology modeling. These also play an important role in structure-based drug design efforts. Developing an accurate scoring function for protein structure discrimination and validation remains a current challenge. Network approaches based on overall network patterns of residue packing have proven useful in soluble protein structure discrimination. It is thus of interest to apply similar approaches to the studies of residue packing in membrane proteins. In this work, we first carried out such analysis on a set of diverse, non-redundant and high-resolution membrane protein structures. Next, we applied the same approach to three test sets. The first set includes nine structures of membrane proteins with the resolution worse than 2.5 Å; the other two sets include a total of 101 G-protein coupled receptor models, constructed using either de novo or homology modeling techniques. Results of analyses indicate the two criteria derived from studying high-resolution membrane protein structures are good indicators of a high-quality native fold and the approach is very effective for discriminating native membrane protein folds from less-native ones. These findings would add information to other similar works being carried out, as membrane proteins accounts for a large part of our genome and are major drug targets.
Infrared Spectroscopy

**Sponsor:** MicroLab, Inc.; Smith Detection  
**Organizer:** Luis Avila Columbia University, New York, NY  
**Organizer:** Leonard Fine Columbia University, New York, NY

**Session Overview:** Infrared Spectroscopists have moved their spectrometers from their benchtops into the fields of homeland security and environmental remediation. They have also refocused IR photons of all ranges into tissue imaging, looking at two-dimensional time-evolving structures. In this symposium we would like to invite you to share your work with us and highlight the versatility of infrared spectroscopy. Fiat Lux!

565. Planar-Array Infrared (PA-IR) Spectroscopy: Evolution, Revolution or Back to the Future???

**John F. Rabolt**, University of Delaware, Newark, DE

With the recent development[1] of planar array infrared (PA-IR) spectroscopy, a re-examination of the usefulness of IR spectroscopy in terms of studying dynamic processes is warranted. This talk will describe an ultrafast, portable PA-IR instrument and its application to the dynamics of polymer organization during assembly of a Langmuir film at the air-water interface.

PA-IR spectroscopy offers a number of advantages over conventional Fourier transform infrared (FT-IR) methods and traditional dispersive infrared instruments, such as a multi-channel advantage, a short integration time, pixel binning options, scaleable optics, and no moving parts. Obtaining a spectrum in the range of 1800-1000 cm\(^{-1}\) of films on the water subphase still remains difficult due to the poor IR reflectivity of water, the extremely low concentration of the ultra thin film and the interference of water bands. In this talk, a new planar array infrared reflection spectrograph (PA-IRRS), which has several advantages over conventional approaches, will be discussed. By splitting the incident infrared beam into two sections on a plane mirror or a water trough, instead of at the front of the globar source, the performance of this instrument is shown to be comparable to that of the dual-beam instrument, although this instrumental setup is the same as that of the single-beam instrument. This PA-IRRS system has significant potential for investigating the time-resolved dynamics of a broad range of Langmuir films, such as cellular membranes or biopolymers, on the water subphase.


566. Membrane Catalyzed hIAPP Folding Followed by 2DIR SPECTROSCOPY

**Yun L. Ling**, Dave B. Strasfeld, Sang-Hee Shim and Martin T. Zanni, University of Wisconsin-Madison, Madison, WI

It is very likely that type 2 diabetes is caused by the human islet amyloid polypeptide (hIAPP) which is proposed to induce pancreatic ß-cell membrane penetration and forms fibrils in the body's pancreas. We studied the structures and kinetics of hIAPP folding in the presence of lipid vesicles using 2DIR spectroscopy. hIAPP accumulates at the water lipid interface through electrostatic interactions and, somehow, the membrane catalyzes beta-sheet amyloid formation. Comparison of the spectra with and without membranes shows that the folding pathway of hIAPP is very different when it is membrane catalyzed. Furthermore, we have preliminary evidence of an intermediate state that is not beta-sheet on the folding pathway with membranes. Our results so far point to 2D IR spectroscopy as a powerful tool for studying amyloid fiber formation.
567. Saint Wolfgang's Secret Past: A Microspectroscopic Analysis of Paints Removed from a Medieval Sculpture

Patricia Lang, Ball State University, Muncie, IN

When looking at a historic work of art, does the word chemistry come to mind? Art historians rely on science for accurate historical information regarding works of art. According to J. Davy in The Collected Works of Sir Humphrey Davy, the marriage of science and art dates back to 1818, when Sir Humphrey Davy chemically analyzed paints removed from the ancient ruins of Pompeii. We report on a more recent study conducted closer to home.

A spectroscopic study of paints removed from a 15th century sculpture depicting Saint Wolfgang, which is housed in Ball State Museum of Art, was performed. Infrared spectra on minute paint samples were obtained, and the spectra were compared to reference spectra of known art pigments and materials. In addition, energy dispersive x-ray spectra were obtained using a scanning electron microscope. The x-ray spectra were used to support the infrared results and, in some cases, allowed for the identification of materials which have infrared absorptions below the detector range or which are infrared inactive. The combined spectral data on the paints, which were layered in several places on the sculpture, allow us to obtain a detailed description of Saint Wolfgang's different appearances throughout the past three hundred years. Although many of the pigments found are relatively modern, the first application of paint is composed of materials consistent with the sculpture's medieval date.


