Contents

41st Middle Atlantic Regional Meeting

Welcome to the Hotel du Pont and Wilmington, Delaware!

On behalf of the organizing committee and the Delaware Section of the American Chemical Society, we are pleased to welcome you to the 41st Middle Atlantic Regional Meeting, MARM 2010.

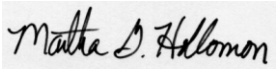
The theme of this meeting is "Chemistry in the First State", reflecting on the history of Delaware and thinking about different states of materials. We have tried to pull together a diverse program while at the same time maintaining all of the fundamental disciplines of chemistry. We have events for all experience levels from the budding young chemists through to our senior chemists. The technical program encompasses analytical, biological, inorganic, organic, medicinal, physical, and polymer chemistry. There are extensive workshops for science teachers including POGIL workshop, career workshops ACS Leadership Development workshop - Fostering Innovation and two popular Chemical, Health, and Safety (CHAS) workshops. In addition, MARM 2010 has an extensive chemistry and law (CHAL) program including a happy hour across the street at Connolly Bove Lodge & Hutz (CBLH) law firm. Our program chair, Narmada Gunawardena and her symposium chairs deserve your congratulations on putting together this exciting program.

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 a warm greeting to all of its members and guest. We hope you will visit the MARM 2010 Expo on Sunday and Monday for exhibits by local, national, and international scientific companies. All are invited to attend the other social events, such as the Directors Breakfast and the Women Chemists Committee Luncheon. We encourage you to attend the MARM 2010 Awards Banquet and Wallace H. Carothers Award Lecture.

We are grateful to our sponsors and advertisers listed on the following pages for their generous support of MARM 2010. This meeting would not have been possible without the tremendous effort of the organizing committee and all of the volunteers who give their time and energy.

Again, welcome to Wilmington, Delaware and we hope that you will find time to relax and enjoy this opportunity to network and learn.

Sincerely,



Martha G. Hollomon
General Chair, MARM 2010

Participating MARM Sections
(Representing Over 30,000 Members)

Washington DC	New York	South Jersey
Delaware	North Jersey	Southeastern Pennsylvania
Lehigh Valley	Philadelphia	Susquehanna Valley
Maryland	Princeton	Trenton
Monmouth County	Ocean County	Western Maryland

American Chemical Society

1155 SIXTEENTH STREET, N.W.
WASHINGTON, D.C. 20036
Phone 202-872-4461
Fax 202-872-6338

OFFICE OF THE PRESIDENT

Joseph S. Francisco, Ph.D.
President-Elect, 2009
President, 2010
Immediate Past President, 2011

April 10, 2010

Dear Middle Atlantic Regional Meeting Participants,

On behalf of the more than 161,000 members of the American Chemical Society, I am pleased to extend greetings to the attendees of the 41st Middle Atlantic Regional Meeting (MARM) at the historic Hotel Du Pont, Wilmington, Delaware.

The theme of the meeting is "Chemistry in the First State." Topical symposia include sessions on medicinal chemistry and the pharmaceutical industry; environmental chemistry; physical/analytical chemistry; materials science/polymer chemistry and engineering; fluorine chemistry; materials science/nanochemistry; sustainability, green chemistry and policy; computers in chemistry; chemical education; food chemistry; issues and resources in chemical health and safety; and more. Please take this opportunity to interact with your colleagues and to discuss developments taking place in your field.

While you're here, I hope you also take the time to fully explore the interesting array of symposia, workshops and special sessions, attend the many social events, visit the exhibition, and some of Wilmington's area attractions.

I am grateful to the many volunteers, especially the members of the ACS Delaware Local Section and the other 14 participating northwest region local sections of the American Chemical Society – representing over 30,000 members in the region! – for their hard work and dedication to create an intellectually stimulating, as well as personally enjoyable experience here in Wilmington.

Sincerely,

Joseph S. Francisco, Ph. D.
President
American Chemical Society

STATE OF DELAWARE
OFFICE OF THE GOVERNOR
TATNALL BUILDING, SECOND FLOOR
WILLIAM PENN STREET, DOVER, DE 19901

JACK A. MARKELL
GOVERNOR

PHONE: 302-744-4101
FAX: 302-739-2775

April 10, 2010

Dr. Martha Hollomon
General Chair, MARM 2010
Delaware Section of the American Chemical Society
203 Robin Redbreast Road
Newark, Delaware 19711

Dear Dr. Holloman and Friends:

I am pleased to welcome you to the American Chemical Society's 41st Middle Atlantic Regional Meeting (MARM 2010), at the historic Hotel du Pont in Wilmington.

Hosted by the American Chemical Society, Delaware Section, this event provides an opportunity for some of the best and brightest in the chemistry field to gather and share their knowledge.

This year's theme, "Chemistry in the First State" is very fitting as the State of Delaware continues to serve as a leader in chemistry and engineering - and a home to many foremost chemical companies and research organizations.

Our state attracts over eight million visitors a year, but we always have room for more. It is my sincere hope that your time in Delaware during this gathering will prove to be educational, enjoyable and relaxing.

Once again, I welcome to you the beautiful State of Delaware.

Sincerely,

Jack Markell

Jack A. Markell
Governor

JAMES M. BAKER
MAYOR

James M. Baker
Mayor

City of Wilmington
Delaware

LOUIS L. REDDING - CITY/COUNTY BUILDING
800 FRENCH STREET
WILMINGTON, DELAWARE
19801 - 3537

April 2010

Dear Friends:

It is with great pleasure that I welcome you to the City of Wilmington for the 41st Middle Atlantic Regional Meeting of the American Chemical Society.

Since its founding, members of the American Chemical Society have made remarkable progress in helping us understand the world in which we live. Today the organization remains as committed as ever to continuing that important legacy by educating and encouraging our young people to pursue careers in the sciences, creating viable community partnerships throughout the nation, and promoting an environment of continuous learning, networking and professionalism throughout its membership.

During your stay, I invite you to experience the rich cultural, historical and social attractions of Wilmington. From tax-free shopping and awe-inspiring collections of art, to sell-out crowds at theatre productions and in the stands of our hometown baseball team, Wilmington is an exciting City with much to offer.

Again, welcome! I hope you enjoy your stay in our beautiful City.

Very truly yours,

James M. Baker
Mayor

THOMAS R. CARPER
DELAWARE

United States Senate

WASHINGTON, DC 20510–0803

April 10, 2010

Dr. Martha Hollomon
General Chair, MARM 2010
Delaware Section of the American Chemical Society
203 Robin Redbreast Road
Newark, DE 19711

Dear Dr. Hollomon and Friends:

It is a great pleasure to welcome the American Chemical Society's 41st Middle Atlantic Regional Meeting to Delaware!

For over 100 years, the American Chemical Society (ACS) has been the leader among professional organizations supporting all fields of chemistry. They have effectively created a network that allows scientists to share information and support each other all over the globe. In addition, the ACS's educational programs, scholarship opportunities, and effective policymaking efforts are second to none.

I am honored to note Delaware's proud past, present, and future as a leader in chemistry and chemical engineering. As a home to many leading chemical companies, the research and development done in Delaware has consistently been at the top of its class. With organizations such as yours to support these companies' efforts, they will surely maintain their standard of excellence.

Again, welcome to the ACS's 41st Middle Atlantic Regional Meeting. I wish you all the best for a productive and successful conference. I hope that you have a great visit and please know that you are always welcome here in Delaware.

With best personal regards, I am

Sincerely yours,

Tom Carper

Thomas R. Carper
United States Senator

EDWARD E. KAUFMAN
DELAWARE

www.kaufman.senate.gov

383 RUSSELL SENATE OFFICE BUILDING
WASHINGTON, DC 20510
(202) 224-5042

United States Senate

JUDICIARY COMMITTEE
MEMBER

FOREIGN RELATIONS COMMITTEE
MEMBER

April 10, 2010

American Chemical Society
C/o John Gavenonis, Ph.D.
DuPont Performance Polymers
Chestnut Run Plaza, Building 713/215
4417 Lancaster Pike
Wilmington, DE 19805

Dear Dr. Gavenonis,

Welcome to the American Chemical Society's 41st Middle Atlantic Regional Meeting (MARM 2010) at the Hotel du Pont in Wilmington!

My hat goes off to the Delaware Section of the American Chemical Society for hosting this year's meeting. Events like this are crucial to professional development and leadership training. America's scientists have a central role to play in developing the innovative technologies that will help our economy recover and promote real job growth. Indeed, I believe the key to the future of our country, and the world, rests on our ability to use science, technology, engineering, and math to solve the major problems we face.

As a fellow engineer, having attained a bachelor's degree in mechanical engineering and worked at DuPont for several years, I am pleased that this year's meeting is hosted in my home state of Delaware. Please accept my heartfelt wishes for a productive and successful event!

Sincerely,

Ted Kaufman

Edward E. Kaufman
United States Senator

24 NORTH WEST FRONT STREET
WINDSOR BUILDING, SUITE 101
MILFORD, DELAWARE 19963
(302) 424-8090

1105 NORTH MARKET STREET
SUITE 2000
WILMINGTON, DELAWARE 19801
(302) 573-6345

MICHAEL N. CASTLE
MEMBER OF CONGRESS

April 10, 2010

American Chemical Society
Attn: Martha Hollomon, Ph.D.
General Chair, MARM 2010
Delaware Section of the American Chemical Society
203 Robin Redbreast Road
Newark, DE 19711

To the members of the American Chemical Society:

It is my honor to welcome all of you to Delaware for the 41st Middle Atlantic Regional Meeting of the American Chemical Society (ACS).

ACS's mission to stay committed to *Improving people's lives through the transforming power of chemistry*, has certainly shone true. Since it was first created more than 100 years ago, it has grown to be the world's largest scientific society, providing invaluable support to all fields of chemistry. ACS certainly sets a sterling example for professional societies everywhere, and you are always welcome in Delaware.

Delaware is a noted leader in the fields of chemistry and chemical engineering, as it is home to numerous companies and bright minds. It is exciting and fitting that your Middle Atlantic Regional Meeting is being held right here in the First State. It is my sincere hope that your conference is rewarding and that it leads to continued success in your endeavor to further the field of chemistry.

Once again-- welcome to Delaware! Please accept my best wishes as you participate in the 41st Middle Atlantic Regional Meeting of the American Chemical Society.

Sincerely,

Mike Castle

Michael N. Castle

NOT PRINTED AT GOVERNMENT EXPENSE

TABLE OF CONTENTS

ACS Board of Directors

The following members of the ACS Board of Directors are expected to be at MARM 2010.

	**Nancy B. Jackson, President Elect** Sandia National Laboratories Manager, International Chemical Threat Reduction Department She received her B.S. degree in chemistry from George Washington University in 1979, and her Ph.D. in chemical engineering from the University of Texas at Austin in 1990. She has been an ACS member since 1979.
	**Thomas H. Lane, Immediate Past President** Dow Corning Corporation, Scientist Emeritus He received B.S. in Chemistry from Purdue University, 1974; M.S. in Chemistry from Central Michigan University, 1979; and Ph.D. in physical chemistry from Open University in England 1990. He has been an ACS member since 1973
	**William F. Carroll, Jr., Director-At-Large** Occidental Chemical Corporation, Vice President He holds a B.A. in chemistry and physics from DePauw University; M.S. from Tulane and a Ph.D. from Indiana University. The latter two degrees are in organic chemistry. He is adjunct professor of chemistry at Indiana, where he teaches polymer chemistry. In 2005, Bill was president of the American Chemical Society. He has been an ACS member since 1974.
	**Dennis Chamot, Director-At-Large** National Research Council, Associate Executive Director He received a B.S. and M.S. from Polytechnic University, Brooklyn, N.Y., in 1964; a Ph.D. from the University of Illinois in 1969; and an M.B.A. from the University of Pennsylvania, Wharton School, in 1974. He is an adjunct assistant professor in the Graduate School of Management & Technology at University of Maryland. He has been an ACS member since 1965.
	**Pat N. Confalone, Director, District III** DuPont, Vice-President, Global Research & Development, Crop Protection, Agriculture & Nutrition Platform He received his B.S. from Massachusetts Institute of Technology in 1967, his M.S. in 1968 and Ph.D. in 1970, both from Harvard University. He has been an ACS member since 1970.
	**Neil D. Jespersen, Director, District I** St. John's University, Professor of Chemistry He received his B.S. from Washington & Lee University in 1967. He received his Ph.D. in 1971 from Pennsylvania State University. He has been an ACS member since 1969.

MARM 2010 Organizing Committee

General Chair	Martha Hollomon	Widener Univ.
Program Chair	Narmada Gunawardena	AstraZeneca R&D
Treasurer	Xiaoli Wang	AstraZeneca R&D
Advertising Manager	Vince Gale	MBO Services
Exhibits Chair	Allen Denio	Retired, Univ. of WI – EC
Awards Chair	Sharon Haynie	DuPont
Fund-Raising	John Gavenonis	DuPont
Careers Chair	Kai Qi	DuPont
Webmaster	Paul Tukey	Bell Laboratories
MARM Executive Board Chair	Yorke Rhodes	Retired, NYU
Delaware Section, Chair 2010	Eric Holowka	DuPont
Delaware Section, Chair 2011	vacant	--
ChemVets, Chair DE ACS, Senior Chemist	Doug Druliner	Retired DuPont
Office of Regional Meetings	Amanda Frederick	ACS

MARM 2010 Logo created by
Miller Mauro Group, Inc.
marketing communications
Creative | Comprehensive | Competitive

MARM 2010 Volunteers

This regional meeting would not have been possible without the invaluable efforts of the volunteers – session chairs and moderators, workshop leaders, event organizers, and everyone else who lent a helping hand along the way.

Anthony Addison	Drexel University
Joshua Ayers	AstraZeneca
Bogdan Barboiu	Infineum
Brian Bidlingmeyer	Agilent
Dean Brown	AstraZeneca
Wayne Brubaker	DuPont
Susan Cheadle	University of Delaware
Margaret Christoph	St. Mark's High School
Frank Creegan	Washington College
Andrew Combs	Incyte
Barbara Dehaven	DE Economic Development Office
Cecil Dybowski	University of Delaware
Alen Denio	DE ACS & DE Acad. Chem. Sci.
Jade Duan	AirLiquide
Marshall Fishman	Eastern Regional Research Center, ARS, USDA
John Gavenonis	DuPont
Terri Quinn Grey	DuPont
Ross Getty	DuPont
Alicia Harris	ACS Staff
Justin Hasford	Finnegan Henderson Farabow Garrett & Dunner, LLP
Sarah Hasford	Connolly Bove Lodge & Hutz LLP
Norman Henry	CHAS
Tiffany Hoerter	AstraZeneca
Elizabeth Howson	Retired
Gary Johansson	DuPont
Denis Kissounko	University of Delaware
Diane Krone	Northern Highlands Regional H.S.
Louise Lawter	ACS Princeton Section
Joanne Long	NJACS-TA
Ester Lovlie	GWCVB
Andrea Martin	Widener University
Erica Martin	Dow Chemical
Joe Mauro	Miller Mauro Group, Inc.
Les McQuire	Novartis
Donald Mencer	Wilkes University
Allison Moore	Ashland
Jeffrey Moore	Siemans Healthcare Diagnostics
Mark Paczkowski	Lubrizol
Simona Percec	DuPont
Kai Qi	DuPont
Nora S. Radu	DuPont
Anis Rahman	Applied Research & Photonics, Inc.
Yorke Rhodes	New York University
Garretta Rollins	ACS Staff
David Rovnyak	Bucknell University
David Sarno	QCC
Greg Shafer	W. L. Gore & Associates
Jennifer Smuts	Connolly Bove Lodge & Hutz LLP
Michael Stemniski	University of Delaware
Bill Suits	ACS North Jersey Section
Paris Svoronos	QCC
Doug Taber	Unversity of Delaware
Jodi L. Wesemann	ACS
Lois Weyer	ATK
Joy Titus-Young	ACS
Zheng P. Yang	GlaxoSmithKline Pharmaceuticals

The volunteer work by local and regional High School and college students

MARM 2010 Sponsors

This regional meeting would not occur without the generous financial contributions from individuals and the corporations or ACS divisions they represent. Please take time to visit sponsors with exhibits and read the sponsor and advertiser pages in this Program book.

Sponsors of the 2010 Carothers Award and Lecture

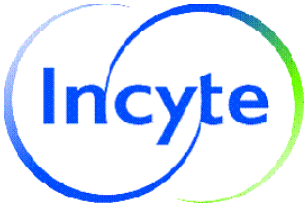
www.dupont.com

www.gore.com

Sponsors of the 2010 Carothers Award and Lecture – Continued

www.cpchem.com

www.infineum.com



www.incyte.com

Sponsors of the Frontiers in Magnetic Resonance in Liquids and Solids Symposium

www.bruker.com

www.varian.com

Cambridge Isotope Lab
www.isotope.com

Sponsor of Computers in Chemistry Symposium

RCH SOLUTIONS www.RCHsolutions.com	Since 1991, RCH Solutions (Products) has served as a trusted, independent advisor in Life Sciences by offering technology and business solutions to a number of organizations across a variety of industries. Our value-added hardware, software and consulting solutions have helped many research and scientific organizations as well as a number of top Fortune 500 and SMB companies achieve measurable business results. These customers truly value our hands on, business and application oriented approach.

We deliver solutions that are supported by an experienced team of professionals. RCH offers a single point of contact to help you navigate and manage your HPC environment. Whether commercial or highly customized, your computer environment should enable you and your people to more effectively conduct research and achieve results. With support and guidance from RCH, your systems will be completely integrated with the necessary security, performance, and availability to meet your changing scientific needs.

Remember, the most dependable and accurate solutions always come from an informed objective resource. RCH customers have relied on us to address the complete technology lifecycle including assessment, design, planning, implementation and support. We have earned a reputation for exemplary client service, intelligent systems design, rapid implementation and unsurpassed industry knowledge.

The RCH solutions have helped a number of research organizations in Life Sciences (Pharmaceutical, Biotech, R&D), Health Care, Education, Chemical, and Financial Services. With our deep knowledge and expertise in scientific research applications, we also offer technology and application consulting utilizing many of the leading technology product manufacturers. Our Preferred partners include: HP, IBM, Isilon, NetApp, Revolution Computing, SGI and, Sun. We also work with RedHat, Intel, AMD, and Microsoft.

We thank our additional symposia and special workshop sponsors.

ACS Chemistry for Life®

American Chemical Society
www.acs.org

C H E D

ACS Division of Chemical Education
CHED
www.divched.org

YAMAZEN SCIENCE, Inc
Japan's *best-selling* Automated Flash Systems

ACS Division of Analytical Chemistry
ANYL

Miller Mauro Group
marketing communications

www.mmg.com

ACS Division of Chemical Health & Safety
CHAS

ACS Division of Medicinal Chemistry
MEDI

ACS Division of Chemistry & Law
CHAL

ACS Division of Computer in Chemistry
COMP

ACS Division of Organic Chemistry
ORGN

ACS Department of Career Management & Development

ACS Board Committee on Local Section Activity
LSAC

ACS Undergraduate Programs Office

ACS Women Chemists Committee

ACS Center for Professional Development

MARM Board

Delaware Section of the American Chemcial Society

Exhibitors at MARM 2010

Come visit the MARM 2010 Expo in the conference center dining and lounge area. In this area, you will find refreshments and it will be a great place to network with colleagues and representatives from the Expo companies. The Expo will take place on Sunday, April 11 and Monday, April 12.

Chemglass Life Sciences
www.chemglass.com
In addition to our wide selection of glassware and equipment for chemistry we have begun adding products for chromatography and cell culture keeping us on the forefront of scientific innovation. CGLS fabricates standard glassware items and components as well as custom glassware. We have the capability to produce not only the most complex glass apparatus, but also intricate electronic equipment and customized machined components. Products include process reactors from 10L-100L, benchtop reactors from 100 mL-5 L.

Delaware Academy of Chemical Sciences
www.delchemistry.org
The Academy is a 501(c)(3) tax-exempt organization of community and leaders and professionals from chemistry and education interested in increasing science literacy through fun and effective public chemistry outreach programs.

Dionex Corp.
www.Dionex.com
It's All About the Chemistry-Dionex delivers breakthrough chromatography solutions for better performance and higher productivity. The UltiMate 300CLi series includes RSLC systems with UHPLC and HPLC capabilities, the new RSLCnano system for proteomics. The titanium solution with bioinert flow paths and ESA detectors expand capabilities for biomolecule detection. Our unique ReagentFree™ IC systems feature Eluent Generation and Regeneration. We lead the industry with selective high-capacity IC and HPLC/RSLC columns and consumables and automated sample preparation and solid-phase extraction systems that significantly reduce labor and waste.

ACS Division of Chemical Education
www.divched.org
The Division of Chemical Education (DivCHED) is one of 33 technical divisions within the American Chemical Society (ACS). Its members come from the entire educational spectrum (pre-secondary, secondary, two- and four-year colleges, universities, research institutions), and include those from industry who are concerned about the education and professional

training of future chemists and other molecular scientists. DivCHED provides a common ground for teachers and students of chemistry to examine chemical education in its broadest sense through its committee and governance structure, website, Newsletter, programs at national and regional ACS meeting, the ACS Exams Institute, the Biennial Conference on Chemical Education (BCCE), and the premier journal in its field, the Journal of Chemical Education.

Glas-Col, LLC
www.glascol.com
Glas-Col offers the largest selection of heating mantles and heating jackets in the world plus temperature controls, monitors, and a range of safety accessories, Glovebags, safety shields, flow monitors and lead stability products. Also, hot plates, magnetic stirrers, hot plate magnetic stirrers and concentrators, evaporators for solvent removal. We now manufacture the Zanntek line of evaporators and the Instruments for Research and Industry line of safety equipment.

Heidolph Brinkmann LLC
www.heidolphbrinkmann.com
Heidolph Instruments, founded in 1938 as a manufacturer of precision drive motors and engineering, is a manufacturer of High Quality laboratory equipment, specializing in rotary evaporation, shakers, overhead stirrers, peristaltic pumps, and magnetic hotplate stirrers. Heidolph Brinkmann was formed as our North American headquarters and includes exclusive partnerships for Tuttnauer™ autoclave sterilizers, Radley™ synthesis solutions, and AirClean™ laboratory ventilation solutions.