David W. Schiering and Dustin Levy, Smiths Detection, Danbury, CT

The need to identify threats in various forms in the post 9/11 world has driven innovation in the development of vibrational spectroscopic instrumentation. Specifically, instruments have been reduced in size and weight and portable, Fourier transform infrared (FT-IR) and Raman spectrometers are prevalent in the hands of First Responders and specialized military teams. These instruments are battery-powered and can be used while the operator is fitted with chemical protective clothing. Software algorithms and methods have been devised to simplify identification of threats by non-chemists. This presentation will concern the state of the art in rugged, portable FT-IR and Raman instruments currently used by homeland security specialists. Key design and performance attributes for these users will be discussed as well as selected applications of the technologies. If time permits, the use of IR and Raman spectroscopies as part of an integrated threat characterization approach will be presented.
**Materials, General Session**

**Sponsor:** Momentive Performance Materials  
**Organizer:** Bhanu P. S. Chauhan, William Paterson University  
**Presider:** Bhanu P. S. Chauhan, William Paterson University, Wayne, NJ  
**Presider:** Elena Galoppini, Rutgers-Newark, Newark, NJ

**569. Functional Polycarbonates**

**James A. Moore,** Rensselaer Polytechnic Institute, Troy, NY

A process for the commercial production of diphenolic acid [4-(bis(hydroxyphenyl))pentanoic acid, DPA] in good yield from cellulose-rich sources such as wood, paper, sewage sludge, paper mill sludge and food processing waste via levulinic acid has been developed.

The preparation of the t-butyl ester of DPA enables the formation of homo- and co-polycarbonates in which the blocking group can be removed to give free carboxyl groups along the polymer backbone. Such materials exhibit classic polyelectrolyte behavior. The sodium salt of the homo polycarbonate carboxylate is surprisingly stable to hydrolysis in alkaline solutions. Neutralization of the carboxyl groups with polyvalent counter ions leads to crosslinked gels. The carboxyl groups can also serve as the locus for grafting reactions leading to materials with unusual properties.

**570. Design of Nitrogen-Containing, Low Molecular-Mass Organogelators Based on (R)-12-Hydroxyoctadecanoic Acid and the Properties of Their Organogels**

**V. Ajay Mallia** and Richard G. Weiss, Georgetown University, Washington, DC

We report the properties of organogels comprised of organic liquids and low molecular mass organogelators (LMOGs) based on nitrogen-containing derivatives of (R)-12-hydroxyoctadecanoic acid ((R)-HSA). The LMOGs are 6 primary and secondary (N-propyl and N-octadecyl) amides and amines of (R)-HSA and the ammonium carbamate salt of the amine, 18-aminooctadecan-7-ol. Some of the LMOGs are extremely efficient, requiring less than 1 wt % in order to gelate several organic liquids at room temperature. Optical polarizing micrographs of gels with 2 wt % of an LMOG in silicone oil, hexane, CCl4 and DMSO show smaller and larger spherulites, respectively, for preparations by fast- and slow-cooling protocols of their sols. X-ray studies have been conducted for the silicone oil gels to elucidate the structures of the fibrous networks responsible for immobilization of the liquid components. They indicate lamellar molecular packing within the fibers of the 3-dimensional LMOG networks. Rheological measurements of representative derivatives of (R)-HSA in their 2 wt % silicone oil gels were also made. Some of the gels were highly thixotropic and exhibited very fast recovery times after being destroyed by high shear. Correlations between the molecular structures of the LMOGs and the properties of their gels, including critical gelator concentrations, periods of stability, and gel-sol transition temperatures will be presented.

We thank the National Science Foundation for its support of this research and Prof. Dan Blair for the use of his rheometer.

**571. Direct White Light from a Single Semiconductor Material: A Unique Approach**

**Wooseok Ki** and Jing Li, Rutgers, The State University of New Jersey, Piscataway, NJ

It has been reported that solid state lighting (SSL) would reduce global electricity consumption by 50%. [1] Specifically, white-light SSL has great potential to replace conventional lighting sources as a much more efficient device. Common approaches are to combine blue, green, and red emitters to achieve a broad spectrum of white light, or by phosphor conversion. But, these procedures lead to
significant energy loss such as self absorption associated with light capture by the phosphor or nonradiative carrier losses.[2] Semiconductor nanocrystals (NCs) provide a new technology platform for developing white light phosphors with improved efficiencies, because self absorption and complex doping process can be avoided, and by tailoring the size of NCs emission properties can be tuned. However, a great challenge for these NCs is the difficulties of achieving high carrier mobility and conductivity required for LEDs.

We have developed a new class of inorganic-organic hybrid nanostructured semiconductors that possess broad band gap tunability and high absorption coefficients desirable for opto-electronic applications, such as photovoltaics and solid state lighting. They exhibit both enhanced semiconductor properties and strong quantum confinement effect similar to the smallest NCs. Here we present a unique approach of generating direct white light from a single semiconductor bulk material, 2D-Cd2S2(ba)](ba=butylamine) based double layer structure. Luminescence properties of this hybrid semiconductor can be tuned systematically by changing its composition and doping level.


572. Aggregation Studies of Tripodal Linkers on Semiconductor Surfaces
Sujatha Thyagarajan and Elena Galoppini, Rutgers-Newark, Newark, NJ
Tripod shaped adamantane derivatives carrying a pyrene sensitizer and three carboxylic acid binding groups (in meta or para positions) with footprint size of 2.7nm² were synthesized to study the effect of the footprint size on the binding and aggregation processes. The photophysical properties were studied in solution and bound to metal oxide surfaces. The UV-vis absorption and fluorescence emission spectra in solution of the pyrene unit were red-shifted due to the extended π-conjugation. Higher extinction coefficients and near unity quantum yields were also observed. Binding to base pre-treated anatase TiO2 films resulted in quenching of the fluorescence indicating electron injection into the semiconductor. Tripods with large footprint, by design, should isolate the pyrene molecule from the nearest neighbors and avoid the formation of excimers on ZrO2 films (ZrO2 is an insulator and the fluorescence is not quenched). However, we observed excimer emission at 505 nm, suggesting contacts between pyrene chromophores from adjacent nanoparticles and necking regions. The effect of aggregation of pyrene chromophores on ZrO2 films studied as a function of surface coverage, solvents, temperature, dyeing times and addition of additives will be discussed.

573. The Role of Aqueous Chemistry in Subcritical Hydrothermal Crystal Growth
Maria C. Gelabert, Wagner College, Staten Island, NY
For subcritical hydrothermal synthesis, crystal habit is sensitive to many experimental parameters, so aqueous conditions influence crystal shapes. However, the current methods for obtaining a particular habit remain largely empirical, relying on a large number of experiments for achieving any degree of prediction and reproducibility. The overall goal in this research is to establish empirical
relationships between aqueous conditions and crystal habit that would enable some degree of predictability for solid state technologies relying on particular crystal habits for optimization of properties. Zincite is being used as a model for its wide technological applicability as well as the ability of Zn2+ to bind to many coordinating species, a primary means by which aqueous conditions are varied. A range of synthesis conditions have used various ligands—EDTA, ethylenediamine-N,N'-diacetic acid (EDDA), , diethylenetriaminepentaacetic acid (DTPA), diethylenetriamine (dien), triethylenetetramine (trien), tetraethylenepentamine (tetren) and pentaethylenehexamine (penten)—and zinc salt counterions acetate, chloride and sulfate. Optical microscopy has revealed that crystal sizes show no apparent correlation with complex stability, even though the presence of a chelating ligand in itself affects crystal size significantly. In order to connect aqueous chemistry to directional growth rates leading to variations in crystal habit, OL Systems speciation software has been used to determine supersaturation levels for zinc ions believed to participate in crystal growth. Comparison of supersaturation calculations with crystal habit will be presented for all studied ligands, in light of establishing a reliable prediction scheme for crystal habit in the subcritical hydrothermal regime.

574. Nanoscale Morphology of Polyaniline and Its Analogs
David M. Sarno1, Steve Da Silva1, Carolina Chaves Prado1 and William L'Amoreaux2, (1)Queensborough Community College - CUNY, Bayside, NY, (2)College of Staten Island - CUNY, Staten Island, NY

For decades, the conducting polymer polyaniline was known as a material with an irregular granular morphology. Recently, a simple modification of the “conventional synthesis” based on rapidly mixing the reagents has proven to be an extremely effective way of producing high yields of uniform nanofibers. We have extended this technique to a series of mono and di-substituted analogs of aniline to examine the influence of ring-substitution on the nanoscale morphology of the resulting material. Scanning electron microscopy has revealed both discrete and interconnected nanofibers; nano/microspheres; and highly porous materials, depending on the monomer. Notably, the morphology of several of these materials is also strongly influenced by reactant concentrations.

575. Synthesis of Exfoliated Functionalized Graphene Sheets
Douglas H. Adamson, Michael J. McAllister, Hannes C. Schniepp and Ilhan A. Aksay, Princeton University, Princeton, NJ

We have developed a process for producing single sheet functionalized graphene by the oxidation and thermal exfoliation of graphite. The oxidation is accomplished by treatment of graphite with a mixture of sulfuric acid, nitric acid and potassium chlorate for 96 hours. The resulting graphite oxide (GO) has an increased layer spacing from the 0.34 nm found in natural graphite to between 0.65 and 0.75 nm. This increase in spacing is found to be critical for the successful exfoliation of the graphite to individual graphene sheets. Rapid heating results in the sheets being forced apart by an abrupt evolution of gas. The thermal treatment also reduces the GO sheets, changing the ratio of carbon to oxygen atoms from 2 to 1 in the graphite oxide to 12 to 1 in the exfoliated graphene sheets (FGS). The high aspect ratio of the produced sheets makes this an exciting nanofiller. In addition, the functionalized surface of the sheets allows for the dispersion of the filler into polymer matrices. We will present results of our investigation into the production of FGS as well as investigations into the use of FGS as a nanofiller in polymer composites.