JULABO USA
www.julabo
The temperature control Company, offers a wide selection of liquid temperature control equipment including: Water Baths, Recirculating Chillers, Immersion Coolers, Calibration & Visco Baths, Heating and Refrigerated Circulators, and the new Presto Plus Highly Dynamic Temperature Control Systems providing up to 36 kW of heating power and 30 kW of cooling power. All JULABO products carry a 2-year warranty.

Mettler-Toledo AutoChem, Inc.
Visit our website at www.mt.com/autochem. View and register for on-line webinars at www.mt.com/ac-webinars. Mettler Toledo provides product and service solutions to enable faster development of robust processes for better chemical and bio-pharmaceutical products. The METTLER TOLEDO worldwide team of technical sales and support experts serve our customers in the Bio-Pharmaceutical, Specialty and Fine Chemical, Petroleum and Petrochemicals, and Polymer industries. Application expertise includes organic

synthesis, process development & safety, crystallization, product formulation, polymerization, Process Analytical Technologies (PAT)/Quality by Design (QbD) and particle processing.

National Lab Day
www.Nationallabday.org
Bring exciting Hands-on Learning to Your Area. It's more than just a day. It's a nationwide initiative to build local communities of support that will foster ongoing collaborations among volunteers, students and educations. These volunteers namely STEM professionals and, more broadly, members of the community ware working together with educators and students to bring discovery-based science experiences to students in grades K-12.

RCH Solutions
www.RCHsolutions.com
Since 1991, RCH Solutions (Products) has served as a trusted, independent advisor in Life Sciences by offering technology and business solutions to a number of organizations across a variety of industries. Our value-added hardware, software and consulting solutions have helped many research and scientific organizations as well as a number of top Fortune 500 and SMB companies achieve measurable business results. These customers truly value our hands on, business and application oriented approach. We deliver solutions that are supported by an experienced team of professionals. RCH offers a single point of contact to help you navigate and manage your HPC environment. Whether commercial or highly customized, your computer environment should enable you and your people to more effectively conduct research and achieve results. With support and guidance from RCH, your systems will be completely integrated with the necessary security, performance, and availability to meet your changing scientific needs.

Remember, the most dependable and accurate solutions always come from an informed objective resource. RCH customers have relied on us to address the complete technology lifecycle including assessment, design, planning, implementation and support. We have earned a reputation for exemplary client service, intelligent systems design, rapid implementation and unsurpassed industry knowledge.

The RCH solutions have helped a number of research organizations in Life Sciences (Pharmaceutical, Biotech, R&D), Health Care, Education, Chemical, and Financial Services. With our deep knowledge and expertise in scientific research applications, we also offer technology and application consulting utilizing many of the leading technology product manufacturers. Our Preferred partners include: HP, IBM, Isilon, NetApp, Revolution Computing, SGI and, Sun. We also work with RedHat, Intel, AMD, and Microsoft.

Thales Nano Inc.

www.thalesnano.com

Thales Nano is the world leader in bench-top flow chemistry reactors. The company has the widest portfolio of continuous process instruments for the pharmaceutical, biotech, fine chemical, petroleum, biofuel, and education markets. Its R&D 100 award winning H-Cube® and scale-up system H-Cube Midi™ are used in hundreds of laboratories globally and have become the new industry standard for hydrogenation. Within three years from the original introduction of its flagship H-Cube product, 20 out of the top 20 pharmaceutical companies have introduced and adopted the technology.

Uniqsis & Asynt

www.uniqsis.com and www.asynt.com

Uniqsis was founded in January 2007 and is an alliance between Asynt, the specialist supplier of organic synthesis apparatus, and Grant Instruments Ltd, the long established scientific equipment manufacturer. Uniqsis' aim is to develop innovative flow chemistry products for customers in both the research and biopharmaceutical sector.

GENERAL MEETING INFORMATION FOR MARM 2010

Registration
On-site registration will begin at 8:00 a.m. Friday, April 9, 2010. Payment can be made by cash, credit card or check. Registration will take place in the Conference Center at Hotel du Pont. The registration schedule is as follows:

Friday	April 9, 2010	8:00 AM - 7:00 PM
Saturday	April 10, 2010	7:30 AM - 7:30 PM
Sunday	April 11, 2010	7:30 AM - 7:30 PM
Monday	April 12, 2010	7:30 AM - 7:30 PM
Tuesday	April 13, 2010	8:00 AM - 10:00 AM

Refreshments at the meeting
Light refreshments will be served during the scheduled morning and afternoon breaks in the dining/lounge area of the conference center. Box lunches may be order in advance at the registration desk. The Grill is an informal cafeteria-style restaurant at the Hotel du Pont, serving breakfast and lunch five days a week. The Lobby Lounge offers a more casual dining option at the Hotel du Pont, serving afternoon tea on weekends, and light fare. A complimentary continental breakfast will be served in the Conference Center Reception Area in the Hotel du Pont on Saturday morning before the start of the technical program. A list of downtown Wilmington restaurants within walking distance from the Hotel du Pont will be available at the registration desk.

Mixers
A welcoming reception (continental breakfast) will be held in the dining/lounge area of the Hotel du Pont conference center from 7:30 – 9:00 AM on Saturday, April 10. All registrants are welcomed to this free event. On Sunday, April 11 and Monday, April 12, a casual mixer reception will be held in the dining/lounge area with the MARM 2010 Expo. On Monday morning, all registered attendees are invited to the du Barry Ballroom to enjoy a complimentary continental breakfast hosted by Neil Jespersen, ACS District I Director and Pat Confalone, ACS District III Director. Other members of ACS Governance will also be present for an informal discussion of the latest information and decisions from the ACS Spring National Meeting. Bring your ideas and concerns. They want to hear from you!

Programming for Students and Educators
MARM 2010 offers a variety of programs for students including ACS Undergraduate Research Symposium, ACS Graduate & Post-Doc Research Symposium, Student Member (undergraduate) luncheon with Neil Jespersen, ACS Director, District I, as the featured speaker, leadership and career workshops.

Programs for educators is Saturday, April 10 with a free POGIL workshop, information about National Lab Day, Chemical Education symposium and chemical demonstration by Dr. Michael Stemniski.

MARM 2010 SPECIAL EVENTS

Friday, 9 April 2010	Time	Room*
On-Site Registration Open	8:00 AM - 7:00 PM	Conference Center
Saturday , 10 April 2010	**Time**	**Room***
On-Site Registration Open	7:30 AM - 7:30 PM	Conference Center
Welcome Reception Continental Breakfast	7:30 AM - 9:00 AM	Dining/ Lounge Area
POGIL Workshop for H. S. Teachers	9:00 AM - 12:00 PM	King/Sullivan
Women Chemist Committee Luncheon	12:00 PM - 1:30 PM	Christiana Room
Chemical Educators (K - 12) Luncheon	12:00 PM - 1:30 PM	King/Sullivan
Chemical Health & Safety (CHAS) Laboratory Waste Management Workshop	1:00 PM -5:00 PM	Marshall
Regional Chemagination Competition	1:30 PM - 4:00 PM	Blake
High School Research Poster Session	1:30 PM - 4:00 PM	Piaget
Project SEED Poster Session	1:30 PM - 4:00 PM	Collins
Plenary - Chemical Demonstrations	4:00 PM - 5:00 PM	King/Sullivan
Spring Meeting of the United States Section of the Royal Society of Chemistry	6:00 PM - 10:00 PM	Delaware Suite

*Rooms are subject to change

Sunday, 11 April 2010	Time	Room*
On-Site Registration Open	7:30 AM - 07:30 PM	Conference Center
Chemical Health & Safety Workshop How to Be a More Effective Chemical Hygiene Officer	8:30 AM – 4:00 PM	Marshall
Exhibition	9:00 AM – 8:00 PM	Dining/Lounge Area
ACS Undergraduate Research Symposium I Poster Session	8:30 AM - 10:00 AM	King/Sullivan
ACS Undergraduate Research Symposium II Poster Session	10:00 AM - 11:30 AM	King/Sullivan
ACS Undergraduate Student Luncheon	12:00 - 1:30 PM	du Barry Ballroom
Chemistry and Law - Your Company Fosters Innovation:	1:00 - 4:30 PM	Greenville
ACS Leadership Development Course	1:00 - 5:00 PM	Montessori
ACS Undergraduate Research Symposium III Poster Session	1:30 - 3:00 PM	King/Sullivan
Plenary Symposium - Sustainability, Green Chemistry, & Policy	3:15 - 4:30 PM	King/Sullivan
Reception Mixer	4:30 PM - 6:30 PM	Dining/Lounge Areas
ACS Graduate & Post-Doc Research Symposium Poster Session	6:30 - 8:00 PM	King/Sullivan

Monday, 12 April 2010	Time	Room*
On-Site Registration Open	7:30 AM - 7:30 PM	Conference Center
Directors' Continental Breakfast	7:30 - 8:30 AM	du Barry Ballroom
University of Delaware - Department of Chemistry & Biochemistry Alumni Breakfast	8:30 - 9:30 AM	Christina Room
ACS Careers Management Workshop - Planning Your Job Search	8:00 - 9:30 AM	Quintanilla
Exhibition	9:00 AM - 8:00 PM	Dining/Lounge Area
Chemistry & Law - What a Chemist Needs to Know About Patent Law	9:00 AM - 1:00 PM	Greenville Suite
Delaware Academy of Chemical Sciences - DuPont's Textile Fiber Dept.	10:00 AM - 12:00 PM	Piaget
ChemVets / Senior Chemist	10:00 AM - 12:00 PM	Collins
ACS Careers Management Workshop - Preparing a Resume	9:30 - 11:00 AM	Quintanilla
ACS Careers Management Workshop - Effective Interviewing	11:00 AM - 12:30 PM	Quintanilla

Monday, 12 April 2010	Time	Room*
Delaware Section 50- and 60- ACS Member Luncheon	12:00 - 1:30 PM	du Barry Ballroom
ACS Careers Management Workshop - ACS Career Consultants	1:00 -5:00 PM	Quintanilla
Delaware Academy of Chemical Sciences - DuPont's Textile Fiber Dept.	2:00 - 4:00 PM	Piaget
Happy Hour - Connolly Bove Lodge & Hutz, LLP Law Firm	4:30 -6:30 PM	1007 N. Orange St.
MARM 2010 Awards Banquet and Carothers Lecture	5:30 - 9:30 PM	du Barry Ballroom

Tuesday, 13 April 2010	Time	Room*
MARM Board Meeting	12:00 - 2:00 PM	

MARM 2010 WORKSHOPS

Saturday, April 10, 2010,

POGIL Workshop for High School Chemistry Teachers 9:00 AM – 12:00 PM
This workshop introduces the philosophy and methodology of Process Oriented Guided-Inquiry Learning (POGIL). This method of teaching actively engages students in learning through working in groups to develop critical thinking skills student use new molds and experimental data to construct new concepts.

Laboratory Waste Management 1:00 PM – 5:00 PM
This course will identify the various regulatory requirements that apply to laboratories that generate hazardous waste, as well as provide insight into the options for on-site management and off-site disposal. Focus will include discussion on recycling/reclamation techniques, economical handling of wastes, and liability issues.

Sunday, April 11, 2010

How to be a More Effective Chemical Hygiene Officer Workshop 8:30 AM – 4:00 PM
Take a close look at the Chemical Hygiene Officer position, and prepare at the same time for the "CHO" Certification exam to be held the next day. The workshop will take a close look at safety issues in the laboratory, focusing on what you do and how you can do it better. You can request an application packet for the Chemical Hygiene Officer Certification examination by National Registry of Certified Chemists online at http://www.nrcc6.org .

ACS Leadership Development Course, Fostering Innovation 1:00 PM – 5:00 PM

This 4-hour facilitated leadership development workshop targets the developing leaders who are constantly challenged to come up with new ideas, approaches, and solutions, yet most of us feel ill-equipped to do this effectively. With a systematic and proven process to generate ideas you can lead your team to develop new ideas.

Monday, April 12, 2010

ACS Career Management Workshop 8:00 AM – 12:30 PM

The following three one-hour modules cover all aspects of managing an effective job search: (1) Job Searching Strategies; (2) Resume Preparation for the Chemical Professional; and (3) Interviewing Skills for the Chemical Professional.

MARM 2010
CHEMAGINATION CONTEST

"Chemagination" is a contest in which 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 2035, looking back at innovations that have occurred since 2010.

The Regional Chemagination Competition will take place on Saturday, April 10, 2010 at Hotel du Pont, Conference Center, Wilmington DE. The tentative agenda is as follows:

12:00 – 1:30 PM	Set-up and Lunch
1:30 – 3:30 PM	Judging
3:30 – 4:00	Awards and Pictures
4:00 – 5:00 PM	Special demonstration by Dr. Michael Stemnisky

First place category winners from LOCAL ACS section competitions are eligible to participate. If a first place winner cannot participate for any reason, sections can elect to send an alternate team. If your section did not hold a local competition, interested students could participate directly at the regional level (contact the Chemagination coordinators for more details).

Contest coordinators Louise Lawter at lawterjr@verizon.net or Vijaya Korlipara at korlipav@stjohns.edu. Event sponsored by the MARM Board.

The Delaware Academy of Chemical Sciences

102 Red Pine Circle • Newark, DE 19711 • 302-455-0389 • DEAcadChemSci@gmail.com

DuPont's Textile Fibers Department: Remembering a Great Moneymaker

The company prospered in the rayon business, but the invention of nylon-66 on February 28, 1935 was a game changer. Dr. Wallace Carothers and his research group came up with a polyamide fiber that was an immediate success. Introduced to the public in 1938, nylon was an impressive replacement for silk in women's hosiery.

The start of World War II at the end of 1941 meant that nylon production quickly was consumed by the war effort. After the war, nylon continued its commercial success. This was followed by the fibers Orlon, Dacron, Lycra, Kevlar and Nomex. The Textile Fibers Department was a goldmine for many years.

In this new century, much of the Department was rebranded as "Invista" and sold to Koch Industries. **The Delaware Academy of Chemical Sciences has organized a Symposium at MARM 2010, to be held on Monday, April 12 from 10 am to noon and from 2 to 4 pm.** Our goal is to have former members of the Department discuss various aspects of "life" in the fiber world, ranging from the research efforts to manufacturing, marketing, sales, etc. Come and hear about triumphs, failures, joys and frustrations. These "survivors" have amazing stories to share.

MARM 2010 Awards Summary

ACS Division of Chemical Education Middle Atlantic Region Award for Excellence in High School Teaching
Stephan Radice, Edward R. Murrow High School, Brooklyn, NY

The E. Emmet Reid Award in Chemistry Teaching at Small Colleges in the ACS Mid-Atlantic Region
Dr. Amber Charlebois, Fairleigh Dickinson University

The E. Ann Nalley Regional Award for Volunteer Service to the American Chemical Society
Dr. Alan B. Cooper, Merck

Delaware ACS Section Wallace H. Carothers Award for Outstanding Contributions and Advances in Industrial Application of Chemistry
Dr. Ronald Knudsen, Chevron Phillips Chemical Company (retired)

The Chromatography Forum of Delaware Valley -Student Award Symposium
Donna Blackney, Drexel University
Jeff Bolstridge, Lafayette College
Neha Gujarati, St. John's University
Shelly McCormack, Bucknell University
Michael Santillo, The Pennsylvania State University
Sarah Schubert, Bucknell University
Kelsey Smith, West Chester University
Joseph Vena, Drexel University
Jenna Yehl, Bucknell University

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

Stephen Radice

Edward R. Murrow High School, Brooklyn, NY

Stephen Radice received his BA in chemistry from Brooklyn College and his Master of Science Education in Secondary Education from The College of Staten Island. Twenty two of his twenty five years of teaching are at his current school, Edward R. Murrow High School. Edward R. Murrow high school is a comprehensive, urban, public, high school of 4,000 students. He has successfully taught all levels of students from self contained special education science classes to advanced placement chemistry. His unique teaching style, infusing humor into difficult material to make it more understandable, is well received by his students, while yielding amazing results, both in terms of student registration for the course and on the Advanced Placement exam itself. Year after year, more students register for the course than there is room. Each year Mr. Radice has two classes of AP Chemistry filled to capacity, 34 students per class. Moreover, the number of students who achieve a 3 or higher on the exam consistently exceeds 80%.

His students do fun and educational projects including celebrating mole day, meeting Nobel Laureates, going to Polytechnic University to do college level laboratory and designing and wearing their own chemistry shirts. In addition to teaching more advanced students, Mr. Radice works with special education students in the laboratory. Here he finds ways to engage students with special needs. He provides hands on activities that are tailored to the needs of this student population. He has enabled these students to be active participants in experimental science. While current students enjoy and succeed in his class, one of his biggest testimonials comes from careers of former students. Mr. Radice's former students include pediatricians, endocrinologists, speech pathologists, chemical engineers, radiologists, teachers, physical therapists and pharmacists. He has motivated these students to create careers based on science.

Stephen has mentored teachers, coordinated the science department, written district curriculum and presented staff developments. He has contributed to the ACS by presenting at MARM in 2008 and as Chairman of the Nichols Award committee. Stephen has received other awards including The New York Times Teacher Who Makes a Difference Award: 2005, Nichols Foundation High School Chemistry Teacher Award: 2007, and the Union College Gideon Halley Teacher Recognition Award: 1998. Stephen is married and has two children.

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

Professor Amber Charlebois

Professor Amber Charlebois received her BS from Syracuse University, her Ph.D. from the University of Buffalo, and completed her post doctoral studies at the University of Illinois Urbana-Champaign. She began her academic career as an Assistant Professor at William Patterson University in Wayne, NJ. After for four years when she moved on to a similar position and is on track to receive tenure at Fairleigh Dickinson University College at Florham. Known by her students as “Dr. C”, Charlebois enthusiastically teaches Organic Chemistry and Biochemistry and the associated laboratories. During her eight years as a faculty member at both institutions, Dr. Charlebois has been consistently rated one of the most effective instructors. In addition, she has mentored over 40 students in various research projects in chemistry and biochemistry, resulting in almost as many student presentations at local and regional meetings. Dr. Charlebois has gone above and beyond the call of duty to excite, engage and challenge her students. She has committed herself to the calling of teaching the future scientists of our world, and she has done so with dedication and excellence. In addition, Dr. Charlebois is an alternate councilor for the North Jersey Section of the ACS, is co-chair of the Local Metro-Women Chemists Committee and is also very active in the National Women Chemists Committee.

The Chromatography Forum of the Delaware Valley Student Award Symposium

The winners will present their work at the DVCF student award symposium on Monday, April 12, from 1:00 PM to 5:00 PM. The scheduled presentations are:

- **Neha A Gujarati**, Bradley J Undem, Vijaya L Korlipara, St. John's University, "Synthesis and characterization of isoquinoline urea derivatives of A-425619 as TRPV1 antagonists"

- **Jeff Bolstridge**, Joseph Sherma, Bernard Fried, Lafayette College, "Effects of temperature on the neutral lipid content of Biomphalaria glabrata as determined by modern, instrumental high-performance thin-layer chromatography with densitometry"

- **Kelsey M Smith**, Mackenzie L Lauro, Karyn M Usher, West Chester University, "QuEChERS as a Sample Preparation Technique for Samples Analyzed by GC/MS"

- **Michael F Santillo**, Michael L Heien, Andrew G Ewing, The Pennsylvania State University, "High-throughput single-cell toxicity screening of biocidal compounds in a microfluidic device"

- **Donna M Blackney**, Joe P Foley, Drexel University, "Evaluation of the precision of dual-opposite injection capillary zone electrophoresis and comparison with conventional capillary zone electrophoresis"

- **Joseph A Vena**, Donna Blackney, Joe P Foley, Drexel University, "Enantiomeric separation of phenylalinine by micellar electrokinetic chromatography using a chiral surfactant, N-dodecoxycarbonylvaline"

- **Jenna B. Yehl**, Greg A Manley, Kyle W. Eckenroad, Christine M. Hebling, Laura E. Thompson, Timothy G. Strein, David Rovnyak, Bucknell University, "Investigating the mechanism responsible for MEKC separations of chiral compounds by bile salt micelles using CE and NMR"

- **Sarah Schubert**, Sarah Findeis, William Napoli, Timothy Strein, Bucknell University, Northwestern University, "Investigation of the effects of buffering and mixing conditions for the in-line jaffe reaction with Chemical reactions within CE capillaries: transferring an antioxidant power assay to the nanoliter level"

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

Alan B. Cooper, Ph.D.

Alan B. Cooper received his B.S degree in chemistry Cum Laude from Rutgers University in 1973. He then joined Schering-Plough Corporation as a member of the Medicinal Chemistry Research Department working in the antibacterial therapeutic area where his main contribution led to the development of aminoglycoside antibiotics resulting in the discovery of Isepamicin which is presently on the market for serious gram negative bacterial infections. He quickly rose through the ranks to the level of Senior Scientist in 1980 (the Ph.D. entree level position). While working at Schering-Plough he continued his education at Rutgers University to obtain his Ph.D. degree in 1984 in synthetic organic chemistry. Within the anti-infective therapeutic area Alan continued his contributions to the discovery of novel antifungal and antiviral agents. He then moved into the anti-tumor therapeutic area where he was the Chemistry Team Leader for the development of a second generation farnesyl protein transferase inhibitor for the inhibition of tumor cell growth that led to a recommendation candidate for further development in 2004. After attaining the level of Research Fellow he was given the responsibility of Chemistry Team Leader, leading a group of 17 chemists across two sites for the development of kinase inhibitors as antitumor agents that resulted in the recommendation of a candidate for further development (4/2009). He now leads a group of 24 chemists at Merck Research Labs across two sites as Chemistry Team Leader for the discovery of anti-tumor agents. Alan is a coauthor of more than 42 research publications and presentations and is co-inventor of over 56 patent and patent publications.

Alan became member of the American Chemical Society in 1974 and has been serving as an active volunteer for the past 15+ years. During this time, he has served on several committees and has contributed significantly at the national, regional and local levels.