576. Luminescence, the Instrumental Key to the Future of Nanotechnology
Adam M. Gilmore, HORIBA Jobin Yvon Inc., Edison, NJ

Horiba Jobin Yvon's Fluorescence Division portrays its instrumental role in the future of semiconductor research and nanoscale applications. Our instrumentation has facilitated observations ranging from the original characterization of quantum dot nanocrystals, single-walled carbon
nanotubes and bucky-balls in addition to major breakthroughs in organic electroluminescence. The significance of these breakthroughs are becoming thoroughly established in the biomedical, material and physical sciences. Quantum dots exhibit a broad palette of realized and potential applications ranging from cancer imaging, ultra-sensitive biosensors, reliable anticounterfeiting agents, enhanced logic-gates for quantum computers, and up to and including the recent, widely-heralded potential to replace conventional ‘light-bulbs’ in economic solid state lighting applications. Carbon nanotubes play a diverse role related to their semiconducting properties ranging from affordable high-definition video display technology, high-efficiency electronic circuitry, improved memory devices, deep-tissue biosensing, and DNA sequence recognition inter alia. OLEDs are currently important in small and portable video displays and show a bright economic future because they have many advantages over conventional LCDs including brighter images, broader viewing angles, and lower power consumption. OLEDs will play a key role in affordable solid state lighting applications because they provide flexible white light substrates with strongly reduced space consumption and thermal waste. Future academic and economic trends for nanotechnology include improved health care, increased energy efficiency, and stronger homeland defense. In particular, spatial and spectral imaging of nanomaterial luminescence at both micro- and macroscopic scales will be discussed in significant detail.

Polymers in Medicine / Bio-Inspired Polymers
Organizer: Jin Montclare SUNY Downstate Medical Center, Brooklyn, NY
Organizer: Richard Gross Polytechnic University, Brooklyn, NY

577. Nanostructured Tri-Block Copolymer Gels for Pain Management
Benjamin Chu, Fen Wan, Chirakkal V. Krishnan and Benjamin S. Hsiao, Stony Brook University, Stony Brook, NY

Local anesthetics are extensively used in medicine with applications including chronic pain, surgery, and post-surgical treatment. However, there is a great need for innovative administration techniques of such anesthetics because the drugs have short half lives, and are currently not very cost effective. Tri-block copolymers with the formula represented by E_xP_yE_z and x,y denoting the number of repeating units in each block, can self-assemble into quasi-crystalline lattice nanostructures including lamellar, hexagonal-packed cylindrical micelles and cubic packed spherical micelles in selective solvents. In our studies, triblock smart gels created from mixtures of F127 (E_99P_69E_99) and F87 (E_61P_40E_61) were investigated for sustained drug-release that can be fine-tuned from hours to several days. Results showed that the sol-gel transition temperature can be manipulated over a wide temperature range from room temperature to 44 ºC by varying the composition of the gels. The nanostructures formed in the gel state were determined by X-ray scattering. Preliminary data of in vitro lidocaine (anesthetics) release showed that a sustained release of about 9 days could be achieved, exhibiting a roughly linear release profile. The rate of release could be slowed down further by incorporating polyelectrolyte complexes (PCs). This novel approach can be used to deliver therapeutics for surgical procedures with tailor-designed release profile.

578. Side-Chain Functionalized Supramolecular Polymers
Marcus Weck, New York University, New York, NY

The design and synthesis of complex polymeric materials such as multifunctional copolymers is of importance for a variety of applications ranging from drug delivery systems to organic light-emitting diodes. We will present a novel methodology inspired by Nature’s biomaterials towards the synthesis of such polymeric materials by using a combination of supramolecular chemistry (including

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hydrogen-bonding, Coulombic interactions and metal-coordination) and a living polymerization technique, ring-opening metathesis polymerization. In particular, we will present the design and realization of so-called 'universal polymer backbones' that are based on random, alternating, or block copolymers and possess recognition moieties that self-assemble with their complementary receptor molecules with very high association strengths. Through the employment of living polymerization techniques, we can control the architecture of such polymeric systems and we have proven that the self-assembly of our polymers is quantitative, reversible, and can be achieved in an orthogonal fashion. Therefore, we can synthesize from a single polymer backbone a large variety of functionally varied polymers, which widely differ in their physical and chemical properties, simply by altering the functionalization strategy. Finally, we will also present a variety of applications of these universal polymer backbones in template polymerizations, the controlled, patterned and reversible functionalization of surfaces and particles and the formation of highly cross-linked polymeric networks.

579. Inherent Antibacterial Activity of a Peptide-Based β-Hairpin Hydrogel

Daphne A. Salick, Juliana K. Kretsinger, Lisa A. Haines-Butterick, Darrin J. Pochan and Joel P. Schneider, University of Delaware, Newark, DE

Among several important considerations for implantation of a biomaterial, a main concern is the introduction of infection. Biomaterial-centered infections are common, accounting for about 45% of all nosocomial infections. We have designed a hydrogel scaffold from the self-assembling peptide, MAX1, for tissue regeneration applications whose surface exhibits inherent antibacterial activity. In experiments where MAX1 gels are challenged with bacterial solutions ranging in concentrations from 2 x 10^3 colony forming units (CFU)/dm^2 to 2 x 10^9 CFU/dm^2, gel surfaces exhibit broad spectrum antibacterial activity. Results show that the hydrogel surface is active against gram positive (Staphylococcus epidermidis, Staphylococcus aureus, and Streptococcus pyogenes) and gram negative (Klebsiella pneumoniae and Escherichia coli) bacteria, all prevalent in hospital settings. Live-dead assays employing laser scanning confocal microscopy show that bacteria are killed when they engage the surface. In addition, the surface of MAX1 hydrogels were shown to cause inner and outer membrane disruption in experiments that monitor the release of β-galactosidase from the cytoplasm of lactose permease-deficient Escherichia coli ML-35. These results suggest a mechanism of antibacterial action that involves membrane disruption. Co-culture experiments indicate the hydrogel surfaces show selective toxicity to bacterial versus mammalian cells. Gel surfaces are non-hemolytic towards human erythrocytes and maintain healthy morphologies when in contact with the surface. Preliminary in vitro studies employing J774 macrophages suggest that MAX1 hydrogels may not provoke an inflammatory immune response after implantation into a host. These material attributes make MAX1 gels attractive candidates for use in tissue regeneration, even in non-sterile environments.

580. Multilayer Multifunctional Magnetic Polymeric Nanoparticles for Imaging and Therapy

Mostafa Sadoqi1, Shah Chintan2, Emilio Squillante2, Sunil Kumar3 and Richard A. Gross3, (1)St. John’s University, Queens, NY, (2)St John’s University, Queens, NY, (3)Polytechnic University, Brooklyn, NY

The objective of this work is to develop multifunctional biocompatible nanoparticulate system that can be used both for imaging and therapy. Although several combinations of visualization and therapeutic strategies can be envisioned, the nanoparticles developed in our lab encapsulate near infrared dye and magnetic nanoparticles. Either or both encapsulates can be used for imaging as well as for therapy.

Indocyanine green loaded multilayer magnetic nanoparticles were prepared by thermal decomposition method followed by spontaneous emulsification solvent diffusion. The prepared
magnetic nanoparticles were characterized for particle size, size distribution, zeta potential and morphology. The successful coatings of poly lactic-co-glycolic acid and poly (ε) caprolactone polymers on the magnetic nanoparticles were confirmed by atomic force microscopy and fourier transform infrared spectroscopy. The magnetic property of nanoparticles was measured by magnetic susceptibility tester, and the entrapment of indocyanine green the magnetic nanoparticles was calculated. The prepared magnetic nanoparticles were observed to be spherical in shape, 160 ± 9 nm in size, with a narrow particle size distribution. The zeta potential was observed to be -12.54 mV. Fourier transform infrared spectroscopy showed peaks at 1760 cm⁻¹ and 1726 cm⁻¹ confirming the successful coating of poly lactic-co-glycolic acid and poly (ε) caprolactone respectively on the magnetic nanoparticles. The effective magnetic movement was found to be 4.98 showing the ferromagnetic nature of the particles. The entrapment efficiency of indocyanine green was found to be 75 % and prepared particles provided aqueous stability to ICG.

581. Morphology, Dynamics, and Mechanics of Cells on Electrospun Scaffolds
Ying Liu, Zhi Pan, Richard Clark, Nadine Pernodet and Miriam Rafailovich, Stony Brook University, Stony Brook, NY

Electrospun scaffolds are gaining increasing popularity in tissue engineering applications. We have produced a systematic study of the effects of fiber diameter, spacing, mechanics and orientation on cell morphology, proliferation, and dynamics. We studied both glassy (Polymethylmethacrylate, PMMA) and elastomeric (Polybutadiene) fibrous scaffolds. We measured in vitro both the modulii of the primary culture dermal fibroblast cells and the fibers and correlated the result to images of the integrin receptors and actin fibrils. Proliferation measurements indicated that much larger cell densities could be achieved on oriented substrates, as compared with flat films or randomly oriented electrospun scaffolds. Furthermore, cell dynamics measurements of en masse or single cell migration showed that the cells move at constant velocity on fibers, as opposed to flat surfaces where the velocity decreases as the radial distance from the droplet center increases. The relevance of these findings to wound healing applications will be discussed.