At the national level, Alan has served on the Committee on Local Sections (2003 to 2008), Committee on Divisional Activities (1996 to 2001) and Task Force on Local Section/Division Interactions (2002 to 2004). He chaired the LSAC-DAC Joint Subcommittee that focused interactions between local sections and divisions. He is presently serving on the Meetings & Expositions national committee. At the regional level, Dr. Cooper served as the Program Chair for MARM 1999 and was the General Co-Chair for MARM 2005. During MARM 2005, Alan was a member of the core group and supervised the work of over 100 volunteers to deliver one of the most successful regional meetings.

At the local level, Alan serves as Councilor (1995-present) representing the North Jersey Section, one of the largest Sections in the ACS. He became Chair of the Organic Topical Group (OTG) in 1995. Under his leadership the OTG invited quality speakers and the symposia were well attended. Dr. Cooper was viewed as someone who could lead the NJACS and in 1997 he became the Chair-elect and served as the Chair in 1998. Under his leadership, the Section received the Chemluminary award for Outstanding Section in the Large Category, which is a testimony to his dedication and effort as a Section Chair. In addition, Alan has served on numerous NJACS committees: Topical Group Planning Committee, Chair (1996-1998); Lifetime Achievement Award Subcommittee (1998); Program Planning Committee, Chair (1999-2008); Finance Committee (1999-2006); National ACS Award for Team Innovation (2001-02); Professional Relations Committee, Chair (2006), to name a few.

The Delaware Section of the American Chemical Society

33rd Annual Carothers Award for Outstanding Contributions and Advances in Industrial Applications of Chemistry

Carothers Award Lecture Presented by 2010 Recipients:

Dr. Ronald Knudsen

Senior Chemistry Consultant, Chevron Phillips Chemical Company LP

Monday, 12 April 2010
Du Barry Ballroom, Hotel du Pont
Reception, 5:30 PM
Dinner, 6:30 PM
Awards Presentation and Carothers Lecture, 7:30 PM

Dr. Ronald D. Knudsen is currently a chemical consultant for the Chevron Phillips Chemical Company. He received his Ph.D. in organic chemistry from Brigham Young University and did post-doctorial work in synthetic organic chemistry with Harold Snyder at the University of Illinois and in the isolation of hypothalmic hormones with Karl Folkers at the University of Texas. He has worked for the Phillips Petroleum Company and Chevron Phillips Chemical Company. During that time he provided the technical direction for the development of the selective 1-hexene technology from the laboratory through the pilot plant to the successful start-up of the commercial plant. The selective 1-hexene technology has been recognized as One of the 100 Most Technologically Significant New Products by *R&D Magazine* and received the Kirkpatrick Award from *Chemical Engineering*. He has received internal technology awards from Phillips Petroleum and Chevron Phillips Chemical as well as being named the Oklahoma Chemist of the Year and was selected for the ACS Heroes of Chemistry Award.

MARM AWARDS CRITERIA

The Stanley C. Israel Regional Award for Advancing Diversity in the Chemical Sciences
Sponsored by the Committee on Minority Affairs of the American Chemical Society
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”.
Send nominations to: Committee on Minority Affairs, American Chemical Society, 1155 16th Street NW, Washington, DC 20036. For information regarding the award, contact Paula Christopher, 800/227-5558, Ext. 6122, or e-mail: p_christopher@acs.org.

The E. Emmet 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 Middle Atlantic Regional Meeting (MARM) of the American Chemical Society for outstanding achievements in teaching chemical sciences at small colleges within the Middle 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 Middle 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 candidate need not be a member of the American Chemical Society.
- The Award committee of the MARM will review the candidates and select the nominee.
- The nominee will be presented the Award during the forthcoming MARM. The nominee is expected to deliver a short acceptance speech.
- 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.
- The Award will consist of $1000 and a major award plaque.

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.

ACS Regional Industrial Innovation Award

Nomination Guidelines:

The 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:
E-mail: cheminnovations@acs.org
Fax: (202) 872-6098
Mail: Attn: Joy Titus-Young
American Chemical Society
Office of Corporation Associates
1155 Sixteenth Street, NW,
Washington, D.C. 20036.

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.
For a paper to be given full consideration for presentation at the Student Award Symposium: submit a title & 250-word abstract to:
Dr. Marshall L. Fishman
Eastern Regional Research Center
600 East Mermaid LN
Wyndmoor, PA 19038-8598
Phone: 215-233-6450
E-mail: marshall.fishman@ars.usda.gov

The Delaware Section Wallace H. Carothers Award for Outstanding Contributions and Advances in Industrial Application of Chemistry

The purpose of the award	To honor scientific innovators who have made outstanding contributions and advances in industrial applications of chemistry
The nature of the award	$2000 cash award and a sculpture which was commissioned by the Delaware Section. It consists of two hands molding a benzene ring, depicting man shaping molecules. The artist is Mr. Domenico Mortellito, a well-known local sculptor, muralist and painter who has pioneered the use of synthetic materials in the fine arts.
The establishment and support of the award	The award was established in 1976 in memory of Wallace H. Carothers, one of the founders of modern polymer chemistry. It is funded by the Delaware Section and local corporations.
The rules of eligibility	A nominee must have made a significant contribution to the industrial application of chemistry. Selection is made by a committee that is separate from the Section Awards Committee.

MARM 2010

Program & Abstracts

Delaware Art Museum

(This page intentionally blank)

PROGRAM

Saturday, April 10, 2010

Saturday, April 10, 2010 7:30 AM – 9:00 AM

Welcome Reception

Conference Center, Dining/Lounge Area

Organizer: Narmada Gunawardena

Saturday, April 10, 2010

Saturday, April 10, 2010 9:00 AM – 11:40 AM

Biological Chemistry I

Conference Center, King Sejong

9:00 AM **1** Insight into cutinase reactivity for biotransformations. **Peter James Baker**,[1] David Feder,[1] Richard Gross,[1] Jin K Montclare.[1,2], [1]Department of Chemical and Biological Sciences, Polytechnic Institute of New York University, Brooklyn, NY, United States; [2]Department of Biochemistry, Downstate Medical College, Brooklyn, New York, United States.

9:20 AM **2** Probing Biology with Chemistry: Targeting the Ubiquitin Pathway for Novel Drugs. **Ping Cao**, Craig Leach., Medicinal Chemistry, Progenra, Malvern, PA, United States.

9:40 AM **3** Use of the Quartz Crystal Microbalance to Investigate Mechanical Viscoelstic Changes in HIV-1 Env upon Ligand Binding. Hyun-Su Lee,[1] Mark Contarino,[2] Isaac Zentner,[2] Umashankara Muddegowda,[2] Srivats Rajagopal,[2] Arne Schon,[3] Ernesto Freire,[3] Amos B Smith, III,[4] Irwin Chaiken,[2] **Lynn S Penn**.[1], [1]Department of Chemistry, Drexel Universtiy, Philadelphia, PA, United States; [2]Department of Biochemistry and Molecular Biology, Drexel University, Philadelphia, PA, United States; [3]Department of Biology, The Johns Hopkins University, Baltimore, MD, United States; [4]Department of Chemistry, The University of Pennsylvania, Philadelphia, PA, United States.

10:00 AM **4** Self-catalyzed DNA depurination mediated by cruciform extrusion in closed circular DNA plasmid. **Olga Amosova**, Veena Kumar, Aaron Deutsch, Jacques R Fresco., Department of Molecular Biology, Princeton University, Princeton, NJ, United States.

10:20 AM **5** Computational and experimental investigation of the formation of cyclodextrin 'host-guest' inclusion complexes. **Clint Stalnecker**, Jeffrey Wolbach, Pamela Artz., Department of Chemistry and Biochemistry, Albright College, Reading, PA, United States.

10:40 AM **6** Giant vesicles as model cells capable of asymmetric division and polarity. **Meghan Andes-Koback**, Christine D. Keating., Department of Chemistry, The Pennsylvania State University, University Park, PA, United States.

11:00 AM **7** Development of Artificial Antennas from the Self-Assembly of Peptide-Porphyrin Complexes. **Gregory A. C**,[1] Darius Kuciauskas.[2], [1]Department of Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States; [2]National Renewable Energy Laboratory, Golden, CO, United States.

11:20 AM **8** Active site conformational changes in the metal dependent phosphatidylinositol-specific phospholipase C (PI-PLC) from Streptomyces antibioticus. **Thomas L Selby**., Chemistry, Bucknell University, Lewisburg, PA, United States.

Saturday, April 10, 2010

Saturday, April 10, 2010 9:00 AM – 12:00 PM

Inorganic Chemistry I

Sponsor: Division of Inorganic Chemistry

Conference Center, Montessori

9:00 AM **9** Molecular modeling of cysteine oxidation. **Craig A Bayse**., Department of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA, United States.

9:20 AM **10** Synthesis and characterization of narrow band gap V-VI hybrid semiconductors. **Mojgan Roushan**,[1] Hisato Yamaguchi,[2] Thomas J Emge,[1] Jing Li.[1], [1]Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, NJ, United States; [2]Department of Materials Science and Engineering, Rutgers University, Piscataway, NJ, United States.

9:40 AM **11** Molecular Based Synthesis of Solid State High Nuclearity Lanthanide Chalcogenide Clusters For Optoelectronic and Scintillation Applications. **Brian F Moore**,[1] Thomas Emge,[1] G A Kumar,[2] Richard E Riman,[2] John G Brennan.[1], [1]Department of Chemistry & Chemical Biology, Rutgers University, Piscataway, NJ, United States; [2]Department of Material Science & Engineering, Rutgers University, Piscataway, NJ, United States.

10:00 AM **12** Mechanism of Dioxygen cleavage by Low valent b-diketiminato chromium compound. **Fang Dai**,[1] Leonard A MacAdams,[2] Glenn P. A. Yap,[1] Klaus H Theopold.[1], [1]Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States; [2]KiON Corporation, Huntingdon Valley, PA, United States.

10:20 AM **13** [2 + 2] Reactions of quintuple bonds Cr compounds with alkynes. **Jingmei Shen**, Glenn P. A. Yap, Klaus H Theopold., Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States.

10:40 AM **14** Synthesis of the sulfur rich Eu(III) compound, $(py)_6Eu_2(SS)_2(OC_6F_5)_2$. **Kieran Norton**, John Brennan, Thomas Emge., Chemistry and Chemical Biology, Rutgers The State University of New Jersey, Piscataway, NJ, United States.

11:00 AM **15** Monolithic porous electron-rich covalent organophosphonitridic frameworks. **Kai Landskron**, Paritosh Mohanty., Chemistry, Lehigh University, Bethlehem, PA, United States.

11:20 AM **16** Late transition metal complexes supported by tris(3-amino-5-methylpyrazolyl) borate ligands. **Ismael Nieto**,[1] Elizabeth T Papish,[1] Matthias Zeller.[2], [1]Department of Chemistry, Drexel University, Philadelphia, PA, United States; [2]Department of Chemistry, Youngstown State University, Youngstown, OH, United States.

11:40 AM **17** Artificial Photosynthesis- Photocatalyzed Conversion of CO_2 to CH_4 by Visible Light. **Edward G Look**,[1] Harry D Gafney,[1] Nicholas F Borrelli.[2], [1]Department of Chemistry and Biochemistry, Queens College, CUNY, Flushing, NY, United States; [2]Sullivan Park, Corning, Inc, Corning, NY, United States.

Saturday, April 10, 2010

Saturday, April 10, 2010 9:00 AM – 11:10 AM

Physical Chemistry

Sponsor: Division of Physical Chemistry

Conference Center, Collins

Organizer: Cecil Dybowski

9:00 AM Introductory Remarks

9:05 AM **18** Theoretical analysis of the molecular dynamics of ionic liquids. **Mark N. Kobrak**., Department of Chemistry, Brooklyn College of CUNY, Brooklyn, NY, United States.

9:25 AM **19** Hole mobility for thin-film organic molecular solids in the presence of defects or surface adsorbates: Theory and implications for gas detection. **Matthew L Rossi**, Karl Sohlberg., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

9:45 AM **20** Substitution effect on the charge mobility of metal free phthalocyanine. **Choongkeun Lee**, Karl Sohlberg., Chemistry, Drexel University, Philadelphia, PA, United States.

10:05 AM **21** Inhibition of histidine ammonia lyase by 8-methoxypsoralen and psoralen oxidized photo-products. **John T Reilly**, Trista T Tryner, Kyle A Troester, Dominick A Vitale, Tiffiany T Risher., Department of Chemistry and Physics, Coastal Carolina University, Conway, South Carolina, United States.

10:25 AM Intermission

10:40 AM **22** Thermochemical Characterization of Biodiesel Fuels Synthesized from Various Oil Feedstocks. **Michael Bell**, **Marc L Richard**., Chemistry Program, The Richard Stockton College of New Jersey, Pomona, NJ, United States.

10:45 AM **23** Effects of viscosity on phase separation of liquid mixtures with a critical point of miscibility. **Filomena Califano**., Chemistry and Physics, St. Francis College, Brooklyn, NY, United States.

10:50 AM **24** Structural and size effects in reactions of CO on O- and NO- covered Ir. **Wenhua Chen**, Robert A Bartynski., Department of Physics and Astronomy, and Laboratory for Surface Modification, Rutgers, The State University of New Jersey, Piscataway, NJ, United States.

10:55 AM **25** Time evolution of an electron in a simple system. **Hae-Won Kim**,[1] Karl Sohlberg.[2], [1]Deaprtment of Chemistry, Penn State Abington, Abington, PA, United States; [2]Department of Chemistry, Drexel University, Philadelphia, PA, United States.

11:00 AM **26** New empirically corrected AM1 method: Accurately and efficiently modeling supermolecular complexes. **Michael Foster**, Karl Solhberg., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

11:05 AM **27** Synthesis, physical characterization, and toxicity studies of a series of room temperature ionic liquids based on 1-methylimidazole. Evgenia Gasumova, **Bradley Zale**, **Hueanh Tran**, **Marc L Richard**., Chemistry Program, The Richard Stockton College of New Jersey, Pomona, NJ, United States.

Saturday, April 10, 2010

Saturday, April 10, 2010 9:00 AM – 12:00 PM

POGIL Workshop for High School Chemistry Teachers

Conference Center, King/Sullivan

Process Oriented Guided Inquiry (GIL) workshop for high school chemistry teachers will be presented by Diane Krone and Joanne Long. This workshop introduces the philosophy and methodology of POGIL. Participants experience the approach from a student's per

Saturday, April 10, 2010

Saturday, April 10, 2010 10:00 AM – 11:30 AM

Organic Chemistry I

Sponsor: Division of Organic Chemistry

Conference Center, Knowles

10:00 AM **28** Effects of cis and trans Isomers of alpha-Linolenic Acid on the Formation Kinetics of Cyclic Fatty Acid Monomers. Amelie Desmarais,[1] Jean-Louis Sebedio,[2] Joseph Arul,[1] **Paul Angers**.[1], [1]Food Science and Nutrition, Universite Laval, Quebec City, Quebec, Canada; [2]Unite de Nutrition Humaine, Institut National de la Recherche Agronomique (INRA), Clermont-Ferrand, France.

10:00 AM **29** Synthesis of Calixarenes Functionalized at the Lower Rim as Potential Host Compounds. **Shimelis T Hailu**, Paul F Hudrlik, Anne M Hudrlik., Department of Chemistry, Howard University, Washington, DC, United States.

10:00 AM **30** Cascade cyclization of acyclic N -sulfinyl b -amino ketone ketals. Franklin A. Davis, **Ram Edupuganti**., Department of Chemistry, Temple University, Philadelphia, PA, United States.

10:00 AM **31** New synthetic method for 5'-capped oligoribonucleotides. **Elizabeth Veliath**, Barbara L. Gaffney, Roger A. Jones., Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, NJ, United States.

10:00 AM **32** New route to g,d-unsaturated nitro compounds via [3,3]-sigmatropic rearrangement of O-Allyl nitronic esters. **Alma Pipic**, Peter Wade., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

10:00 AM **33** Surfactant modified carbon nanotubes: Effect of surfactant and surfactant content on electrical conductivity. **Juliet Hahn**., Department of Chemistry & Biochemistry, University of Delaware, Newark, DE, United States.

10:00 AM **34** Skin cancer reaction in a test tube: Solvent effect on the photodimerization of a derivative of thymine. **Juliet Hahn**., Department of Chemistry & Biochemistry, University of Delaware, Newark, DE, United States.

10:00 AM **35** Aromatic ring strain and carbon 13 NMR. **Donald D Clarke**,[1] James Foresman.[2], [1]Department of Chemistry, Fordham University, New York, NY, United States; [2]Department of Physical Sciences, York College of Pennsylvania, York, PA, United States.

10:00 AM **36** Efficient Synthesis of Vinyl allene and Its Application to Carbocycles. **Subin Choi**, **Su-sung Oh**, Phil Ho Lee., Chemistry, Kangwon National University, Chuncheon, Kangwon-do, Republic of Korea.

10:00 AM **37** Nucleomistry video lectures: Humorous internet presentations teaching nuclear chemistry. **Isaac Shomer**., Nucleomistry Research Institute, Arlington, Virginia, United States.

10:00 AM **38** Regio-selective electrophilic fluorination of pyridine derivatives with SelectfluorTM. **Daniel Smith**,[1] Jianqing Li,[1] Bang-Chi Chen,[2] John Kadow,[1] Balu Balasubramanian,[2] Nicholas Meanwell,[1] Joel C. Barrish.[2], [1]Department of Chemistry, Bristol-Myers Squibb, Wallingford, CT, United States; [2]Department of Chemistry, Bristol-Myers Squibb, Princeton, NJ, United States.

10:00 AM **39** Study of student learning in a conductivity lab using real world samples. **James C Rieben Jr.**, Daniel B. King., Chemistry, Drexel University, Philadelphia, Pennsylvania, United States.

10:00 AM **40** Towards the total synthesis of (-)-veratramine. **James F. Berry**, Peter W. DeMatteo, Douglass F. Taber., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

10:00 AM **41** Progress toward the synthesis of a functional Bis-peptide Oligomer that mimics Carbonic Anhydrase. **Sharad Gupta**, Christian E Schafmeister., Department of chemistry, Temple University, Philadelphia, PA, United States.

Saturday, April 10, 2010

Saturday, April 10, 2010 12:00 PM – 1:30 PM

Science Teachers (K-12) Luncheon

Conference Center, King/Sullivan

12:00 PM **42** What is National Lab Day?. **Tom Lane**., Dow Corning, United States.

Saturday, April 10, 2010

Saturday, April 10, 2010 12:00 PM – 1:30 PM

Women Chemist Committee Luncheon

Main Hotel Floor, Christina Room

Saturday, April 10, 2010

Saturday, April 10, 2010 1:00 PM – 5:00 PM

Laboratory Waste Management Workshop

Sponsor: Division of Chemical Health & Safety

Conference Center, Marshall

Presider: Russell Phifer

This course will identify the various regulatory requirements that apply to laboratories that generate hazardous waste, as well as provide insight into the options for on-site management and off-site disposal. Focus will include discussion on recycling/re

Saturday, April 10, 2010

Saturday, April 10, 2010 1:30 PM – 3:00 PM

Biological Chemistry II

Conference Center, King Sejong

1:30 PM **43** Cloning and expression of a putative ligand gated ion channel from Nostoc punctiforme and its extramembranous domain. **Stephanie Reichardt**, Barry S Selinsky., Department of Chemistry, Villanova University, Villanova, PA, United States.

1:30 PM **44** Allosteric regulation of dynamic, dissociating homo-oligomeric enzymes. **Trevor Selwood**, Eileen K. Jaffe., Fox Chase Cancer Center, Philadelphia, PA, United States.

1:30 PM **45** Effects of Amino Acid Sequence on Structure, Membrane Binding, and Activity of an Antimicrobial Peptide. **Lubov Arotsky**, Laura Hagens, Gregory A. Caputo., Department of Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States.

1:30 PM **46** Characterization of an unusual beta-hydroxybutyrate dehydrogenase from the parasite Trypanosoma brucei. **Tina D Shah**, **Kathryn Capasso**, Meghan Hickey, Jennifer Palenchar., Department of Chemistry, Villanova University, Villanova, PA, United States.

1:30 PM **47** Functional Amino Acid Navigator. **Jason K Cargill**, Sal Gomez, Peter Palenchar., Chemistry, Rutgers University, Camden, NJ, United States.

1:30 PM **48** Synthesis of Stercobilin and its Deuterated Isotopomer: ESI and MS/MS of a Potential Autism Biomarker. Troy Wood,[2] Amber F Charlebois,[1] **Gregory F Pirrone**.[1], [1]Department of Chemistry and Pharmaceutical Sciences, Fairleigh Dickinson University, Madison, New Jersey, United States; [2]Department of Chemistry, SUNY University at Buffalo, Buffalo, New York, United States.

1:30 PM **49** Structure-function studies of the putative protease TM0727 from Thermotoga maritima. **James D Berstler**, Thomas L Selby., Chemistry, Bucknell University, Lewisburg, PA, United States.

1:30 PM **50** Effects of Ionizable Amino Acids in the Hydrophobic Core of Model Transmembrane a-helices. **David Bauer**, Benjamin Nixon, Gregory A. Caputo., Department of Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States.

1:30 PM **51** Chemoenzymatic synthesis of conjugate polysialic acid vaccines. **Pumtiwitt C. McCarthy**, Sylvester L. Mosley, Rina Saksena, Dwight C. Peterson, Justine Vionnet, Willie F. Vann., Laboratory of Bacterial Polysaccharides, Center for Biologics Evaluation and Research, U.S. Food and Drug Administration, Bethesda, MD, United States.

Saturday, April 10, 2010

Saturday, April 10, 2010 1:30 PM – 5:15 PM

Chemical Education

Sponsor: Division of Chemical Education

Conference Center, Quintanilla

Organizer/Presider: Andrea Martin

1:30 PM Introductory Remarks

1:35 PM **52** Using POGIL in the laboratory. **Frank J. Creegan**., Department of Chemistry, Washington College, Chestertown, MD, United States.