582. Functional Nanofibrous Scaffolds for Biomedical Applications
Benjamin S. Hsiao and Benjamin Chu, Stony Brook University, Stony Brook, NY

Within the last few years, there has been an explosive growth in published reports on the use of electrospinning as a method of generating functional scaffolds intended for biomedical applications. Specific advantages of electrospun scaffolds (high surface-to-volume ratio, controlled porosity, and flexibility to conform to a wide variety of sizes and shapes) make them superior to scaffolds generated by most other techniques. In addition, electrospun scaffold composition and fabrication can also be used to design explicit utility and functionality of scaffolds. Even after fabrication, the physical properties of scaffolds can further be altered to closely match those of native tissues. Collectively, these advantages are reflected in the wide diversity of scaffolds generated with the intended purposes of delivering cells, as well as bioactive agents including drugs, proteins and DNA. In this talk, we outline the current state-of-art fabrication of nanofibrous scaffolds by electrospinning and electro-blowing technologies, as well as describe recent advances made in the production, in vitro and in vivo testing and future potential applications of electrospun scaffolds in biomedical applications such as prevention of surgery-induced adhesion and tissue engineering.

583. Self-Assembling Protein Polymers
Jin Montclare, Polytechnic University, Brooklyn, NY

Traditional methods for polymer synthesis rely on conventional polymerization chemistries that lead to products that are polydisperse. Nature, on the other hand, has been able to generate biopolymers in the form of proteins with varied monomer units that are highly sequence specific and monodisperse. Here we offer an alternative to synthetic polymer synthesis by exploiting nature's
biosynthetic mechanisms to generate protein polymers that may serve as biodegradable materials. We have designed genetically engineered artificial protein co-polymers based on natural extracellular matrix proteins: elastin and cartilage oligomeric matrix protein. We will discuss the synthesis and characterization of the various engineered co-polymers.

**Organic Chemistry, General Session II**
Organizer: JaimeLee Rizzo Pace University

**Session Overview:** This session is for general contributions in the field of organic chemistry.

584. Preparation, Antibacterial Activity and Absorption Spectra of Pyrazolo-Oxadiazine Derivatives
Fayez M. Eissa, Awan Faculty of Science, Aswan, Egypt

The new pyrazolo[4,3-e][1,3,4]oxadiazine heterocyclic ring system was prepared and employed to synthesize cyanine dyes of different methine types, (mono, tri, penta and hepta). The antibacterial activity of all the newly synthesized compounds was investigated against some bacterial strains. The electronic absorption spectra of the dyes were also studied in ethanol. The structure of all the synthesized compounds was identified via elemental and spectroscopic analysis.

585. Oxazolone Cycloadducts as Versatile Scaffolds for Alkaloid Synthesis
Charnsak Thongsornkleeb and Stephen Philip Fearnley, The City University of New York - York College, Jamaica, NY

We have recently developed a series of intramolecular Diels-Alder reactions with oxazolone as the dienophilic species. These initial cycloadducts offer functionalized scaffolds reminiscent of several key alkaloid structural motifs, each well-suited to further elaboration as required. Application to the synthesis of several bioactive alkaloid targets is currently underway. For example, the common n-propyl cycloadduct shown features not only the decahydroquinoline framework of pumiliotoxin C, but could also allow entry to the corresponding indolizidine system via a novel reorganization strategy.

586. Conformational Analysis of cADPR and cADPR Analog Agonists and Antagonists Using PSEUROT, Molecular Mechanics, and Ab Inito Calculations
Steven M. Graham, St. John's University, Queens, NY

Cyclic adenosine diphosphate ribose (cADPR), a cyclic metabolite of NAD⁺, is a second messenger that causes release of calcium from intracellular stores. For some time our lab has been attempting to unravel the structure-activity relationships in cADPR and cADPR analogs, in particular the conformation of the 5-membered furanose rings. The key feature of the PSEUROT program is its ability to convert ¹H⁻¹H NMR coupling constants, via a Karplus equation, to exocyclic H-C-C-H torsion...
angles ($\phi_{\text{exo}}$); these angles are then converted to the endocyclic ring torsions ($\phi_{\text{endo}}$) needed to describe the conformation of the furanose ($\phi_{\text{exo}} = A \cdot \phi_{\text{endo}} + B$). The “A” and “B” parameters are specific to a particular furanose configuration (e.g. ribose, arabinose, deoxyribose, etc.) and are supplied by the PSEUROT program, at least for the common furanoses. In the event that a particular furanose is not in the PSEUROT database, or if one suspects the supplied parameters may not be appropriate (as in cADPR), then the “A” and “B” parameters must be calculated, typically from a survey of in silico structures obtained from molecular modeling. This talk will focus on our efforts to determine the appropriate “A” and “B” parameters for cADPR via molecular mechanics, semi-empirical, and ab initio calculations, and their effect on the PSEUROT calculations.


Steven M. Graham, St. John’s University, Queens, NY and Debra A. Swoboda, York College of the City University of New York, Jamaica, NY

A major issue that students struggle with in organic chemistry is cognitive organization: given a particular problem, what, in the great mass of content covered, is needed to solve the problem? Faculty experts, on the other hand, routinely use knowledge transformations to solve chemistry problems, but they do not always emphasize them in teaching and thus these strategies remain hidden to students.