1:55 PM **53** Freshman Summer Research Experience. **Andrea E Martin**, **Louise M Liable-Sands**, Loyd Bastin, Shirley Fischer-Drowos., Department of Chemistry, Widener University, Chester, PA, United States.

2:15 PM **54** Molecular oxygen in organic chemistry. **Parvathi S. Murthy**., Chemistry and Biochemistry, Georgian Court University, Lakewood, NJ, United States.

2:35 PM **55** Clicker use in general chemistry: Who uses them and is there a benefit?. **Daniel B King**., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

2:55 PM Intermission

3:10 PM **56** Spoken Polymer. **Thomas E Twardowski**, Nadine McHenry., Department of Chemical Engineering, Widener University, Chester, PA, United States.

3:30 PM **57** Baiting the hook: The Chemistry of Beer. **Roger Barth**., Department of Chemistry, West Chester University, West Chester, Pennsylvania, United States.

3:50 PM **58** Student test scores in math computation in some mid-Atlantic states and school districts and the implications for chemistry instruction. **Eric Nelson**., Retired Instructor, United States.

4:10 PM Concluding Remarks

4:15 PM **59** Fundamental chemical demonstrations. **Michael A. Stemniski**., Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States.

Saturday, April 10, 2010

Saturday, April 10, 2010 1:30 PM – 3:00 PM

High School Research Poster Session

Conference Center, Piaget

Organizer: Martha Hollomon

Saturday, April 10, 2010

Saturday, April 10, 2010 1:30 PM – 5:10 PM

Organic Chemistry II

Sponsor: Division of Organic Chemistry

Conference Center, Knowles

1:30 PM **60** Portable device based on a fiber-optic singlet-oxygen [$^1O_2$ (^1d_g)] generator (FOSG). David Aebisher, Matibur Zamadar, Adaickapillai Mahendran, Goutam Ghosh, Catherine McEntee, **Alexander Greer**., Chemistry, Brooklyn College of the City University of New York, Brooklyn, NY, United States.

1:50 PM **61** Metalla-Cope rearrangements: Bridging organic and inorganic chemistry. **Edyta Greer**, Roald Hoffmann., Natural Sciences, Baruch College of the City University of New York, New York, NY, United States.

2:10 PM **62** Progress Towards the Total Synthesis of (-) Veratramine. Douglass F. Taber, James F. Berry, **Peter W. DeMatteo**., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

2:30 PM **63** The Total Synthesis of (-) Deoxynupharidine. Douglass F. Taber, **Peter W. DeMatteo**, **Patrick J. Straney**., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

2:50 PM **64** Allylic Substitution versus Suzuki Cross-Coupling: Capitalizing on Chemoselectivity with Bifunctional Substrates. **Mahmud M. Hussain**, Byeong-Seon Kim, Nusrah Hussain, Patrick J. Walsh., Department of Chemistry, University of Pennsylvania, Philadelphia, PA, United States.

3:10 PM **65** Olefin and fullerene sulfurations with thiozone (S_3). A theoretical study. **Alvaro Castillo**, Alexander Greer., Chemistry Department, The City University of New York, Brooklyn College and The Graduate Center, Brooklyn, NY, United States.

3:30 PM **66** Examining the role of helicity in salen catalysis. **James N Plampin III**, Joseph M Fox., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

3:50 PM **67** Synthesis, Characterization, Stability, and Antiproliferative Activity of a New PEGylated Benzopolysulfane, 4-$CH_3(OCH_2CH_2)_3NHC(O)$-C_6H_4-1,2-S_5. **Adaickapillai Mahendran**,[1] Angela Vuong,[1] David Aebisher,[1] Yaqiong Gong,[2] Robert Bittman,[2] Gilbert Arthur,[3] Akira Kawamura,[4] Alexander Greer.[1], [1]Department of Chemistry, Brooklyn College and Graduate Center of The City University of New York, Brooklyn, New York, United States; [2]Department of Chemistry and Biochemistry, Queens College and Graduate Center of The City University of New York, Flushing, New York, United States; [3]Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, Manitoba, Canada; [4]Department of Chemistry, Hunter College and Graduate Center of The City University of New York, New York, New York, United States.

4:10 PM **68** Copper-free Sonogashira coupling of aryl bromides and chlorides using highly active Pd catalysts in API development. **Hongbo Li**, Thomas Colact., Johnson Matthey Catalysts, West Deptford, NJ, United States.

4:30 PM **69** Synthesis of PABA derivatives: The Fischer Esterification reaction revisited, Part IV: An adventurous Pathway for teaching and learning research through Organic Synthesis!. **Nagarajan Vasumathi**,[1] Kristin Shirey,[1] Thai Huynh,[1] Caterina Lazaroni.[2], [1]Department of Physical and Earth Sciences, Jacksonville State University, Jacksonville, AL, United States; [2]Physical and Earth Sciences, Jacksonville State University, Jacksonville, AL, United States.

4:50 PM **70** Effect of nonionic co-surfactants on corrosion inhibition effect of cationic gemini surfactant in acid medium. **Dourna Asefi**,[1] Mokhtar Arami,[2] Niyaz Mohammad Mahmoodi.[3], [1]Polymer Engineering, Islamic Azad University South Branch of Tehran, Iran (Islamic Republic of); [2]Textile Engineering, Amirkabir University of Technology, Iran (Islamic Republic of); [3]Environmental Research, Institute for Color Science and Technology, Iran (Islamic Republic of).

Saturday, April 10, 2010

Saturday, April 10, 2010 1:30 PM – 3:00 PM

Project SEED Poster Session

Conference Center, Collins

Saturday, April 10, 2010

Saturday, April 10, 2010 1:30 PM

Regional Chemagination Competition

Conference Center, Blake

Presider: Vijaya Korlipara

Saturday, April 10, 2010

Saturday, April 10, 2010 6:00 PM – 9:00 PM

Spring Meeting of the US Section of the RSC

Sunday, April 11, 2010

Sunday, April 11, 2010 8:30 AM – 10:00 AM

ACS Undergraduate Research Symposium - I

Sponsor: American Chemical Society

Conference Center, King/Sullivan

Organizer/Presider: Narmada Gunawardena

Posters may be set up any time between 8:00 - 8:30. The symposium provides an excellent opportunity for undergraduate chemistry students to present the results of their research. Presenters should be by their posters from 8:30 - 10:00.

8:30 AM **71** Quantitative determination of gallic acid in commercial tea and juice beverages using HPLC. **Christine Casas**, Soraya Svoronos, Pedro Irigoyen, Paris Svoronos., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

8:30 AM **72** Determination of the total phenol content in commercial bottled beverages via the Folin-Ciocalteau Micromethod. **Kyu-Ree (Katie) Lee**, Soraya Svoronos, Pedro Irigoyen, Paris Svoronos., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

8:30 AM **73** Probing the interaction of gold nanoparticles with nanofibers of polyaniline and its analogs. **Bhawanie Persaud**,[1] David M. Sarno,[1] Mathew M. Maye.[2], [1]Department of Chemistry, Queensborough Community College of CUNY, Bayside, NY, United States; [2]Department of Chemistry, Syracuse University, Syracuse, NY, United States.

8:30 AM **74** Temperature effect of alcohols on refractive index measured by a laser pointer. **Ernest Choi**, Esther Yang, Jun H Shin., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

8:30 AM **75** Refractive index of hydrocarbons at various temperatures measured by a laser pointer. **Esther Yang**, Ernest Choi, Jun H Shin., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

8:30 AM **76** Ring-contraction of 3 H -1-benzazepine to 1,2-diarylquinoline. **Sasan Karimi**,[1] **Prakash Prasad**.[2], [1]Department of Chemistry, Queensborough Community College, Bayside, New York, United States; [2]Department of Chemistry and Biochemistry, Queens College of CUNY, Flushing, New York, United States.

8:30 AM **77** Detection of nitrofuran metabolites in imported shrimp: An internship experience at the Food and Drug Administration. **Timothy Fitzgerald**,[1] LeRae Graham,[2] Paris Svoronos,[1] Michael Fazio.[2], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]158-15 Liberty Avenue, Food and Drug Administration Regional Office, Jamaica, NY, United States.

8:30 AM **78** Antibiotic resistance and chemical profiling of actinomycetes in New York soils.. **Krisna Sricharoon**, Ruth Lee, Monica Rivera, Monica Trujillo, Mangala Tawde., Department of Biological Sciences and Geology, Queensborough Community College, Bayside, NY, United States.

8:30 AM **79** Determination of the ionization constant of weak carboxylic acids using microscale freezing point depression measurements. **Parsa Sharifi**,[1] Gopal Subramaniam,[2] Pedro Irigoyen,[1] Paris Svoronos.[1], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Department of Chemistry and Biochemistry, Queens College, Flushing, NY, United States.

8:30 AM **80** Computational studies of methylcobalamin binding to aminoacids in solution. **Jerry Kouloumbes**, Jordan Verdis., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

8:30 AM **81** Preparation of poly(o-toluidine) as porous micron-scale spheres. **Mauricio Murillo**, David M. Sarno., Department of Chemistry, Queensborough Community College of CUNY, Bayside, NY, United States.

8:30 AM **82** Determination of a solute's molecular weight using microscale freezing point depression measurements. **Shiran Zhavian**, Pedro Irigoyen, Paris Svoronos., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

8:30 AM **83** Determination of acid and base concentrations using a laser pointer: Refractive index vs. concentration. **Rebecca Cho**, Esther Yang, Jun H Shin., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

8:30 AM **84** Determination of chlorine residual in water by the DPD method.. **Grace Song**,[1] Sophia Mezina,[2] Panayiotis Meleties,[3] Paris Svoronos.[1], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Bureau of Wastewater Treatment, New York City Department Environmental Protection, Wards Island, NY, United States; [3]Office of Academic Affairs-Math and Science Division, York College, Jamaica, NY, United States.

8:30 AM **85** EFFECT of CARNITINE and CO-ENZYME Q10 on ASTROCYTE MITOCHONDRIA. **Jose Zhagnay**, Regina Sullivan, Marisa Cotrina., Department of Biology, Queensborough Community College, Bayside, NY, United States.

8:30 AM **86** The effect of outdoor smoking on an indoor environment: A Brookhaven National Laboratories experience.. **Christine Casas**,[1] John Heiser.[2], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Environmental Research & Technology Division, Brookhaven National Laboratories, Upton, NY, United States.

8:30 AM **87** Analysis of milk for fat, protein, and lactose Authors Waddah Guneid , Bruce Montalbano, Joe Iorio, Irina Rutenberg,. **Waddah Guneid**, Irina Rutenburg, Pedro Irigoyen, Bruce Montalbano, Joseph Iorio, TianChun Xu., Chemistry, Queensborough Community College, Bayside, New York, United States.

8:30 AM **88** A summer internship at the DEP: An application of what I learned in class to the real world.. **Kyu-Ree (Katie) Lee**,[1] Panayiotis Meleties,[2] Sophia Mezina,[3] Paris Svoronos.[1], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Office of Academic affairs-Math and Science Division, York College, Jamaica, NY, United States; [3]Owls Head Park, New York City Department Environmental Protection, Brooklyn, NY, United States.

8:30 AM **89** DNA Isolation and phosphate detection: An undergraduate chemistry experiment. **Noor Sardar**, Jordan Verdis., Department of Chemistry, Queensborough Community College of CUNY, Bayside, NY, United States.

8:30 AM **90** Analysis Of Antibiotic Induced Evolutionary Changes In E.coli .. **Elana Santos**, Omid Khalpari, Nidhi Gadura., Department of Biology, Queensborough Community College, Bayside, New York, United States.

8:30 AM **91** Optimizing Plant cell walls for Biofuels: Role of carbohydrate binding proteins in wall polymer assembly. **Ahsan Waqar**,[1] Desigan Kumaran,[2] Mangala Tawde,[1] Paul Freimuth.[2], [1]Department of Biological Sciences and Geology, Queensborough Community College, Bayside, New York, United States; [2]Biology Department, Brookhaven National laboratory, Upton, New York, United States.

8:30 AM **92** Creating a structure based searchable database for FDA approved chemotherapy drugs using KnowItAll®. **Ghada J. Alabed**, Jordan Wheatley, Malcom J. D'Souza., Department of Chemistry, Wesley College, Dover, DE, United States.

8:30 AM **93** Copper Surface-Mediated Toxicity Correlates With Memebrane Lipid Peroxidation In E.coli .. **Rachel Hammer**, Nidhi Gadura., Department of Biology, Queensborough Community College, Bayside, New York, United States.

8:30 AM **94** Is food labeled "Organic" in our supermarkets "Genetically Modified"?. **Athanasia Pavlou**, Nidhi Gadura., Department of Biology, Queensborough Community College, Bayside, New York, United States.

8:30 AM **95** Computational studies of the Bergman reaction in substituted oxabicyclo[7.2.1] dodecaenediynes. **Sahar Refua**, Jordan Verdis., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

8:30 AM **96** Reactivity of tris (trimethyl silyl) phosphate(TMSP): Synthesis of the bisphosphonate derivatives of b-alanine. **Anibal Davalos-Morinigo**, Luis Vargas., Department of Chemistry, Queensborough Community College, Bayside, Ny, United States.

8:30 AM **97** Computational and experimental studies of the reaction of aryl chlorothionoformates with tris(trimethylsilyl)phosphite. **Byung-Min Shin**, Tresa Ambooken, Luis Vargas, Jordan Verdis., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

8:30 AM **98** Formation of [Tris(3-trimethoxysilylpropyl) Isocynurate] (TTPI) capped Palladium Nanoparticles onto Single-Walled Carbon Nanotubes. **Esther Ahn**, Chi Kwan Wong, Eunchul Kim, Moni Chauhan, Tirandai Hemraj-Benny., Department of Chemistry, Queensborough Community College, Bayside, New York, United States.

8:30 AM **99** Antimicrobial activity of Nano Silver versus Silver Salts. **Ruth Lee**,[2] **Eunchul Kim**,[1] Moni Chauhan,[1] Mangala Tawde.[2], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Department of Biology, Queensborough Community College, Bayside, NY, United States.

8:30 AM **100** Determination of Caffeine Content in Energy Drinks by High Pressure Liquid Chromatography.. **Xiaomei Ye**, TianChun Xu, Pedro Irigoyen., Department of Chemistry, Queensborough Community College of CUNY, Bayside, NY, United States.

8:30 AM **101** Analyzing commercial discharges for various pollutants: A DEP industrial pretreatment program internship.. **Gerasimos Kouloumbes**,[1] Faye Jacques,[2] Panayiotis Meleties,[3] Paris Svoronos.[1], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Bureau of Wastewater Treatment, New York City Department Environmental Protection, Wards Island, NY, United States; [3]Office of Academic Affairs-Math and Science Division, York College, Jamaica, NY, United States.

8:30 AM **102** ANALYSIS OF HOLISTIC FISH BASED DRY DOG FOOD FOR HEAVY METALS using X-ray Fluorescence Spectrophotometry. **Andre Smithson**, Pedro Irigoyen, Irina Rutenburg, TianChun Xu., Chemistry, Queensborough Community College of CUNY, Bayside, NY, United States.

8:30 AM **103** Importance of Linear Free Energy Relationships LFERs in studying solvolytic behavior in Thio- and Thionocarbonyl Esters. **Brian Mahon**., Department of Chemistry, Wesley College, Dover, DE, United States.

8:30 AM **104** Kinetic Evaluation of s -Isobutyl Chlorothioformate. **Matthew McAneny**, Malcolm D'Souza., chemistry, Wesley College, Dover, Delaware, United States.

8:30 AM **105** High pressure synthesis of water splitting oxynitrides. **Parsa Sharifi**,[1] William Woerner,[2] Lars Ehm.[3], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Department of Giosciences, Stony Brook University, Stony Brook, NY, United States; [3]Mineral Physics Institute, Stony Brook University, Stony Brook, NY, United States.

8:30 AM **106** Bacterial metabolism of ionic liquid-pretreated lignocellulose: production of biofuels. **Firmause Payen**,[1] Samanta Boursiquot,[1] Sharon I Lall-Ramnarine,[1] Marie Thomas,[2] James F. Wishart.[2], [1]Department of Chemistry, Queensborough Community College, CUNY, Bayside, NY, United States; [2]Department of Chemistry, Brookhaven National Laboratory, Upton, NY, United States.

8:30 AM **107** Si-H bond activation in models of siloxanes – a DFT study. **Daniel Sangobanwo**, Mihaela Diana Bojin., Chemistry, Queensborough Community College, CUNY, Bayside, NY, United States.

Sunday, April 11, 2010

Sunday, April 11, 2010 8:30 AM – 11:35 AM

Analytical Chemistry I

Executive Business Center, Newark

8:30 AM Introductory Remarks

8:35 AM **108** Imaging of impact modifier dispersion in plastics with an optical microscope. **Gunter Moeller**, George Papakonstantopoulos., Department of Analytical and Systems Research, Arkema Inc., King of Prussia, Pennsylvania, United States.

8:55 AM **109** Characterization of degradation pathways of modified therapeutic oligonucleotides using mass sequencing via UPLC MS. **Ann M O'Brien**,[1] Natalie A Daurio,[2] Anthony M Leone.[1], [1]Merck Co. Inc., West Point, PA, United States; [2]College of Arts & Sciences, Syracuse University, Syracuse, NY, United States.

9:15 AM **110** Multivariate analysis for resolving tryptophan and tyrosine emissions. **Carol A. Roach**, Sharon L. Neal., Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

9:35 AM **111** Probing light-harvesting with photo-induced chronoamperometry. **Jonas I Goldsmith**., Department of Chemistry, Bryn Mawr College, Bryn Mawr, PA, United States.

9:55 AM **112** High pressure direct protein extraction from tissue. **Nicholas Sobol**, Jennifer Oprihory, Parth Kothiya, Zeineen A. Momin, Naresh Vasani, Vladamir Kachalov, Tiffany Remsen, Faraj Al Qaraghuli, Paul H Pevsner., Department of Pathology, University of Missouri School of Medicine, Columbia, MO, United States.

10:15 AM **113** Maldi imaging, ims, of tissue field defects in colorectal carcinoma. **Tiffany Remsen**, Parth Kothiya, Zeineen A. Momin, Naresh Vasani, Vladamir Kachalov, Jafar Imanpour, Siddharth Mathur, Chethana Kanaparthi, Sury Anand, Paul Pevsner., Department of Pathology, University of Missouri School of Medicine, Columbia, MO, United States.

10:35 AM **114** Maldi and lcms protein biomarkers of ionizing radiation. **Tiffany Remsen**, Vladamir Kachalov, Parth Kothiya, Zeineen A. Momin, Naresh Vasani, Jason Chouake, Douglas C. Miller, Paul Pevsner., Department of Pathology, University of Missouri School of Medicine, Columbia, MO, United States.

10:55 AM **115** Maldi imaging and diagnosis of prostate cancer. **Tiffany Remsen**, Adair Seager, Jonathan Melamed, Paul Pevsner., Department of Pathology, University of Missouri School of Medicine, Columbia, MO, United States.

11:15 AM **116** Application of principal component analysis and two dimensional correlation spectroscopy to investigate drug-polymer miscibility. **David Heaps**, Alfred Rumondor, Lynne Taylor., Department of Analytical Chemistry, AstraZeneca Pharmaceuticals LP, Wilmington, DE, United States.

Sunday, April 11, 2010

Sunday, April 11, 2010 8:30 AM – 4:30 PM

How to Be a More Effective Chemical Hygiene Officer

Sponsor: Division of Chemical Health & Safety

Conference Center, Marshall

Presider: Russell Phifer

Take a close look at Chemical Hygenie Officer position, and prepare at the same time for the NRCC-CHO Certification exam to be held the next day. Phifer gives a different slant to safety issues in the laboratory, focusing on what you do and how you can d

Sunday, April 11, 2010

Sunday, April 11, 2010 9:00 AM – 3:00 PM

Computers in Chemistry

Conference Center, King Sejong
Sponsor: RCH Solutions
Organizers: Sandeep Patel, Zheng Yang

NOTE: The order of the presenters has changed. The corrected schedule will be available at MARM.
Or click here

9:00 AM		Introductory Remarks
9:05 AM	**117**	Computational alanine scanning with linear scaling semi-empirical quantum mechanical methods. **David J Diller**,[1] Christine Humblet,[1] Xiaohua Zhang,[2] Lance M Westerhoff.[2], [1]Consultant, East Windsor, NJ, United States; [2]QuantumBio Inc., State College, PA, United States.
9:35 AM	**118**	Molecular description of flexibility in an antibody combining Site. **Ian F. Thorpe**., Department of Chemistry and Biochemistry, University of Maryland, Baltimore County, Baltimore, MD, United States.
10:05 AM	**119**	Development of the Next Generation of the Shape Signatures Technique for Molecular Shape Comparison. **Randy J Zauhar**,[1] William J Welsh.[2], [1]Depts of Chemistry & Biochemistry/ Bioinformatics & Computer Science, University of the Sciences, Philadelphia, PA, United States; [2]Department of Pharmacology, University of Medicine & Dentistry of New Jersey, Piscataway, NJ, United States.
10:35 AM		Intermission
11:00 AM	**120**	CADD methodologies for lead optimization: Recent advances. **Richard D Cramer**., CSO, Tripos Intl, St. Louis, MO, United States.
11:30 AM	**121**	Molecular systems biology through multiscale modeling and high-performance computing. **Ravi Radhakrishnan**., Department of Bioengineering, University of Pennsylvania, Philadelphia, PA, United States.
12:00 PM	**122**	Fluctuation dynamics analysis of gp120 envelope protein reveals a topologically based communication network. **Judith M. LaLonde**,[1] Indira Shrivastava.[2], [1]Chemistry, Bryn Mawr College, Bryn Mawr, PA, United States; [2]Department of Computational Biology, School of Medicine, University of Pittsburgh, Pittsburgh, PA, United States.

12:30 PM **123** Coarse-grained molecular dynamics simulations of fullerines interacting with lipid bilayers.. **Preston Moore**,[1] Steven Nielsen,[2] Russel DeVane.[3], [1]Department of Chemistry & Biochemistry, University of the Sciences in Philadelphia (USP), Philadelphia, PA, United States; [2]Department of Chemistry, University of Texas at Dallas, Richardson, TX, United States; [3]Institute for Computational Molecular Science and Department of Chemistry, Temple University, Philadelphia, PA, United States.

1:00 PM **124** Role of electrostatics in modulating hydrophobic interactions and barriers to hydrophobic assembly. **Brad A. Bauer**, Sandeep Patel., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

1:30 PM Intermission

1:55 PM **125** Binding pocket analysis of seven helical transmembrane proteins: Is sequence identity alone suitable for modeling GPCRs as drug targets?. **Vagmita Pabuwal**,[1] Zhijun Li.[1,2,3], [1]Department of Chemsitry & Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, United States; [2]Department of Bioinformatics and Computer Science, University of the Sciences in Philadelphia, Philadelphia, PA, United States; [3]Institute for Translational Medicine and Therapeutics, University of Pennsylvania, Philadelphia, PA, United States.

2:25 PM **126** Molecular Dynamics Simulation of Protein-Carbohydrate Interactions in Hen Egg White Lysozyme Complex Using a Polarizable Force Field. **Yang Zhong**, Sandeep Patel., Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States.

2:55 PM Concluding Remarks

Sunday, April 11, 2010

Sunday, April 11, 2010 9:00 AM – 1:40 PM

Nano Science, Technology, & Material Science I

Conference Center, Piaget

9:00 AM **127** Catalyst-free, one-pot synthesis of monodisperse, high-quality PbSe nanorods. **Weon-kyu Koh**,[1] Adam C Bartnik,[3] Frank W Wise,[3] Christopher B Murray.[1,2], [1]Department of Chemistry, University of Pennsylvania, Philadelphia, PA, United States; [2]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, United States; [3]School of Applied and Engineering Physics, Cornell University, Ithaca, NY, United States.

9:20 AM **128** Hexagonal Nanopillars of Melamine-Cyanuric Acid Complex Prepared by A Crystallization After Mixing on Surfaces (CAMS) Method. **Hai-Feng JI**., Chemistry, Drexel University, Philadelphia, PA, United States.

9:40 AM **129** Synthesis and properties of conjugation extended phenanthrolines. **Hyungsock Suh**, Dominick J Casadonte, Jr., Chemistry, Texas Tech University, Lubbock, TX, United States.

10:00 AM **130** Novel patterned protein assay to measure differential extracellular matrix protein affinities for cellular attachment and axonal outgrowth. **William Theilacker**,[1] Amy Styer,[1] Dianna Willis,[2] Holt Bui,[1] Jeffery L. Twiss,[2] Thomas P. Beebe.[1], [1]Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States; [2]Alfred I. DuPont Hospital for Children, Nemours Biomedical Research, Wilmington, DE, United States.

10:20 AM **131** Using electrochemical impedance spectroscopy to determine the geometry of radially symmetric nano-channels. **Michael J Vitarelli**, David S Talaga., Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, New Jersey, United States.

10:40 AM **132** Characterization of natural fiber welded biopolymer composites. **Zane A Fayos**,[1] Luke M Haverhals,[1] Hadley M Sulpizio,[1] W Matthew Reichert,[1] Matthew P Foley,[1] Hugh C De Long,[2] Paul C Trulove.[1], [1]Department of Chemistry, United States Naval Academy, Annapolis, MD, United States; [2]Mathematics, Information and Life Sciences Directorate, Air Force Office of Scientific Research, Arlington, VA, United States.

11:00 AM **133** Particle reformation in small anisotropic silver nanocolloids. **Stuart T. Gentry**, Mark W. Bezpalko., Department of Chemistry and Biochemistry, La Salle University, Philadelphia, PA, United States.

11:20 AM **134** Characterization of Tethered Bilayer Lipid Membranes (tBLMs) with Unsaturated Lipidic Anchor Molecules with Comparison to tBLMs with Saturated Lipidic Anchors. **David J Vanderah**,[1] Gintaras Valincius,[2] Frank Heinrich,[3,4] Rima Butvytyte,[2] Prabhanshu Shekhar,[4] Gediminas Niaura,[2] Vlada Voiciuk.[2], [1]Biochemical Science Division, National Institute of Standards & Technology, Gaithersburg, MD, United States; [2]Institute of Biochemistry, Vilnius, Lithuania; [3]Center for Neutron Research, National Institute Of Standards & Technology, Gaithersburg, MD, United States; [4]Department of Physics, Carnegie Mellon University, Pittsburgh, PA, United States.

11:40 AM **135** Highly stabilized nanoparticles fuctionalized with GdDTPASH as magnetic resonance imaging contrast agent. **Talha S Siddiqui**,[1] Lindsay K Hill,[2] Youssef Zaim Wadghiri,[2] Marc A Walters.[1], [1]Chemistry, New York University, New York, NY, United States; [2]Radiology, New York University Langone Medical Center, New York, NY, United States.

12:00 PM **136** Surface-enhanced Raman spectroscopy with silver nanocube dimers: Experiment and calculations. **Seung Yong Lee**,[1] Jane E Cornett,[1] Garrett S Lang,[2] Ling Hung,[2] Isaak D Mayergoyz,[2,3] Oded Rabin.[1,3], [1]Department of Materials Science & Engineering, University of Maryland, College Park, MD, United States; [2]Department of Electrical & Computer Engineering, University of Maryland, College Park, MD, United States; [3]Center for Applied Electromagnetics, University of Maryland, College Park, MD, United States.

12:20 PM **137** Characterization of the fractal geometry of SBA-15, and its use as a vanadia oxide support for the partial oxidation of methanol. **Thomas M Baldassare**, Michael A Smith., Department of Chemical Engineering, Villanova University, Villanova, PA, United States.

12:40 PM **138** Novel fluorescent nanomaterials, via assembly of anionic poly(phenylene vinylene) with lipid vesicles, divalent cations, and/or silica beads. **An T Ngo**, Pierre Karam, Kai L Lau, Melanie Burger, Jeffrey Quesnel, Gonzalo Cosa., Department of Chemistry, McGill University, Montreal, QC, Canada.

1:00 PM **139** Determining the mechanical response of propellants for large caliber ammunition. **Stephanie M Piraino**, Michael Leadore, Melissa Meyer, Rob Lieb., Energetic Materials Science Branch, Army Research Laboratory, Aberdeen Proving Ground, MD, United States.

Sunday, April 11, 2010

Sunday, April 11, 2010 9:00 AM – 10:40 AM

Polymer, Colloid, and Emulsion Chemistry

Sponsor: Division of Polymer Chemistry

Conference Center, Collins

9:00 AM **140** Microencapsulation of gentamicin sulphate using chitosan and alginate for time-released drug delivery systems (DDS). **Shakera M Guess**, Cherese Winstead., Department of Chemistry, Delaware State University, Dover, Delaware, United States.

9:20 AM **141** Preparation of Poly(lactic acid) Brush for dynamic surface. **Lebo Xu**, Chris B. Gorman., Department of Chemistry, North Carolina State University, Raleigh, North Carolina, United States.

9:40 AM **142** Synthesis of conjugates of camptothecin and phosphorycholine polymers for cancer therapeutics. **Xiangji Chen**, Samantha McRae, Sangram Parelkar, Todd Emrick., Department of Polymer Science & Engineering, University of Massachusetts, Amherst, Amherst, MA, United States.

10:00 AM **143** Drug elution kinetics and structure of absorbable matrix coatings. **Srilekha Sarkar Das**, Martin K McDermott, Anne D Lucas, Timothy E Cargal, Lakir Patel, David M Saylor, Dinesh V Patwardhan., Division of Chemistry and Materials Science, US FDA/CDRH/OSEL, Silver Spring, MD, United States.

10:20 AM **144** Synthesis and characterization of metal loaded plastic and liquid scintillator composites of cobalt benzne dithiolate, tetra phenyl butadine and poly(tegdma). **DEVIN M MCKELVEY**, **Kristin R Jones**, **Brittney Wass**, Mohit P Patel, Susan Jansen Varnum., Chemistry, Temple University, Philadelphia, PA, United States.

10:30 AM **145** Modifying Chitosan for biomedical purposes. **Elza Chu**, Alexander Sidorenko., Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, United States.

Sunday, April 11, 2010

Sunday, April 11, 2010 10:15 AM – 11:45 AM

ACS Undergraduate Research Symposium - II

Conference Center, King/Sullivan

Organizer/Presider: Narmada Gunawardena

Posters may be set up around 10:00. The symposium provides an excellent opportunity for undergraduate chemistry students to present the results of their research. Presenters should be by their posters from 10:15 - 11:45.

10:15 AM **146** Detection of PSA antigen on carbon nanotubes using fluorescence microscopy. **Seo-Young Kwon**, Amos M Mugweru., Department of Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States.

10:15 AM **147** Time-dependent DFT studies of the photoluminescence of amine-decorated 1-D CuCN chains. **Jasprina L Ming**,[1] Craig A Bayse,[1] Robert D Pike.[2], [1]Department of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA, United States; [2]Department of Chemistry, College of William and Mary, Williamsburg, VA, United States.

10:15 AM **148** Theoretical investigation of the gas-phase polymerization of ethylene by the chromium hydroxide cation ($CrOH^+$). **Patrick O'Kane**, Timothy J Dudley., Department of Chemistry, Villanova University, Villanova, PA, United States.

10:15 AM **149** Investigating a tandem cyclization-coupling reaction between o-ethynylbenzoic acids with p-iodoanisole as part of an approach to the Aristolactam alkaloids. **David M. Degan**, **Erin T. Pelkey**., Department of Chemistry, Hobart and William Smith Colleges, Geneva, NY, United States.

10:15 AM **150** Convergent method towards thiophene substituted 3-pyrrolin-2-ones. **Jacob P. MacDonald**, Jessica G. Greger, **Erin T. Pelkey**., Department of Chemistry, Hobart and William Smith Colleges, Geneva, NY, United States.

10:15 AM **151** Synthesis of a Macrocyclic Ligand and a New Copper Complex. **Erika D Druckenmiller**, **Brittney L Offenbacker**, Andrea E Martin, Louise M Liable-Sands., Department of Chemistry, Widener University, Chester, PA, United States.

10:15 AM **152** Synthetic approach to staurosporinone utilizing pyrrole Weinreb amides. **Jessica G. Greger**, Jacob P. MacDonald, **Erin T. Pelkey**., Department of Chemistry, Hobart and William Smith Colleges, Geneva, NY, United States.

10:15 AM **153** Thermodynamic investigation of $LiNTF_2$ dissolution in ionic liquids. **Angelo Andriola**, Lei Yu., Department of Chemistry and Biochemistry, Rowan University, Glassboro, New Jersey, United States.

10:15 AM **154** Synthesis and characterization of magnetic nanoparticles for drug delivery applications. **John Kong**, Amos Mugweru., Department of Chemistry & Biochemistry, Rowan University, Glassboro, NJ, United States.

10:15 AM **155** Ferrocenium trifluoroborate: An unexpected product. **Paul F. Smith**, Joseph J. Grzybowski., Department of Chemistry, Gettysburg College, Gettysburg, PA, United States.

10:15 AM **156** Self assembled multilayer films of cytochrome C and DNA for bio-activation studies. **Marc Iuliucci**, Amos Mugweru Mugweru., Department of Chemistry & Biochemistry, Rowan University, Glassboro, United States.

10:15 AM **157** Synthesis and characterization of molecular switch containing organic bridging compounds and their effects on the fluorescence process. **Thomas J Comey**, Ann Lezama, Kenneth Yamaguchi., Department of Chemistry, New Jersey City University, Jersey City, NJ, United States.

10:15 AM **158** Determination of hydrogen peroxide concentration in dental bleaching gel. **Kaitlyn Grosso**, Ryan Sours., Department of Chemistry, Towson University, Towson, Maryland, United States.

10:15 AM **159** Use of multicomponent coupling reactions for the synthesis of lipophilic a-acetoxyamides. **Subash C Jonnalagadda**, Christopher M Bashian, Joseph R Schafer, Anthony Cirri., Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States.

10:15 AM **160** Synthesis and characterization of spiropyran polymers. **Kelechi Chikeka**, **Phuong Ha**, Shannon E Stitzel., Department of Chemistry, Towson University, Towson, MD, United States.

10:15 AM **161** Automated Detection of GNRA Tetraloop Prevalence Using 3DNA and Python. **Prerana Pradhan**,[2] Mauricio Esguerra,[1] Wilma K Olson.[1], [1]Department of Chemistry and Chemical Biology, Rutgers, the State University of New Jersey, Piscataway, New Jersey, United States; [2]Department of Biomedical Engineering, Rutgers, the State University of New Jersey, Piscataway, NJ, United States.

10:15 AM **162** Effectoftheionicliquid1-butyl-1-methylpyrrolidiniumbis(trifluoromethylsulfonyl) imide on small peptide structure. **Karson Schmidt**, Leigh Murray, Michael Noss, Jia Huang, **Michelle R Bunagan**., Department of Chemistry, The College of New Jersey, Ewing, NJ, United States.

10:15 AM **163** Preparation of ionic liquids and their use in electrophilic aromatic substitution reactions with naphthalene and guaiazulene. **Ryan Ludwig**, Francis C. Mayville., Department of Natural Science - Chemistry, DeSales University, Center Valley, PA, United States.

10:15 AM **164** Squeeze Flow of Shear Thickening Fluids as a Possible Protective Garment. **David E Barlaz**,[1] Charles Swanik,[2] Richard Dombrowski,[1] Norman Wagner.[1], [1]Department of Chemical Engineering, University of Delaware, Newark, DE, United States; [2]Department of Health, Nutrition, & Exercise Science, University of Delaware, Newark, DE, United States.

10:15 AM **165** Investigation of various effects on gold nanoparticle aggregation. **Allison Sturm**, **Rodger E. Berg**., Natural Science, DeSales University, Center Valley, PA, United States.

10:15 AM **166** The extraction and isolation of the active ingredient, resveratrol, from grapes and various red wines. **Stephanie A. Lee**, **Laura A. Smith**, **Francis C. Mayville**., Natural Science, DeSales University, Center Valley, PA, United States.

10:15 AM **167** Investigation of the effect that different drying methods have on the release mechanism of naproxen from ethyl cellulose/microcrystalline cellulose beads. **Julianne Berger**, **Jonathan Fura**, **Francis C. Mayville**., Natural Science, DeSales University, Center Valley, PA, United States.

10:15 AM **168** Aerosol preparation of spherical zirconia (ZrO_2) and polymer coated zirconia particles. **Alyssa Maltese**, **Francis C. Mayville**., Natural Science, DeSales University, Center Valley, PA, United States.

10:15 AM **169** Python Graphical User Interface (GUI) for Control of the Levitated Dipole. **David Z Jacome**., Department of Applied Science and Technology, Saint Peter's College, Jersey City, New Jersey, United States.

10:15 AM **170** Characterization of self-assembled monolayer on gold electrode in ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate. **An D Le**, Lei Yu., Department of Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States.

10:15 AM **171** Towards structural characterization of the catalytic domain of bacteriophage T4 primase by NMR. **Thomas H Mann**, Mark D Sarcone, Lauren E Manning, William Tsai, Jayne A Kubat, Gregory A Manley, David Rovnyak., Chemistry, Bucknell University, Lewusburg, PA, United States.

10:15 AM **172** Adsorption of Lanthanides on Cellulose Carbamate - Silica Hybrid Materials. **Ivana McNeal**., Chemisty, Prairie View A&M University, Priarie View, TX, United States.

10:15 AM **173** Synthesis of a Pentaphenyl Benzene Bridging Ligand. **Adolfo Pertuz**, Ken Yamaguchi., Department of Chemistry, New Jersey City University, Jersey City, NJ, United States.

10:15 AM **174** Systematic Investigation of Phage Elution from Calcite Crystal Suraces. **Stephanie Stanley**, Ryan Sours., Department of Chemistry, Towson University, Towson, MD, United States.

Sunday, April 11, 2010

Sunday, April 11, 2010 12:00 PM – 1:30 PM

ACS Undergraduate Student Luncheon

1st Floor, du Barry Room

Dr. Jespersen, ACS District I Director, will discuss the financial benefits of being an ACS student member - reduced meeting registration fees, special student rates on journals and courses, and discounted prices with selected companies. ACS studen

Sunday, April 11, 2010

Sunday, April 11, 2010 1:00 PM – 3:20 PM

Frontiers in Magnetic Resonance in Liquids and Solids

Sponsors: Varian, Inc. (NMR); Bruker Corporation - Bruker BioSpin NMR; Cambridge Isotape Labs

Conference Center, Quintanilla

Organizer/Presider: David Rovnyak

Applications of nuclear magnetic resonance spectroscopy (NMR) continue to expand into new disciplines, while new NMR technologies and methods are emerging at a rapid pace. In this session, a diverse selection of highlights of nuclear magnetic resonance s

1:00 PM Introductory Remarks

1:05 PM **175** Characterization of cation-exchanged NH4NaY and USY zeolites by ^{27}Al MAS NMR spectroscopy. **David J. Aurentz**,[1] Kevin J. Sutovich.[2], [1]Division of Science, Penn State Berks College, Reading, PA, United States; [2]Refining Technologies, Grace Davison, Columbia, MD, United States.

1:25 PM **176** Solid-state NMR studies of CAP-Gly domain of mammalian dynactin and the CAP-Gly/microtubule complex. **Shangjin Sun**,[1] Si Yan,[1] Amanda E Siglin,[3] John C williams,[2,3] Tatyana Polenova.[1], [1]Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States; [2]Department of Molecular Medicine, Beckman Research Institute at City of Hope, Duarte, CA, United States; [3]Department of Biochemistry and Molecular Biology, Thomas Jefferson University, Philadelphia, PA, United States.

1:45 PM **177** Structures of Phospholamban Monomer and Pentamer by a Hybrid Solution and Solid-State NMR Refinement Protocol. **Nathaniel Traaseth**, Raffaello Verardi, Lei Shi, Martin Gustavsson, Gianluigi Veglia., Biochemistry, Molecular Biology and Biophysics, University of Minnesota, Minneapolis, MN, United States.

2:05 PM Intermission

2:20 PM **178** Structural switch model for Group II Intron RNA catalytic function. **T. Kwaku Dayie**., Chemistry and Biochemistry, University of Maryland, College Park, MD, United States.

2:50 PM **179** NMR based screening tool for quality control of botanical dietary supplements. **Kimberly L. Colson**,[1] Joshua M. Hicks,[1] Jan A. Glinski,[2] Stefan Gafner,[3] Jonathan Ferrier,[4] Kristina McIntyre,[4] John T. Arnason,[4] Alain Cuerrier,[5] Brian Killday.[1], [1]R&D, Bruker BioSpin, Billerica, MA, United States; [2]Planta Analytica LLC, Danbury, CT, United States; [3]Tom's of Maine, Kennebunk, Maine, United States; [4]Department of Biology, University of Ottawa, Ontario, Canada, United States; [5]Montreal Botanical Garden, Montreal, Quebec, Canada.

3:20 PM **180** A fresh look at triosephosphate isomerase reaction mechanism. **Sharon Rozovsky**., Department of Chemistry & Biochemistry, University of Delaware, Newark, DE, United States.

3:40 PM **181** Database mining applications for NMR protein structure determination. **Frank Delaglio**., Software Science Consultant, NMR Science, North Potomac, MD, United States.

Sunday, April 11, 2010

Sunday, April 11, 2010 1:00 PM – 5:00 PM

Your Company Fosters Innovation - Now how do you protect it?

Sponsor: Division of Chemistry & the Law

Executive Conference Center, Greenville Suite

Organizer: Sarah Perlinger Hasford

1:00 PM **182** Whether And How To Protect Your Innovations: Initial Considerations. **Roberte Makowski**., Connolly Bove Lodge & Hutz LLP, United States.

1:20 PM **183** Drafting your Patent Application to Avoid Written Description, Enablement, and Obviousness Rejections. **Eamonn Morrison**., Connolly Bove Lodge & Hutz LLP, United States.

1:40 PM **184** A Former Examiner's Guide to the Patent Office: How to Work Effectively and Efficiently with Examiners to Patent Your Innovations. **Sarah Hasford**, **James Balls**., Connolly Bove Lodge & Hutz, LLP, United States.

2:00 PM **185** Potential Pitfalls to Protecting Innovation: Activities Now that Can Affect Patentability in the Future. **Geoffrey Zelley**., Connolly Bove Lodge & Hutz, LLP, United States.

2:20 PM **186** IP Strategy: Licensing, Legal Opinions and Due Diligence. **Mark Freeman**., Connolly Bove Lodge & Hutz, LLP, United States.

Sunday, April 11, 2010

Sunday, April 11, 2010 1:30 PM – 3:00 PM

ACS Undergraduate Research Symposium - III

Conference Center, King/Sullivan

Organizer: Narmada Gunawardena

Posters may be set up time around 1:15. The symposium provides an excellent opportunity for undergraduate chemistry students to present the results of their research. Presenters should be by their posters from 1:30 - 3:00.

1:30 PM **187** Synthesis of a Ruthenium Complex of a Chiral Tetradentate Aminosulfoxide Ligand. **Krista N. Taylor**,[1] Tim J. Brunker,[1] Arnold L. Rheingold.[2], [1]Department of Chemistry, Towson University, Towson, MD, United States; [2]Department of Chemistry, University of California, San Diego, La Jolla, CA, United States.

1:30 PM **188** Cloning, expression, and purification of a putative acetylcholine binding protein from Nostoc punctiforme. **Kasey M Johnson**, Victoria Pisciella, Barry S Selinsky., Department of Chemistry, Villanova University, Villanova, PA, United States.

1:30 PM **189** Synthesis of new Heterocyclic Inhibitors of the Helicase of Hepatitis C Virus. **Kevin W. O'Malley**, Dawn N. Ward, Paul J. Smith., Department of Chemistry and Biochemistry, University of Maryland, Baltimore County, Baltimore, Maryland, United States.

1:30 PM **190** Explorations in the synthesis of new Troger's base derivatives. **Alyson DeStefano**, Donald L Jameson., Department of Chemistry, Gettysburg College, Gettysburg, PA, United States.