The See-Think-Predict (STP) method, a problem-solving strategy developed to improve students' chemistry understanding and performance, will be presented. Results indicate that use of STP improves students' problem-solving performance and increases their sense of chemistry mastery. STP use appears to enhance student ability because it assists students in understanding and applying expert knowledge transformations. In order to think and solve chemistry problems like an expert, students engage in: 1) visual interpretation of information; 2) meaningful organization of content and facts; 3) consistent application of strategies; 4) cognitive organization (active monitoring of "knowing" versus "not knowing").

This work has implications for both classroom teaching and student learning. STP appears to be a useful instructional tool for making the expert knowledge transformations involved in solving chemistry problems more explicit. Utilization of STP also infuses the teaching of metacognitive skills into the subject matter, and development of this skill is useful both within and beyond organic chemistry.
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Saturday, May 17, 2008

56th NY-ACS Undergraduate Research Symposium

POGIL Workshop
8.00AM-3.00PM

Chemagination Competition
8.30AM-4.00PM

Project SEED Poster Session
1.00PM-5.00PM

Making the Most of Being a Student Affiliate
2.00PM-4.00PM

Spring Meeting of the United States Section of the Royal Society of Chemistry
2.00PM-4.00PM

ACS Leadership Development Workshop: Involving Volunteers
6.00PM-10.00PM

ACS Leadership Development Workshop: Leading Change

Chemical Education, I
8.00AM-12.00PM

Clinical Chemistry I
8.30AM-12.00PM

Forensic Chemistry
8.30AM-12.00PM

Organic Chemistry, General Session I
8.30AM-12.00PM

NY Section Nichols Teacher Forum
8.30AM-12.00PM

Tapping into the Excitement: Strategies for Building – or Rebuilding – a Student Affiliates Chapter
9.00AM-12.00PM

ACS Leadership Development Workshop: Leading Change

BioTherapeutics
1.00PM-5.00PM

Chemical Education, II
1.00PM-5.00PM

Clinical Chemistry II and Clinical Chemistry Workshop
1.00PM-5.00PM

H I V/ AIDS
1.00PM-5.00PM

Ionic Liquids I: Synthesis and Reactions in Ionic Liquids
1.00PM-5.00PM

Medicinal Chemistry
1.00PM-5.00PM

Process Chemistry
1.00PM-5.00PM

Probeware Workshop and Chemical Demonstrations for Pre-College Educators
1.30PM-5.00PM

Plenary Lecture I: Ronald Breslow, Columbia University
5.30PM-6.30PM

Sunday Night Barbecue/mixer
6.30PM-8.30PM

Poster Session I
7.00PM-8.30PM

Student Union Building Upper

Library Building, Rm LB-6

Medical Arts Building, Rm M-136

Medical Arts Building, Rm M-136

Medical Arts Building, Rm MC-29

Oakland Building

Sunday, May 18, 2008

ACS Leadership Development Workshop: Involving Volunteers

Chemical Education, I
8.00AM-12.00PM

Clinical Chemistry I
8.30AM-12.00PM

Forensic Chemistry
8.30AM-12.00PM

Organic Chemistry, General Session I
8.30AM-12.00PM

NY Section Nichols Teacher Forum
8.30AM-12.00PM

Tapping into the Excitement: Strategies for Building – or Rebuilding – a Student Affiliates Chapter
9.00AM-12.00PM

ACS Leadership Development Workshop: Leading Change

BioTherapeutics
1.00PM-5.00PM

Chemical Education, II
1.00PM-5.00PM

Clinical Chemistry II and Clinical Chemistry Workshop
1.00PM-5.00PM

H I V/ AIDS
1.00PM-5.00PM

Ionic Liquids I: Synthesis and Reactions in Ionic Liquids
1.00PM-5.00PM

Medicinal Chemistry
1.00PM-5.00PM

Process Chemistry
1.00PM-5.00PM

Probeware Workshop and Chemical Demonstrations for Pre-College Educators
1.30PM-5.00PM

Plenary Lecture I: Ronald Breslow, Columbia University
5.30PM-6.30PM

Sunday Night Barbecue/mixer
6.30PM-8.30PM

Poster Session I
7.00PM-8.30PM

Student Union Building Upper

Library Building, Rm LB-8

Medical Arts Building, Rm M-133

Library Building, Rm LB-14

Library Building, Rm LB-6

Science Building, Rm S-112

Library Building, Rm LB-15

Medical Arts Building, Rm MC-29

Library Building, Rm LB-8

Medical Arts Building, Rm M-146

Medical Arts Building, Rm M-133

Library Building, Rm LB-14

Medical Arts Building, Rm M-136

Library Building, Rm LB-6

Science Building, Rm S-111

Science Building, Rm S-112

Science Building, Rm S-405

Medical Arts Building, Rm M-136

Student Union Building, Upper

Student Union Building, Upper

Student Union Building, Upper

Student Union Building, Upper
Monday, May 19, 2008

Polymer I (Materials Synthesis)
  Analysis of Biomolecules
  Antimicrobials
  Bioinorganic Chemistry
  Frontiers in Nanoscience and Nanotechnology – I
  Green Chemistry
  Ionic Liquids II: Properties and Applications
  Physical Chemistry, I
  Tools for Entrepreneurs- from the Kauffman Foundation.
  ACS Career Management and Development Workshops
  ACS Resume Reviews
  Professional Analytical Chemists in Industry: What Does An Analytical Chemist Do?