1:30 PM **191** Simple and efficient green methylation of phenols, carboxylic acids and heteroaromatic nitrogen compounds using dimethyl carbonate. **Marc Fialkoff**, **Andrew Krasley**, Donald L Jameson, Timothy W Funk., Department of Chemistry, Gettysburg College, Gettysburg, PA, United States.

1:30 PM **192** Electrochemical sensors based on poly[4-vinylpyridine Os(bipyridine)$_2$Cl]-co-ethylamine on glassy carbon electrode for glucose analysis. **Phong Trinh**, Amos Mugweru., Chemistry & Biochemistry, Rowan University, Glassboro, NJ, United States.

1:30 PM **193** Synthesis of functionalized cyclic boronic acids via hydroxy assisted Baylis Hillman reaction of a-boronoaldehydes. Sravan K Jonnalagadda,[2] **Subash C Jonnalagadda**,[1] Michael A Corsello,[1] Chase P Gomez,[2] **Venkatram R Mereddy**.[2], [1]Department of Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States; [2]Department of Chemistry and Biochemistry, University of Minnesota Duluth, Duluth, MN, United States.

1:30 PM **194** Synthesis and Quantization of Z-(9)-Pentacosene, A Honey Bee Pheromone Given Off During The Waggle Dance. **Yonaton N Heit**, Spyros Mavropoulos, Amber F. Charlebois., Department of Chemistry and Pharmaceutical Science, Fairleigh Dickinson University College at Florham, Madison, New Jersey, United States.

1:30 PM **195** Effects of Osmotic Stress and Macromolecular Crowding on the B-to-Z Transition in DNA. **Crista Nguemeta**, Richard S. Preisler, Alan J. Pribula., Department of Chemistry, Towson University, Towson, MD, United States.

1:30 PM **196** Computational analysis of aromatic oligoamide foldamers. **Marc Luong**, Jhenny Galan, Zhiwei Liu, Christian Tooley, Vojislava Popristic Popristic., West Center for Computational Chemistry and Drug Design, University of the Sciences in Philadelphia, Philadelphia, PA, United States.

1:30 PM **197** Biodiesel: From the Frier to the Laboratory. **Joseph G Jablonski**, Amber F Charlebois., Department of Chemistry, Fairleigh Dickinson University, Madison, NJ, United States.

1:30 PM **198** Core-shell hydrogel particles incorporating Acid Black 48. **Tiffany Ha**,[1] Alexis Patanarut,[1] Prianka Debnath,[1] Davide Tamburro,[2] Alessandra Luchini,[2] Emanuel F. Petricoin,[2] Lance Liotta,[2] Barney Bishop.[1], [1]Department of Chemistry and Biochemistry, George Mason University, Fairfax, VA, United States; [2]Center for Applied Proteomics and Molecular Medicine, George Mason University, Fairfax, VA, United States.

1:30 PM **199** Characterization of Sacharolyticum degradans xylanases activity. **Richard Negri**, Brittany Nixon, Gbekeloluwa B. Oguntimein., Civil Engineering, Morgan State University, Baltimore, Maryland, United States.

1:30 PM **200** Studies of the conformational rigidity of monomer units of arylamide oligomers with H-bond acceptors embedded in the aromatic ring. **Chi Ngong Tang**, Jhenny F Galan, Zhiwei Liu, Vojislava Pophristic., Department of Chemistry & Biochemistry/West Center for Computational Chemistry and Drug Design, University of the Sciences in Philadelphia, Philadelphia, PA, United States.

1:30 PM **201** Computational function annotation of structural genomics proteins in the enolase superfamily using THEMATICS. **Ee Leng Terng**,[1] Jaeju Ko,[1] Mary Jo Ondrechen.[2], [1]Department of Chemistry, Indiana University of Pennsylvania, Indiana, PA, United States; [2]Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA, United States.

1:30 PM **202** Drug-lipid interaction studies via fluorescence anisotropy and molecular dynamics simulations. **Harsh Amin**, Nicolas Chen, Jhenny Galan, Zhiwei Liu, Preston Moore, Julian Snow., Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, Pennsylvania, United States.

1:30 PM **203** Synthesis, structure and reactivity of an Azaferrocene-borane sandwich complex. **Benjamin T. Roembke**,[1] Tim J. Brunker,[1] James Golen,[2] Arnold L. Rheingold.[2], [1]Department of Chemistry, Towson University, Towson, MD, United States; [2]Department of Chemistry, University of California, San Diego, La Jolla, CA, United States.

Sunday, April 11, 2010

Sunday, April 11, 2010 3:15 PM – 4:55 PM

Sustainability, Green Chemistry, and Policy Symposium

Sponsor: American Chemical Society

Conference Center, King/Sullivan

Organizer: Martha Hollomon

3:15 PM **204** Sustainability – What is it and what does it mean to me?. **Frankie K Wood-Black**., Trihydro Corporation, Ponca City, OK, United States.

3:35 PM **205** Enhancements of enzymatic saccharification of hardwood biomass using oxalic acid pretreatments. **David W Berke-Schlessel**, Robert Wexler, Sudipto Das, Yen Wei., Department of Chemistry, Drexel University, Philadephia, PA, United States.

3:55 PM **206** Sustainability from innovative chemistries to legislative policy. **Catherine T. Hunt**., Technology Collaboration Development, The Dow Chemical Company, Spring House, PA, United States.

4:15 PM **207** Sustainable future: century of challenge and change for our plant. **Pat N. Confalone**., Crop Agriculture and Nutrition Platform, DuPont, Newark, DE, United States.

4:35 PM **208** Sustainability and the chemical enterprise. **William F. Carroll**., Occidental Chemical Corporation, Dallas, TX, United States.

Sunday, April 11, 2010

Sunday, April 11, 2010 6:30 PM – 8:00 PM

ACS Graduate and Post-Doc Research Symposium - Poster Session

Sponsor: American Chemical Society

Conference Center, King/Sullivan

Organizer: Narmada Gunawardena

6:30 PM **209** Master of the 7 C's. **Thomas Lane**., Director of Global Science and Technology Outreach, Dow Corning Corporation, Midland, MI, United States.

6:50 PM **210** Molecular dynamics of amphiphathic peptides embedded in a lipid bilayer. **Thuy Hien T Nguyen**, Zhiwei Liu, Preston B Moore., Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, United States.

6:50 PM **211** Asymmetric transfer hydrogenation of allylic alcohols with chiral ruthenium catalysts. **Ruoqiu Wu**, Marie G. Beauchamps, Joseph M. Laquidara, John R. Sowa., Department of Chemistry and Biochemistry, Seton Hall University, South Orange, NJ, United States.

6:50 PM **212** Role of Dichloromethane and Phenol in Chemical Paint Strippers. **Kelly E. Watson**,[1] James H. Wynne,[2] James P. Yesinowski,[2] Christopher N. Young,[3] Clive R. Clayton.[3], [1]Science Applications International Corporation, Washington, DC, United States; [2]Department of Chemistry, Naval Research Laboratory, Washington, DC, United States; [3]Department of Materials Science and Engineering, Stony Brook University, Stony Brook, NY, United States.

6:50 PM **213** Progress towards a light activated self-decontaminating coating. **Jeffrey G Lundin**,[1,2] Robert F Cozzens,[2] Kelly E Watson,[3] James H Wynne.[1], [1]Chemistry Division, Naval Research Laboratory, Washington, DC, United States; [2]Department of Chemistry, George Mason University, Fairfax, VA, United States; [3]Science Applications International Corporation, Washington, DC, United States.

6:50 PM **214** Characterization of a novel, putative trypanosome transcription factor. **Allison Sing**, Kellie Whitecavage, Jennifer Palenchar., Chemistry, Villanova University, Villanova, Pennsylvania, United States.

6:50 PM **215** Atmospheric oxidation mechanisms of trichloroethylene and tetrachloroethylene: ab initio studies. **Carrie J Christiansen**, Joseph S Francisco., Department of Chemistry, Purdue University, West Lafayette, Indiana, United States.

6:50 PM **216** OxyR dependent stress response. **Salvador Gomez**, Matthew Harter, Peter M Palenchar., Department of Chemistry, Rutgers, The State University of New Jersey - Camden, Camden, New Jersey, United States.

6:50 PM **217** Theoretical study on protonated water clusters: enumeration of structures and classification of OH bonds. **Maihemutijiang Jieli**, Misako Aida., Center for Quant Life Science & Chemistry Deapartment of Graduate School of Science, Hiroshima University, Hiroshima University, Higashi-Hiroshima, Hiroshima, Japan.

6:50 PM **218** Mechanism of anesthetic binding to lipid bilayer. **Nicolas Chen**., Chemistry & Biochemistry, University of Science in Philadelphia, Philadelphia, PA, United States.

6:50 PM **219** Engineering magnetic hydrogel microspheres for the capture and concentration of dilute proteins and peptides: Application as biomarker harvesting platforms. **Alexis Patanarut**,[1] Tiffany Ha,[1] Elissa H. Williams,[1] Emanuel F. Petricoin,[2] Lance A. Liotta,[2] Barney Bishop.[1], [1]Department of Chemistry and Biochemistry, George Mason University, Fairfax, VA, United States; [2]Center for Applied Proteomics and Molecular Medicine, George Mason University, Fairfax, VA, United States.

6:50 PM **220** Carbon nanotube-based electrochemical sensors for single-cell NO detection. **R. Venkat Kalyana Sundaram**,[1] Fei Li,[3] Roozbeh Ghavami,[3] Riju Singhal,[2] Zulfiya Orynbayeva,[2] Eric Borguet,[3] Yury Gogotsi,[2] Elisabeth S Papazoglou,[1] **Michael G Schrlau**.[2], [1]School of Biomedical Engineering, Drexel University, Philadelphia, Pennsylvania, United States; [2]Department of Materials Science and Engineering, Drexel University, Philadelphia, Pennyslvania, United States; [3]Department of Chemistry, Temple University, Philadelphia, Pennsylvania, United States.

6:50 PM **221** Synthesis of imidazole and pyrrolidine containing ionic liquids and study of their biodegradation properties. **Samanta Boursiquot**,[1] Firmause Payen,[1] Sharon I. Lall-Ramnarine,[1] Marie Thomas,[2] James F. Wishart,[2] Cleveland J. Dodge,[2] A. J. Francis.[2], [1]Department of Chemistry, Queensborough Community College, CUNY, Bayside, NY, United States; [2]Department of Chemistry, Brookhaven National Laboratory, Upton, NY, United States.

6:50 PM **222** Immobilization of horseradish peroxidase on modified chitosan beads. **Mohammed Monier**,[1] Yen Wei,[1] A Sarhan.[2], [1]department of chemistry, Drexel University, United States; [2]Mansoura University, Egypt.

6:50 PM **223** Hydration effects on ion polarizability: Insights from iterative Hirshfeld partitioning. **Brad A. Bauer**, Timothy R. Lucas, Sandeep Patel., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

6:50 PM **224** Solvation Properties of N-acetyl-beta-hexosaminides: A Molecular Dynamics Study Incorporating Electrostatic Polarization. **Yang Zhong**, Sandeep Patel., Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States.

6:50 PM **225** Molecular dynamics simulation of hydrated DPPC monolayers using charge equilibration force fields. **Timothy R Lucas**, Sandeep Patel., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

6:50 PM **226** Effect of ions on hydrophobic assembly and properties at the water/hydrophobe interface. **Shuching Ou**, Brad A. Bauer, Sandeep Patel., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

6:50 PM **227** Investigating intramolecular hydrogen bonding in aromatic oligoamide foldamers. **Jessica Amber Geer**, Zhiwei Liu, Vojislava Pophristic, Jhenny Galan., Chemistry & Biochemistry, Univeristy of the Sciences in Philadlephia, Philadlephia, PA, United States.

6:50 PM **228** Development of a coarse-grain intramolecular forcefield for proteins. **Kenny Nguyen**,[1] Jhenny Galan,[1] Zhiwei Liu,[1] Russell DeVane,[2] Preston Moore.[1], [1]Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, Pennsylvania, United States; [2]Department of Chemistry, Temple University, Philadelphia, Pennsylvania, United States.

6:50 PM **229** Novel method to control pressure in molecular dynamics simulations. **D Vladimir Perez**,[1] Preston B Moore,[1] Steve O Nielsen.[2], [1]Department of Chemistry & Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, United States; [2]Department of Chemistry, University of Texas at Dallas, Richardson, TX, United States.

6:50 PM **230** Targeting the human Andorgen Receptor with steroidal CYP17 inhibitors: A Molecular Docking approach. **Eleonora Gianti**,[1] Randy J. Zauhar,[1] Puranik Purushottamachar,[2] Vincent C. O. Njar.[2], [1]Departments of Chemistry & Biochemistry, Bioinformatics & Computer Science, University of The Sciences in Philadelphia, Philadelphia, PA, United States; [2]Department of Pharmaceutical Sciences, Jefferson School of Pharmacy, Thomas Jefferson University, Philadelphia, PA, United States.

6:50 PM **231** Synthesis and cycloaddition reactions of diethyl (E)-2-fuoromaleate. **Mehrdad Shadmehr**, Timothy B Patrick., Department of Chemistry, Southern Illinois University, Edwardsville, IL, United States.

Monday, April 12, 2010

Monday, April 12, 2010 8:00 AM – 5:30 PM

ACS Career Management Workshop

Sponsor: American Chemical Society

Conference Center, Quintanilla

Presider: Administrator ACS

8:00 AM **232** Today's Job Searching Strategies. **James D. Burke**., Career Consultant, American Chemical Society, Washington, DC, United States.

9:30 AM **233** Preparing your résumé or CV. **James D. Burke**., Career Consultant, American Chemical Society, Washington, DC, United States.

11:00 AM **234** Effective Interviewing. **James T. Burke**., Department of Career Management and Development, American Chemical Society, Washington, DC, United States.

12:30 PM Intermission

1:30 PM **235** Resume reviews and career assistance. **James D. Burke**., Department of Career Management and Development, American Chemical Society, Washington, DC, United States.

Monday, April 12, 2010

Monday, April 12, 2010 9:00 AM – 10:30 AM

Analytical Chemistry II

Conference Center, King

Organizer: Narmada Gunawardena

9:00 AM **236** Analysis and determination of the chemical constituents of turmeric and its anti-microbial activity. **Bibi Javeria**, Aheda Saber., Department of Chemistry, Governors State University, University Park, IL, United States.

9:00 AM **237** Antibacterial activity determination and extraction quantification of cuminaldehyde in cuminum cyminum seeds. **Divya Varadarajan**, Aheda Saber., Department of Chemistry, Governors State University, Univeristy Park, IL, United States.

9:00 AM **238** Analysis of mineral contents in seed coat in relation to canning quality of selected cultivars of dark red kidney beans (Phaseolus Vulgaris L .). **Alfred Anderson**., Department of Family Sciences, Kuwait University, Safat, Kuwait.

9:00 AM **239** Analysis of polyhexamethylene biguanide in multipurpose contact lens solutions. **Anne D Lucas**, Edward A Gordon., Center for Devices and Radiological Health, US Food and Drug Administration, Silver Spring, MD, United States.

9:00 AM **240** Evaluation of the oxidative metabolites of w-6 and w-3 fatty acids by LC-ESI-MS and their implication in the progression of rheumatoid arthritis. **Deepti R Varma**, Susan Jansen Varnum., Chemistry, Temple University, Philadelphia, PA, United States.

9:00 AM **241** Tuning of nanohole array surface plasmon resonance wavelength by varying nanohole diameter and array periodicity. **Laurel L Kegel**, Karl S. Booksh., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

9:00 AM **242** Implementation of liquid chromatography and UV-Vis spectrometry for the quantification of a low level colored impurity formed during the process optimization of Trityl Losartan. **Stephen M Marcinko**, Robert Hartman, Tony Hudgens., Analytical Development and Commercialization, Merck Manufacturing Division, Merck and Company, Rahway, NJ, United States.

Monday, April 12, 2010

Monday, April 12, 2010 9:00 AM – 1:05 PM

What a Chemist Needs to Know About Patent Law

Sponsor: Division of Chemistry & the Law
Organizer: Sarah Perlinger Hasford

9:00 AM Introductory Remarks

9:05 AM **243** Requirements for Patentability: Utility, Novelty, Nonobvious, Enablement, and Written Description. **Christine Hlavka**., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

9:35 AM **244** What Constitutes an Invention: Conception, Reduction to Practice, and Inventorship. **Krista Bianco**., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

10:05 AM **245** Best Practices in Drafting and Prosecuting a Patent Application. **Maureen Queler**., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

10:35 AM **246** A Patent Litigation Primer. **Krista Bianco**., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

11:05 AM **247** Overview of ANDA Pharmaceutical Patent Litigation in the United States. **Justin Hasford**., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

11:35 AM Panel Discussion

12:05 PM Reception

Monday, April 12, 2010

Monday, April 12, 2010 9:30 AM – 10:50 AM

Chemical Engineering/AIChE Symposium

Conference Center, Knowles

9:30 AM **248** Evaluating Miscibility Tests for Planning Gas Injection Projects for Four Major Kuwaiti Oil Reservoirs. **Adel Elsharkawy**,[1] Osamah Al-Omair,[1] Moudi Al-Ajmi.[1], [1]Petroleum Engineering, Kuwait University, Safat, Kuwait, Kuwait; [2]Kuwait University, Kuwait; [3]Kuwait Oil Company, Kuwait.

9:50 AM **249** Colloidosomes: Controlling transport from alginate hydrogels. **Rachel Rosenberg**, Nily Dan., Department of Chemical and Biological Engineering, Drexel University, Philadelphia, PA, United States.

10:10 AM **250** Cross-dimerization of isoamylene and a-methylstyrene in a microreactor using Filtrol-24 catalyst. **Obiefuna C. Okafor**,[1] Sunitha Tadepalli,[2] Geatesh Tampy,[2] Adeniyi Lawal.[1], [1]Department of Chemical Engineering and Material Sciences, Stevens Institute of Technology, Hoboken, New Jersey, United States; [2]R&D Center, International Fragrances and Flavors, Union Beach, New Jersey, United States.

10:30 AM **251** Vascularized scalable networks: Electrohydrodynamic viscous fingering and electrical treeing. **Kristopher D. Behler**, Eric D. Wetzel., Composite and Hybrid Materials Branch, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, United States.

Monday, April 12, 2010

Monday, April 12, 2010 9:30 AM – 11:30 AM

Medicinal Chemistry I

Sponsor: Division of Medicinal Chemistry

Conference Center, King Sejong

9:30 AM **252** Using computer-aided drug design to identify new antimicrobial lead compounds. **Malela Werner**,[1] Mohammed Bamajboor,[2] Randy Zauhar.[1,2], [1]Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, United States; [2]Department of Bioinformatics and Computer Science, University of the Sciences in Philadelphia, Philadelphia, PA, United States.

9:50 AM **253** Benzylthiocarbamate inhibitors of endothelial lipase: A drug target for atherosclerosis. **D. J. Hlasta**, A. Darrow, M. Hawkins, Z. Huang, J. Kranz, G. Leo, M. Olson, E. Powell, C. Smith, W. Sun, H. Xin, M. Connelly, M. Greco., Johnson & Johnson Pharmaceutical Research & Development, Spring House, Pennsylvania, United States.

10:10 AM **254** Design and structure-activity relationships of a dipeptidyl peptidase-1 inhibitor series. **D. J. Hlasta**, R. Alexander, S. Ghosh, Y. Huang, D. Johnson, A. Jordan, J. Kervinen, J. Kirkpatrick, L. Kuo, E. Lawson, R. Malaviya, M. Parker, I. Petrounia, A. Reitz, C. Schubert, R. Steele, E. Strobel, B. Tounge, K. White, M. Winters., Johnson & Johnson Pharmaceutical Research & Development, Spring House, Pennsylvania, United States.

10:30 AM **255** Synthesis and anti-inflammatory acitivity in a lipophilic vanilloid amide platform. **Abhilash N Pillai**,[1] Carl J Lacey,[1] Cynthia A Fianu Velgus,[1] Sherri C Young,[1] Karine M Fabio,[1] Christophe D Guillon,[1] Ned D Heindel,[1] Jeffrey Laskin,[2] Diane Heck,[3] Irene Wohlman,[2] Mou-Tuan Huang,[2] Anna Vetrano.[4], [1]Chemistry, Lehigh University, Bethlehem, PA, United States; [2]UMDNJ / EOHSI, Rutgers University, Piscataway, NJ, United States; [3]Environmental Health Science, New York Medical College, Valhalla, NY, United States; [4]of Pediatrics, Rutgers University, School of Pharmacy, Piscataway, NJ, United States.

10:50 AM **256** Novel tricyclic inhibitors of IKK2: Synthesis, SAR, PK/PD and activity in a preclinical model of rheumatoid arthritis. **Alaric J. Dyckman**, Charles M. Langevine, Claude Quesnelle, James Kempson, Junqing Guo, Patrice Gill, Steven H. Spergel, Scott H. Watterson, Tianle Li, David Nirschl, James R. Burke, Kathleen Gillooly, Mark A. Pattoli, Kim W. McIntyre, Laishun Chen, Punit H. Marathe, Zheng Yang, David Wang-Iverson, Murray McKinnon, John H. Dodd, Joel C. Barrish, William J. Pitts., Research and Development, Bristol-Myers Squibb, Princeton, NJ, United States.

11:10 AM **257** Novel inhibitors of basal glucose transport as potential anticancer agents. **Weihe Zhang**,[1] Yi Liu,[2] Xiaozhuo Chen,[2,3,4] Stephen C Bergmeier.[1], [1]Department of Chemistry and Biochemistry, Ohio University, Athens, OH, United States; [2]Department of Biological Science, Ohio University, Athens, OH, United States; [3]Department of Biomedical Science, Ohio University, Athens, OH, United States; [4]Edison Biotechnology Institute, Ohio University, Athens, OH, United States.

Monday, April 12, 2010

Monday, April 12, 2010 1:00 PM – 2:45 PM

Advances in Infra-red (IR) and Terahertz (THz) Spectrometry Symposium

Conference Center, Piaget

Organizer/Presider: Anis Rahman

1:00 PM Introductory Remarks

1:05 PM **258** Applications of terahertz spectrometry in biopharmaceutical reagent quantification and characterization. **Trevor L. Broadt**,[1] Anis Rahman.[2], [1]Biopharmaceutical Development Program, SAIC-Frederick, Frederick, MD, United States; [2]Applied Research and Photonics, Inc., Harrisburg, PA, United States.

1:35 PM **259** Terahertz spectral analysis of FCGR3A genotypes. **Gulshan Ara**,[1] Aunik K Rahman,[1] Bruce A Stanley,[2] Anis Rahman.[1], [1]Applied Research Photonics, Inc., Harrisburg,, PA, United States; [2]Penn State College of Medicine, Hershey, PA, United States.

1:55 PM **260** Terahertz study of transdermal drug delivery. **Aunik K Rahman**,[1] Anis Rahman,[1] Diksha Kaushik,[2] Bozena Michniak-Kohn.[2], [1]470 Friendship Road, Ste 10, Applied Research & Photonics, Harrisburg, PA, United States; [2]Department of Pharmaceutics/Pharmacy, Rutgers-The State University of New Jersey, Piscataway, NJ, United States.

2:15 PM **261** Mid-IR reflectance spectroscopy for surface analysis: in-situ applications of grazing-angle methods. **Mary Thomson**., Remspec Corporation, Sturbridge, MA, United States.

Monday, April 12, 2010

Monday, April 12, 2010 1:00 PM – 4:20 PM

Chromatography Forum of Delaware Valley Student Award Symposium

Conference Center, Quintanilla

Organizer/Presider: Marshall Fishman

1:00 PM Introductory Remarks

1:05 PM **262** Synthesis and characterization of isoquinoline urea derivatives of A-425619 as TRPV1 antagonists. **Neha A Gujarati**,[1] Bradley J Undem,[2] Vijaya L Korlipara.[1], [1]College of Pharmacy & AHP, St. John's University, Queens, NY, United States; [2]John's Hopkins Asthma and Allergy Center, Baltimore, MD, United States.

1:25 PM **263** Effects of temperature on the neutral lipid content of Biomphalaria glabrata as determined by modern, instrumental high-performance thin-layer chromatography with densitometry. **Jeff Bolstridge**,[1] Joseph Sherma,[1] Bernard Fried.[2], [1]Department of Chemistry, Lafayette College, Easton, PA, United States; [2]Department of Biology, Lafayette College, Easton, PA, United States.

1:45 PM **264** QuEChERS as a Sample Preparation Technique for Samples Analyzed by GC/MS. **Kelsey M Smith**, Mackenzie L Lauro, Karyn M Usher., Department of Chemistry, West Chester University, West Chester, PA, United States.

2:05 PM **265** High-throughput single-cell toxicity screening of biocidal compounds in a microfluidic device. **Michael F Santillo**,[1] Michael L Heien,[1] Andrew G Ewing.[1,2], [1]Department of Chemistry, The Pennsylvania State University, University Park, PA, United States; [2]Department of Chemistry, University of Gothenburg, Goteborg, Sweden.

2:25 PM Intermission

2:40 PM **266** Evaluation of the precision of dual-opposite injection capillary zone electrophoresis and comparison with conventional capillary zone electrophoresis. **Donna M Blackney**, Joe P Foley., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

3:00 PM **267** Enantiomeric separation of phenylalinine by micellar electrokinetic chromatography using a chiral surfactant, N-dodecoxycarbonylvaline. **Joseph A Vena**, Donna Blackney, Joe P Foley., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

3:20 PM **268** Investigating the mechanism responsible for MEKC separations of chiral compounds by bile salt micelles using CE and NMR. **Jenna B. Yehl**, Greg A Manley, Kyle W. Eckenroad, Christine M. Hebling, Laura E. Thompson, Timothy G. Strein, David Rovnyak., Department of Chemistry, Bucknell University, Lewisburg, PA, United States.

3:40 PM **269** Investigation of the effects of buffering and mixing conditions for the in-line jaffe reaction with capillary electrophoresis. **Sarah Schubert**, Sarah Findeis, William Napoli, Timothy Strein., Department of Chemistry, Bucknell University, Lewisburg, Pennsylvania, United States.

4:00 PM **270** Chemical reactions within CE capillaries: transferring an antioxidant power assay to the nanoliter level Shelly A. McCormack, Adam D. Catherman, Timothy G. Strein PhD. **Shelly A McCormack**,[1] Timothy G Strein,[1] Adam D Catherman.[2], [1]Department of Chemistry, Bucknell University, Lewisburg, Pennsylvania, United States; [2]Department of Chemistry, Northwestern University, Chicago, Illinois, United States.

Monday, April 12, 2010

Monday, April 12, 2010 1:00 PM – 2:30 PM

Medicinal Chemistry II

1:00 PM **271** X-ray imaging contrast agent based on nanoparticles of bismuth compounds. **Oded Rabin**.[1,2], [1]Department of Materials Science and Engineering, University of Maryland, College Park, MD, United States; [2]IREAP, University of Maryland, College Park, MD, United States.

1:00 PM **272** Antitrypanosomal activities of some novel imido- substituted 1,4-naphthoquinone derivatives. **Mozna H Khraiwesh**,[2] Clarence M Lee,[2] Yakini Brandy,[1] Emmanuel S Akinboye,[1] Solomon Berhe,[1] Genelle Gittens,[1] **Oladapo Bakare**.[1], [1]Department of Chemistry, Howard University, Washington, DC, United States; [2]Department of Biology, Howard University, Washington, DC, United States.

1:00 PM **273** Investigations of heterocyclic sulfones as medicinal compounds. **Kristen N Barrett**, James McKee, Murray Zanger., Department of Chemistry & Biochemistry, University of the Sciences in Philadelphia, Philadelphia, Pennsylvania, United States.

1:00 PM **274** Free radical scavenging assay for comprehensive analysis of individual and multi-component anti-oxidants. **Michael M Koganov**, Artyom Duev., Integrated Botanical Technologies, Ossining, NY, United States.

1:00 PM **275** SAR of tertiary carbinamine derived BACE1 inhibitors: role of aspartate ligand amine pK_a in enzyme inhibition. **Hemaka A. Rajapake**,[1] Philippe G. Nantermet,[1] Harold G. Selnick,[1] James C. Barrow,[1] Georgia B. McGaughey,[2] Sanjeev Munshi,[3] Stacey R. Lindsley,[1] Mary Beth Young,[1] Phung L. Ngo,[1] M. Katherine Holloway,[2] Ming-Tain Lai,[4] Amy S. Espeseth,[4] Xiao-Ping Shi,[4] Dennis Colussi,[4] Beth Pietrak,[4] Ming-Chih Crouthamel,[4] Katherine Tugusheva,[4] Qian Huang,[4] Min Xu,[4] Adam J. Simon,[4] Lawrence Kuo,[3] Daria J. Hazuda,[4] Samuel Graham,[1] Joseph P. Vacca.[1], [1]Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA, United States; [2]Department of Structural Biology, Merck Research Laboratories, West Point, PA, United States; [3]Department of Molecular Systems, Merck Research Laboratories, West Point, PA, United States; [4]Department of Alzheimer's Research, Merck Research Laboratories, West Point, PA, United States.

Monday, April 12, 2010

Monday, April 12, 2010 1:00 PM – 3:00 PM

Industrial Innovation Award Symposium

Conference Center, Sullivan

Monday, April 12, 2010

Monday, April 12, 2010 1:00 PM – 2:30 PM

Nano Science, Technology, & Material Science II

Conference Center, King

1:00 PM **276** Neurite Outgrowth on Gradients of Extracellular Matrix Proteins. **William Theilacker**,[1] Dianna Willis,[2] Lisa Capriotti,[1] Holt Bui,[1] Glen O'Neil,[1] Ying Len,[1] Jeffery Twiss.[2], [1]Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States; [2]Alfred I. DuPont Hospital for Children, Nemours Biomedical Research, Wilmington, DE, United States.

1:00 PM **277** Surfactant mediated electrochemical polymerization of polythiophene fibers. **Ian de Albuquerque**,[2] Eduard Nasybulin,[1] Kalle Levon.[1], [1]Department of Chemical and Biological Sciences, Polytechnic Institute of NYU, United States; [2]Department of Chemical and Biological Engineering, Polytechnic Institute of NYU, United States.

1:00 PM **278** Carbon Nanotube-Bioglass nanocomposite for Bone Tissue Engineering Applications. **Leah E Mitchell**, Aderemi Oki., Department of Chemistry, Prairie View A&M University, Prairie View, Texas, United States.

1:00 PM **279** New inorganic-organic hybrid materials based on III-VI semiconductors. **Ruibo Zhang**, Derek Le, Thomas J. Emge, Jing Li., Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, New Jersey, United States.

1:00 PM **280** Genetically encodable methods for controlling the orientation of the proteins ubiquitin, eGFP and protein G on gold nanoparticles. **Alison M. Williams-Reed**, Steven J. Metallo., Department of Chemistry, Georgetown University, Washington, DC, United States.

Monday, April 12, 2010

Monday, April 12, 2010 1:00 PM – 5:00 PM

Recent Updates in Patent Law

Sponsor: Division of Chemistry & the Law

Executive Conference Center, Greenville Suite

Organizer: Sarah Perlinger Hasford

1:00 PM **281** Bilski and Patent Eligibility of Processes in the Chemical and Biological Arts. **Charles Collins-Chase**., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

1:20 PM **282** Omission Without Intent is Not Inequitable Conduct: AstraZeneca Pharmaceuticals LP v. Teva Pharmaceuticals USA, Inc. (Fed. Cir. 2009). **Casey Dwyer**., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

1:40 PM **283** In re '318 Patent Litigation : The Enablement and Utility Requirements. **Shana Mattson**., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

2:00 PM **284** Implications of Wyeth v. Kappos. **Sheetal Patel**., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

2:20 PM **285** Product-by-Process: What You Say Is What You Get. **Mary Chlebowski**., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

2:40 PM **286** Preventing premature patent retirement: Is your invention working and earning up to its full potential?. **Patricia A. Carson**, **Christopher T. Jagoe**, **Graham M. Pechenik**., Kaye Scholer LLP, New York, NY, United States.

Monday, April 12, 2010

Monday, April 12, 2010 6:00 PM – 9:00 PM

Carothers Award Symposium

1st Floor, du Barry Room

Tuesday, April 13, 2010

Tuesday, April 13, 2010 9:00 AM – 11:00 AM

Cope Scholars Award Symposium

Conference Center, Knowles

Organizer: Narmada Gunawardena

Tuesday, April 13, 2010

Tuesday, April 13, 2010 9:00 AM – 11:00 AM

Environmental Chemistry

Sponsor: Division of Environmental Chemistry

Conference Center, Quintanilla

Monday, April 12, 2010

Monday, April 12, 2010 3:00 PM – 4:05 PM

Polymer and Nanomaterials based Photonics, Electro-optics and Tetrahertz Spectrometry

Conference Center, Piaget

Organizer: Anis Rahman

3:00 PM		Introductory Remarks
3:05 PM	**287**	Polymers for long range photoinduced proton transfer. **Richard P Brown**, Paul J Smith., Department of Chemistry and Biochemistry, University of Maryland Baltimore County, Baltimore, Maryland, United States.
3:25 PM	**288**	Fabrication of Polycyclic aromatic hydrocarbons nanostructures from 1D to 3D by gas phase self-Assembly. **Hong Wang**, Karen Xu, Haifeng Ji., Department of Chemistry, Drexel University, Philadelphia, PA, United States.
3:45 PM		Panel Discussion

Tuesday, April 13, 2010

Tuesday, April 13, 2010 9:00 AM – 10:55 AM

Fluorine Chemistry

Sponsor: Division of Fluorine Chemistry

Conference Center, Piaget

9:00 AM		Introductory Remarks
9:05 AM	**289**	Synthesis of ethyl cis-2-fluoroproenoate and its use in the Diels-Alder reaction. **Joshua Neumann**, Timothy Patrick., chemistry, southern illinois university edwardsville, edwardsville, illinois, United States.
9:25 AM		Panel Discussion

Tuesday, April 13, 2010

Tuesday, April 13, 2010 9:00 AM – 10:30 AM

Inorganic Chemistry II

Sponsor: Division of Inorganic Chemistry

Conference Center, King Sejong

9:00 AM **290** Imine chelates of copper, nickel, and zinc. **Molly A. O'Connor**, Anthony W. Addison., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

9:00 AM **291** A New Microporous Metal Organic Framework (MMOF) Material for Small Gas Separation. **Jingming Zhang**, Haohan Wu, Thomas Emge, Jing Li., Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, NJ, United States.

9:00 AM **292** Comparison of the coordination chemistry of tripod ligands possessing three pyridine donors and three imidazole donors. **Julie Vrana**,[1] **Kathleen McGuinn**,[1] Donald L Jameson,[1] Christopher J Ziegler,[2] James Engle.[2], [1]Department of Chemistry, Gettysburg College, Gettysburg, PA, United States; [2]Department of Chemistry, University of Akron, Akron, OH, United States.

9:00 AM **293** Nearly-Zero Anisotropic Thermal Expansion in II-VI Based Inorganic-Organic Hybrid Semiconductor Materials. **Xiao Zhang**,[1] Yang Ren,[2] Mojgan Roushan,[1] Jing Li.[1], [1]Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, NJ, United States; [2]Advanced Photon Source, Argonne National Laboratory, Argonne, IL, United States.

9:00 AM **294** Tolerance of Biomphalaria glabrata to Triorganotins. **James Ferguson**,[1] Xueqing Song,[1] Andargachew Negash,[1] Carolyn Cousin,[2] Stephanie Graves,[2] George Eng.[1], [1]Department of Chemistry & Physics, University of the District of Columbia, Washington, DC, United States; [2]Department of Biological & Environmental Sciences, University of the District of Columbia, Washington, DC, United States.

9:00 AM **295** Luminescent MOFs for Detection of Explosives and Other Aromatic Compounds. **Sanhita Pramanik**,[1] Anjian lan,[2] Jing Li.[1], [1]Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, New Jersey, United States; [2]Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian, China.

9:00 AM **296** Toxicity of Triorganotins against Escherichia coli. **Hirut Yimer**,[2] Russell Knighton,[1] Joni Robinson,[2] Xueqing Song,[1] George Eng.[1], [1]Chemistry & Physics, University of the District of Columbia, Washington, DC, United States; [2]Biological & Environmental Sciences, University of the District of Columbia, Washington, DC, United States.

9:00 AM **297** Studies on asymmetric bis(imino)pyridines and their synthetic precursors. **Rachel Hardie**, Margaret D. Kennedy, Jonathan C. Axtell, Janelle E. Steves, William S. Kassel, William G. Dougherty, Timothy J. Dudley, Deanna L. Zubris., Department of Chemistry, Villanova University, Villanova, PA, United States.

9:00 AM **298** Synthesis and Study of $[Ru(bpy)_2(bpy(OH)_2)][PF_6]_2$. **Samantha Klein**, Jared J. Paul., Department of Chemistry, Villanova University, Villanova, Pennsylvania, United States. (Data courtesy of William G. Dougherty & W. Scott Kassel)

9:00 AM **299** Synthesis, characterization and electronic properties of $[Ru(tpy)(tpyOH)]^{2+}$. Alessa B. Wood, Kent A. Maghacut, Walter J. Boyko, **Jared J. Paul**., Department of Chemistry, Villanova University, Villanova, PA, United States.

9:00 AM **300** Long Fluorinated alkyl chains protects Iron(III) porphyrins from self-oxidative degradation during the catalytic process. **Amit Aggarwal**,[1] Charles M Drain.[1,2], [1]Department of Chemistry and Biochemistry, Hunter College, New York, NY, United States; [2]The Rockefeller University, New York, NY, United States.

9:00 AM **301** Ground and excited-state coordination chemistry of $Ru(bpy)_2(ppz)^{2+}$ (ppz-4'7'-phenanthrolino-5'6':5,6-pyrazine). **Anthony Perri**, Harry D Gafney, John Kalambogias., Department of Chemistry and Biochemistry, Queens College-City University of New York, Flushing, NY, United States.

9:00 AM **302** Computational study of the electronic structure and function of a novel class of cyclic Phosphazenes. **Whelton A. Miller**, Vincent S. Pagnotti, Edward R. Birnbaum, Preston B. Moore., Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, United States.

9:00 AM **303** On the road to controlled phosphazene dendrimers: Steps along the way. Part III. **Vincent S. Pagnotti**, Edward R. Birnbaum., Department of Chemistry & Biochemistry, The University of the Sciences in Philadelphia, philadelphia, Pa, United States.

9:00 AM **304** Construction of metal-organic frameworks with enhanced properties. **Yonggang Zhao**, Thomas J Emge, Jing Li., Department of chemistry and chemical biology, Rutgers University, Piscataway, NJ, United States.

9:00 AM **305** Use of underutilized bulky Ttz ligands for the formation of zinc based biomimetic structures. **Mukesh Kumar**,[1] Elizabeth T. Papish,[1] Matthias Zeller.[2], [1]Chemistry, Drexel University, Philadelphia, PA, United States; [2]Chemistry, Youngstown State University, Youngstown, OH, United States.

9:00 AM **306** Departmental Hirsch Index values scale linearly with Chemistry department size. **A. W. Addison**, Thuong H. Tran., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

ABSTRACTS

Biological Chemistry I

1. Insight into cutinase reactivity for biotransformations

Peter James Baker,[1] David Feder,[1] Richard Gross,[1] Jin K Montclare.[1,2], [1]Department of Chemical and Biological Sciences, Polytechnic Institute of New York University, Brooklyn, NY, United States; [2]Department of Biochemistry, Downstate Medical College, Brooklyn, New York, United States.

Cutinases are enzymes secreted by phytopathogens that allow for the penetration of the plant surface barrier. These enzymes effectively hydrolyze their natural substrates, w-hydroxyl fatty acids and epoxy-fatty acids, and have been exploited for a broad range of biotransformations. To date much of the data has focused on the cutinase from *Fusarium solani* (FsC). To further broaden the biotechnological applications of cutinases we have begun to explore cutinases from other species; *Humicola insolens* (HiC), *Alternaria brassicicola* (AbC), *Aspergillus fumigatus* (AfC) and *Aspergillus oryzae* (AoC). These enzymes were over expressed in *Pichia pastoris* and purified using nickel-affinity chromatography. Michaelis-Menten kinetics reveals the AoC has a higher affinity towards soluble esters and is capable of hydrolyzing them in a more efficient manner. Furthermore, we have found that HiC has a higher thermostability and is capable of degrading polymers in a broad range of environments. Finally, molecular modeling has provided structural insight into the functional behavior of these molecules, expanding the repertoire of cutinases for biotransformations.

2. Probing Biology with Chemistry: Targeting the Ubiquitin Pathway for Novel Drugs

Ping Cao, Craig Leach., Medicinal Chemistry, Progenra, Malvern, PA, United States.

The Ubiquitin-proteasome pathway plays a critical role in number of normal cellular functions; for example, polyubiquitylation of proteins typically results in protein degradation by the proteasome and monoubiquitylation is involved in signal transduction and protein localization. Because of its fundamental importance, the pathway is particularly attractive for innovative and selective drug development; nevertheless, the lack of faithful biological assays has led to a lag in the utilization of this pathway for drug development. Ubiquitin is removed from proteins by deubiquitylating enzymes (DUBs) and many of these enzymes have been implicated in a wide range of pathologies including cancer, neurodegeneration, inflammation, metabolic disease and viral infection. Modulation of a particular DUB activity is predicted to result in a more targeted and selective therapy with reduced toxicity, as compared to global proteasome inhibition.

Progenra has been engaged in the discovery of small molecules that modulate a number of important DUBs. A novel, physiologically relevant, highly sensitive and scalable suite of assays has been developed to measure isopeptidase activities. Fortunately, similar assays can be applied to ubiquitin-like proteins (UBLs) such as SUMO, NEDD8 or ISG15; thus Progenra is able to exploit the assay platform for de-SUMOylase, de-NEDDylase and de-ISGinylases. More than 100 isopeptidases have been reported in the literature and Progenra has expressed and characterized the majority of DUBs in the human genome with this assay platform.

HAUSP/USP7 is one of the best validated DUB anti-cancer targets. This DUB is responsible for regulating MDM2, a ubiquitin ligase that modulates p53 levels. Potent and selective inhibitors of USP7 have been characterized and shown to be active in *in vivo* models. The success of this program provided a proof of principle that a potent, specific non-covalent cystein protease inhibitor can be developed. Data will be presented that describe the insights and approaches used to characterize USP7 inhibitors: (a) Development and application of a physiologically relevant isopeptidase assay

for HTS; (b) multiplex assays to screen more than one target per well;(c) suites of assays for rapid characterization of down stream effects secondary to USP7 inhibition; (d) development of families of DUBs for selectivity screening; and (e) development of other protease family assay tools for rapid counter screening.

3. Use of the Quartz Crystal Microbalance to Investigate Mechanical Viscoelstic Changes in HIV-1 Env upon Ligand Binding

Hyun-Su Lee,[1] Mark Contarino,[2] Isaac Zentner,[2] Umashankara Muddegowda,[2] Srivats Rajagopal,[2] Arne Schon,[3] Ernesto Freire,[3] Amos B Smith, III,[4] Irwin Chaiken,[2] **Lynn S Penn**.[1], [1]Department of Chemistry, Drexel Universtiy, Philadelphia, PA, United States; [2]Department of Biochemistry and Molecular Biology, Drexel University, Philadelphia, PA, United States; [3]Department of Biology, The Johns Hopkins University, Baltimore, MD, United States; [4]Department of Chemistry, The University of Pennsylvania, Philadelphia, PA, United States.