Analytical Chemistry, General Session I
  Best Practices for the Chemical Entrepreneur
  Biocatalysis and Biomimetic Catalysis
  Delaware Valley Chromatography Forum Student Award
  Frontiers in Nanoscience and Nanotechnology - Nanoscience, II
  Ionic Liquids III: Dynamical Effects in Ionic Liquids
  Metal Complexes in Chemotherapy and Diagnostics
  Physical Chemistry, II

Polymer II (Material Synthesis)
  Synthesis of Complex Biologically Active Molecules
  Probeware Workshop for Undergraduate Educators
  Plenary Lecture II: Roald Hoffmann, Cornell University

Monday Night Barbecue/mixer
Poster Session II
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<th>Location</th>
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<tr>
<td>Directors Breakfast</td>
<td>7.30AM-8.30AM</td>
<td>Oakland Cafeteria</td>
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<tr>
<td>Polymer III (Functional Materials)</td>
<td>8.00AM-12.30PM</td>
<td>Library Building, Rm LB-6</td>
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<tr>
<td>Applications of Organometallic Chemistry</td>
<td>8.30AM-12.00PM</td>
<td>Medical Arts Building, Rm M-134</td>
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<tr>
<td>Chemistry and the Arts</td>
<td>8.30AM-12.00PM</td>
<td>Medical Arts Building, Rm M-143</td>
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<tr>
<td>Computational Chemistry for the Health of Humanity and the Planet, I</td>
<td>8.30AM-12.00PM</td>
<td>Medical Arts Building, Rm M-146</td>
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<td>&amp; Dynamics</td>
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<tr>
<td>Frontiers in Nanoscience and Nanotechnology – Bioapplications</td>
<td>8.30AM-12.00PM</td>
<td>Medical Arts Building, Rm M-142</td>
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<tr>
<td>HPLC Methods Development</td>
<td>8.30AM-12.00PM</td>
<td>Medical Arts Building, Rm M-136</td>
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<tr>
<td>Industrial Chemistry Symposium, I</td>
<td>8.30AM-12.00PM</td>
<td>Medical Arts Building, Rm M-133</td>
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<td>Photochemistry, I</td>
<td>8.30AM-12.00PM</td>
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<td>Spectroscopy of Biological Systems</td>
<td>8.30AM-12.00PM</td>
<td>Library Building, Rm LB-15</td>
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<tr>
<td>Panel Discussion: Traditional and Non-Traditional Careers in Chemistry</td>
<td>9.00AM-11.00AM</td>
<td>Library Building, Rm LB-16</td>
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<td>Women Chemists Committee Luncheon</td>
<td>12.00PM-1.30PM</td>
<td>Oakland Cafeteria</td>
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<td>Analytical Chemistry, General Session II</td>
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<td>Library Building, Rm LB-14</td>
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<tr>
<td>Arthur C. Cope Scholar Symposium</td>
<td>1.30PM-5.00PM</td>
<td>Medical Arts Building, Rm M-136</td>
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<td>Computational Chemistry for the Health of Humanity and the Planet, II</td>
<td>1.30PM-5.00PM</td>
<td>Medical Arts Building, Rm M-146</td>
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<td>– Energetics, Structure, and Functionality</td>
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<tr>
<td>Environmental Chemistry – in Honor of Frances S. Sterrett</td>
<td>1.30PM-5.00PM</td>
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<tr>
<td>Frontiers in Nanoscience and Nanotechnology – Fabrication</td>
<td>1.30PM-5.00PM</td>
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<td>Industrial Chemistry Symposium, II</td>
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<td>Inorganic Chemistry, General Session</td>
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<td>Photochemistry, II</td>
<td>1.30PM-5.00PM</td>
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<td>Polymer IV (Functional Polymers)</td>
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<td>Industrial Innovation Award Symposium and Reception</td>
<td>4.30PM-7.00PM</td>
<td>Oakland Cafeteria</td>
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<td>Poster Session III</td>
<td>5.30PM-7.00PM</td>
<td>Student Union Building, Upper</td>
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<td>Awards Banquet</td>
<td>7.00PM-9.00PM</td>
<td>Oakland Cafeteria</td>
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<tr>
<td>Event</td>
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<td>Computational Chemistry for the Health of Humanity and the Planet, III - Complexity and Accuracy</td>
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<td>Infrared Spectroscopy</td>
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<td>Materials, General Session</td>
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<td>Polymers in Medicine/ Bio-Inspired Polymers</td>
<td>8.30AM-12.00PM</td>
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<td>Organic Chemistry, General Session II</td>
<td>9.00AM-11.00AM</td>
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