We have been exploring the usefulness of the quartz crystal microbalance to qualitatively detect conformational rearrangements of glycoprotein gp120 in response to exposure to various ligands. This glycoprotein, found on the envelope of the HIV-1 virus, is known to participate in coordinated interactions and conformational changes with host cell receptors that lead to virus entry into cells and consequent infection. For our investigation, the Env glycoprotein was immobilized on the surface of the vibrating quartz crystal, which is the sensing element of the quartz crystal microbalance. A flow cell was used for exposing the immobilized glycoprotein to solutions of different ligands, and the resultant changes in vibrational frequency and dissipation were monitored in real time. The data were interpreted in terms of changes in the viscoelastic properties of the layer, from which the general nature of conformational changes in the glycoprotein could be inferred. Both the monomeric and the trimeric form of the gp120 were investigated by means of the quartz crystal microbalance and preliminary results showed similar ligand-specific responses with both protein forms. Thus, it appears that the quartz crystal microbalance can provide a sensitive, label-free method to measure mechanical (viscoelastic) properties of the Env protein.

4. Self-catalyzed DNA depurination mediated by cruciform extrusion in closed circular DNA plasmid

Olga Amosova, Veena Kumar, Aaron Deutsch, Jacques R Fresco., Department of Molecular Biology, Princeton University, Princeton, NJ, United States.

DNA damage is a major threat to genome integrity and a source of disease-causing mutations. One of its main varieties is endogenous spontaneous generation of apurinic (AP) sites due to the loss of purine residues from the DNA backbone. Depurination rates vary widely across genomes, occurring with higher frequencies at so-called "depurination hot spots". Until now, the underlying mechanism for this wide variation has received little attention. Recently (1), we reported a site-specific self-catalytic G-depurinating activity in short (14-18nt) DNA stem-loop structures with a 5'G-T/A-G-G3' loop and T A or G C as the first base pair of the stem; the 5' G residue of the loop self-depurinates at a rate 10^4-10^5 faster than random "spontaneous" depurination. The remaining *base pair* sequence of the stem-loop catalytic intermediate has little effect on this activity. The human genome contains ~ 1, 250,000 sites distributed over all chromosomes, ~ 6 fold higher than expected on a random basis. Consequently, if such self-catalyzed depurination were to occur *in vivo*, it would be a major source of endogenously generated mutagenic apurinic sites. Self-depurination in genomic DNA requires a stem-loop catalytic intermediate to extrude as part of a cruciform from the DNA duplex. As a step towards demonstrating the potential of this mechanism *in vivo*, we have investigated its occurrence in supercoiled plasmid DNA *in vitro*. Sequences containing either the self-depurinating loop 5'G-T-G-G3' or a non-depurinating 5'T-T-T-T3' loop, surrounded by an $(A\text{-}T)_{16}$ stretch with the potential to form a stem-loop structure were cloned into a pUC19 vector. It is not irrelevant that the self-depurinating loop exhibited "resistance" to cloning and propagation in *E.coli*, i.e., very few clones were obtained, and those initially positive for the cruciform-forming self-depurinating insert

"lost" it when the culture was grown for large scale plasmid purification. Thus, sequencing of 7 clones containing the insert revealed acquired mutations in the loop of two of them, i.e., 5'G-T-G-G3' was replaced by non-depurinating 5'-G-G-T-G3'. In contrast, there were neither mutations nor cloning problems with the non-depurinating insert. Cruciform extrusion from the plasmid was confirmed and quantitated by its digestion with single-strand-specific Mung Bean (MB) nuclease, followed by restriction and equencing of the MB-generated fragments. Additionally, appearance of the apurinic site in the self-depurinating stem-loop was confirmed by digestion with apurinic endonuclease IV (AP), followed by primer extension and/or PCR amplification to detect the AP-generated strand break and its location. Self-catalyzed depurination was contingent on the supercoiled state of the plasmid, consistent with the presence of the extruded cruciform and its absence in the linear plasmid; and its rate of depurination was similar to that of the stem-loop-forming deoxyoligonucleotide. These results indicate that self-catalytic depurination is not unique to single-stranded DNA, and is relevant to the principal genomic form, that of the duplex.

1)Amosova, O., Coulter, R. and Fresco, J.R. Self-catalyzed site-specific depurination of guanine residues within gene sequences. *Proc Natl Acad Sci U S A* 2006; 103**:** 4392-4397.

5. Computational and experimental investigation of the formation of cyclodextrin 'host-guest' inclusion complexes

Clint Stalnecker, Jeffrey Wolbach, Pamela Artz., Department of Chemistry and Biochemistry, Albright College, Reading, PA, United States.

A host-guest carrier system for small molecules was explored as a model for studying the host-guest complex for small hydrophobic drugs. Three cyclodextrins (b-cyclodextrin, 2,6-O-methyl-b-cyclodextrin and g-cyclodextrin) were examined as host molecules for the inclusion complex because of their unique cylindrical structure and solubility properties. Cyclodextrins are cyclic oligosaccharides formed from various numbers of a-D-glucopyranoside subunits. The cyclodextrins used in this study consist of seven (b-cyclodextrin and 2,6-O-methyl-b-cyclodextrin) or eight (g-cyclodextrin) subunits. The 3guest molecules studied were benzene, difluorobenzene, vitamin K_3, caffeine, 5-fluorouracil, and 5-fluorotryptophan. These guest molecules were chosen to model drug interactions due to side chain arrangement, hydrophobicity, and/or actual therapeutic usage.

Inclusion complexes were investigated computationally by calculating the energy of complexation using the ONIOM method of the Gaussian '03 software. The ONIOM method has the advantage of allowing the host molecule, which is significantly larger than the guest molecule, to be treated using a different model chemistry than the guest molecule. Using different model chemistries for the two interacting molecules allows the computations to be conducted in a reasonable amount of time while retaining a high level of accuracy. The 'guest' molecules were studied in different cyclodextrin 'host' molecules in order to compare relative complex energies for the various cyclodextrin cavities. The calculated energies of the inclusion complexes were found to be between -10 and 10 Kcal/mol, which was in the expected range for favorable interactions to occur. These computational predictions were used as a basis for laboratory investigations.

NMR and UV-vis spectroscopy were the primary instrumental methods implemented to study the complexes in the laboratory. With NMR spectroscopy, host-guest complexes were analyzed through changes in chemical shift dispersion due to interaction and through the Rotating frame Overhauser Enhancement (ROE) to determine through space interactions of the host and guest molecules. Both proton and fluorine chemical shift changes were observed for fluorinated 'guest' molecules. The ratio of guest/host was varied from 1:5 to 1:1 with host in excess as well as with guest in excess. The trend in chemical shift changes with respect to the various ratios of guest/host elucidated inclusion complex stoichiometries and orientations. UV-vis spectroscopy was employed to find formation constants using the modified Benesi-Hildebrand equation. The formation constants found for guest molecules in different cyclodextrin hosts were compared with the trends predicted by the computational study. The computational results are complemented and expanded by the instrumental results. The

optimized computational and instrumental methods can be utilized to model and verify various host-guest inclusion complex systems, particularly pharmacologically interesting drugs in complex with cyclodextrins and cyclodextrin derivatives to affect drug protection and delivery.

6. Giant vesicles as model cells capable of asymmetric division and polarity

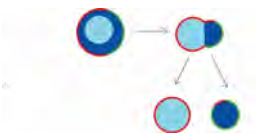
Meghan Andes-Koback, Christine D. Keating., Department of Chemistry, The Pennsylvania State University, University Park, PA, United States.

The long term goal of this research is to elucidate possible consequences of cell differentiation by developing an experimental model capable of generating and maintaining (bio)chemical polarity. Biological cells polarize, or asymmetrically organize sub-cellular components to opposite poles of the cell, in response to internal or external stimuli. Polarity is an essential step for cellular processes such as growth, division, differentiation, and migration. Researchers have examined a number of uni- and muticellular organisms to study polarity, but even the simplest cell is vastly complex.

Cell models are an alternative and useful tool for the examination of cellular structures such as the plasma membrane and for the elucidation of complex processes such as polarity. Giant lipid vesicles (GVs) are attractive cell models as they contain a lipid bilayer membrane surrounding an aqueous core, are cell sized, and can be optically visualized via microscopy and individually manipulated. The membrane of GVs provides an accurate biological membrane model, but the interior aqueous core of GVs poorly represents the crowded milieu found in biological cells.

Our model cytoplasm is a phase separated polymer solution. Aqueous two-phase systems (ATPS) have long been used for the separation of biomaterials as they provide a gentle, non-denaturing environment compared to conventional extraction methods. An ATPS is composed of two dissimilar polymers such as polyethylene glycol (PEG)/dextran, or a polymer and a salt, in water or buffer. A phase diagram is generated to determine the conditions under which phase separation will occur. Polymer weight percent, temperature and ionic strength are all factors that can be manipulated to control mixing or phase separation of the polymer solutions. When added to ATPS, biomolecules will partition into one of the two polymer phases.

We have utilized the separation and crowding properties of ATPS in a novel way, as a cytoplasm mimic for cell modeling studies. When encapsulated in GVs, an ATPS mimics the macromolecular crowding and chemical heterogeneity of biological cytoplasm. Biomolecules such as proteins or DNA can be localized to sub-regions of the vesicle interior by partitioning between the aqueous phases, and the degree of localization is controlled by slight adjustments in temperature, osmotic pressure, or pH. We are able to generate a simple model of polarity by exposing ATPS GVs to external stimuli. For instance, by increasing the external osmolarity and/or temperature of the system we can generate asymmetrically "budded" vesicles resembling pre-divisional bacterial cells. Exposure of ATPS-containing GVs to extremely hypertonic conditions results in fission of the budded vesicles to produce two non-identical daughter vesicles that are different in both membrane and interior composition, which will be further discussed here. [figure1]



7. Development of Artificial Antennas from the Self-Assembly of Peptide-Porphyrin Complexes

Gregory A. C,[1] Darius Kuciauskas.[2], [1]Department of Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States; [2]National Renewable Energy Laboratory, Golden, CO, United States.

Simple model systems designed to mimic the excitonic interactions between light harvesting complexes in plants have focused on the self-assembly of charged porphyrins in aqueous solution. These porphyrins require harsh conditions to self-assemble into excitonically coupled aggregates (pH < 1). Following a biomimetic approach, we are using synthetic polypeptides to induce porphyrin self-assembly to nanostructures. Because of their stability and favorable spectroscopic properties, peptide-porphyrin aggregates could be applied as light harvesting antennas in dye-sensitized nanocrystalline solar cells.

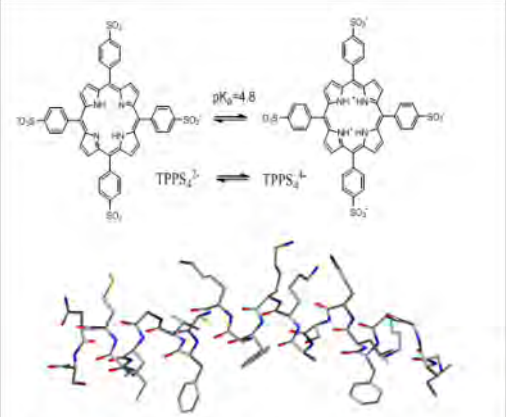


Figure 1. Tetra(4-sulfonatophenyl) porphyrin and α-helical structure of a cationic peptide.

In particular, polypeptides with positively charged side chains are likely to bind anionic porphyrins, such as $TPPS_4^{2-}$ (Figure1). This new antimicrobial 22 residue peptide has 9 lysine residues (positively charged at pH = 1.8). Normally under these pH conditions, $TPPS_4^{2-}$ does not form aggregates. UV-vis absorbance and Circular Dichroism (CD) spectra in the Soret band region (specifically peaks seen at at 490 nm, 434 nm, and 417 nm) indicate the formation of J aggregates when only 83 nM of peptide is added to 5 mM $TPPS_4$ solution ($[TPPS_4^{2-}]/[peptide] = 60$ or $[TPPS_4^{2-}]/[Lys] = 6.6$). This is indicative that peptide-porphyrin nanostructure formation is highly cooperative and binding constant is very high. A detailed spectroscopic study of peptide-porphyrin aggregates is presented using UV-vis, CD, fluorescence, and resonance light scattering. Ultrafast optical spectroscopy will be applied to study excited state dynamics, energy and electron transfer in these systems as well as resonance energy transfer experiments to probe the binding order of multiple $TPPS_4^{2-}$ molecules to the peptide.

8. Active site conformational changes in the metal dependent phosphatidylinositol-specific phospholipase C (PI-PLC) from Streptomyces antibioticus

Thomas L Selby., Chemistry, Bucknell University, Lewisburg, PA, United States.

The objective of this study focused on understanding the pH dependent conformational changes in the metal dependent phosphatidylinositol-specific phospholipase C (PI-PLC) from *Streptomyces antibioticus (*hereafter referred to as SaPLC). The first crystal structure produced by our lab was completed at pH 4.5 and showed a well-ordered active site that was very similar to the mammalian

enzyme. A second crystal form completed at high pH shows some significant conformational changes relative to the low pH structure that may relate to the conformational changes that appear to occur with calcium and inositol binding.

These conformation changes were corroborated using ^{15}N-HSQC NMR studies in an attempt to understand the global conformational changes associated with substrate and cofactor binding. Taken together, these two structures, and the binding data demonstrate a flexible active site that is able to adopt a specific conformation to support an inverted cyclic 1,6 inositol intermediate. Future studies include additional NMR experiments and fluorescent studies using terbium as an acceptor for the tryptophan fluorescence emission to better understand these active site conformational changes and elucidate a formal mechanism.

Inorganic Chemistry I

Sponsor: Division of Inorganic Chemistry

9. Molecular modeling of cysteine oxidation

Craig A Bayse., Department of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA, United States.

Oxidation of cysteine and other biological thiols is important to oxidative stress and biochemical signaling. We have modeled the activation barriers of the sequential oxidation of cysteine and of disulfide coupling using DFT and solvent-assisted proton exchange (SAPE). SAPE is a method of microsolvation that includes explicit solvent molecules in a gas-phase quantum-chemical model to represent the catalytic role of solvent in proton transfer processes. Activation barriers obtained using SAPE are lower than computational models that do not include explicit solvent molecules and generally consistent with experimental rate constants. For example, the DFT-SAPE activation energies for oxidation of cysteine sulfenic acid (CysSOH) to the sulfinic acid ($CysSO_2H$) to the coupling of the sulfenic acid and the sulfhydryl to the disulfide are consistent with the experimental observation that [O]:[Cys] ratios < 10:1 favors disulfide formation and > 10:1 favor over-oxidation.

10. Synthesis and characterization of narrow band gap V-VI hybrid semiconductors

Mojgan Roushan,[1] Hisato Yamaguchi,[2] Thomas J Emge,[1] Jing Li.[1], [1]Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, NJ, United States; [2]Department of Materials Science and Engineering, Rutgers University, Piscataway, NJ, United States.

We have developed a class of narrow band gap V-VI based inorganic-organic hybrid semiconductors for potential applications in energy conversion. Group V-VI binary compounds are well known for their high conductivity and thermoelectric properties. Our previous studies on the II-VI based hybrid systems show that inserting the organic amines in the II-VI crystal lattices decreases the thermal conductivity and as a result it may give rise to an increase in the figure of merit. While II-VI based hybrid semiconductors have relatively wide band gaps and may not be suitable for thermoelectric applications, V-VI based hybrid systems are more promising in this regard. Here, we report synthesis, crystal structure analysis, electrical and thermal conductivity study of several new hybrid structures containing one-dimensional chains or two-dimensional layers of V-VI motifs.

11. Molecular Based Synthesis of Solid State High Nuclearity Lanthanide Chalcogenide Clusters For Optoelectronic and Scintillation Applications

Brian F Moore,[1] Thomas Emge,[1] G A Kumar,[2] Richard E Riman,[2] John G Brennan.[1], [1]Department of Chemistry & Chemical Biology, Rutgers University, Piscataway, NJ, United States; [2]Department of Material Science & Engineering, Rutgers University, Piscataway, NJ, United States.

The room temperature synthesis and characterization of a new series of Heptadecanuclear lanthanide chalcogenide ($(Py)_{16}Ln_{17}Se_{18}$ $(SePh)_{16}Na$) clusters, will be presented, (Ln = Ce, Pr, Nd; Py = Pyridine). The 17 member core consists of a single Ln(III) center encapsulated by 10 m_3 Se^{2-} ions that are then surrounded by Ln, with the surface of the cluster capped with additional Se^{2-}, py, and SePh. The ($(Py)_{16}Nd_{17}Se_{18}$ $(SePh)_{16}Na$) system exhibits NIR emissions with the highest Quantum Efficiency (Q.E.), of any molecular based lanthanide system to date, while the ($(Py)_{16}Ce_{17}Se_{18}$ $(SePh)_{16}Na$) system shows remarkable potential as a highly efficient scintillator.

12. Mechanism of Dioxygen cleavage by Low valent b-diketiminato chromium compound

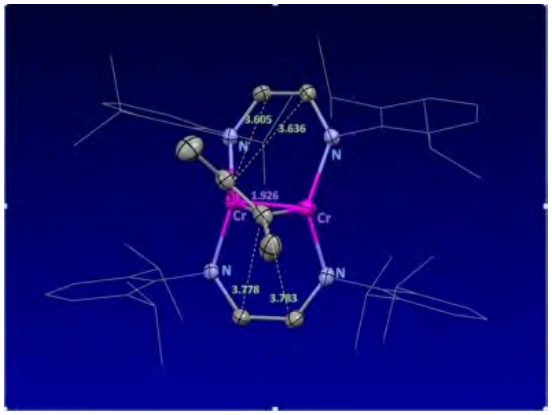
Fang Dai,[1] Leonard A MacAdams,[2] Glenn P. A. Yap,[1] Klaus H Theopold.[1], [1]Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States; [2]KiON Corporation, Huntingdon Valley, PA, United States.

Monomeric Cr(V) dioxo compound (i-$Pr_2Ph)_2$nacnac$Cr(O)_2$ (**1**), can be formed by treatment of monomeric low valent Cr acetylene complexes, e.g., ((i-$Pr_2Ph)_2$nacnac)Cr(h^2-$Me_3SiCCSiMe_3$) (**2**) with dioxygen . The mechanism of this oxygen cleavage process was studied experimentally. *In situ* IR spectra show a gradual change from starting material **2** to **1** in toluene or THF solution. Upon treatment with a $^{16}O_2/^{18}O_2$ mixture, mass spectroscopy indicated statistical formation of ((i-$Pr_2Ph)_2$nacnac)Cr($^{16}O)_2$, ((i-$Pr_2Ph)_2$nacnac)Cr($^{18}O)_2$ and ((i-$Pr_2Ph)_2$nacnac)Cr(^{16}O) (^{18}O) in approximately 1:1:2 ratio. Reaction of **1** with **2** formed an unusual asymmetrical bridging oxo compound, namely [((i-$Pr_2Ph)_2$nacnac)Cr]$_2$ μ-$O)_2$ (**3**). **3** react with excess dioxygen to yield **1**. Reaction of **1** and PPh_3 slowly formed $OPPh_3$ and **3**.

13. [2 + 2] Reactions of quintuple bonds Cr compounds with alkynes

Jingmei Shen, Glenn P. A. Yap, Klaus H Theopold., Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States.

Quintuply bonded Cr dimmer, [(Ar-N=C(H)-(H)C=N-Ar)$_2Cr_2$] (Cr-Cr=1.80Å) (where Ar = 2,6 – diisopropylphenyl ("iPr")), reacts with acetylenes RCºCR in hydrocarbon solvents to form 1:1 adducts ($^{H}L^{iPr}{}_2Cr_2$)(RCCR), where R= Me, Et, Ph, CF_3. The rates of the decomposition of the adducts are decreasing in the order of CF_3CºCCF_3 > PhCºCPh > EtCºCEt > MeCºCMe. The single crystal X- ray structures have been obtained. All the complexes feature short Cr-Cr distances of 1.926 - 1.936 Å and elongated multiple C-C bonds of 1.313 - 1.436 Å. For R= Me, Et, Ph, the structures show distinctly skewed bridging alkynes with respect to the Cr-Cr axis, q=24°,36°,42°. These three complexes were also characterized by infrared, UV-vis, MS and NMR (^1H, ^{13}C) spectroscopes. Variable temperature NMR spectroscopic studies of the adducts for R= Me, Et indicate the occurrence of a fluxional process. Interestingly, the CF_3CºCCF_3 adduct has the alkyne bonded not only to the two Cr centers but also to the backbone of the diimine ligand. This reactivity is a reflection of the nature of HOMO of the starting material which is essentially ligand localized.



14. Synthesis of the sulfur rich Eu(III) compound, $(py)_6Eu_2(SS)_2(OC_6F_5)_2$

Kieran Norton, John Brennan, Thomas Emge., Chemistry and Chemical Biology, Rutgers The State University of New Jersey, Piscataway, NJ, United States.

The novel dimer $(py)_6Eu_2(SS)_2(OC_6F_5)_2$ has been synthesized. The tendency of europium ions bound to sulfur to take the 2+ oxidation state is balanced by the oxidizing strength of the aryloxy ligands. The resulting compound is deeply colored due to the allowed ligand to metal charge transfer from the disulfido. The electronic properties of this unsual class of compounds will be discussed as well as the difficulties in sysnthesis due to the thermodynamic drive towards disproportionation.

15. Monolithic porous electron-rich covalent organophosphonitridic frameworks

Kai Landskron, Paritosh Mohanty., Chemistry, Lehigh University, Bethlehem, PA, United States.

Hexachlorocyclotriphosphazene (HCP) and diaminobenzidine (DAB) have been polycondensed in DMF and DMSO to produce porous electron-rich phosphonitridic frameworks. In DMF the materials are obtained as spherical non-porous particles with irregular size distribution. In the presence of PVP the size of the spheres becomes nearly monodisperse. The size of the particles can be varied between 80 and 1500 nm by adjusting the concentration of DAB and HCP in the solution. When DMSO is used as solvent shape-stable monolithic gels form which are micro-macroporous and exhibit surface areas of up to 850 m^2 g^{-1}. The gels show high CO2 sorption capacities of up to 3.5 mmol/g at 1 atm and 273 K. The CO2 adsorption is fully reversible. The materials exhibit a CO2 : N2 gas selectivity of 86: 1 and are thermally stable up to ca. 700 K in air.

16. Late transition metal complexes supported by tris(3-amino-5-methylpyrazolyl)borate ligands

Ismael Nieto,[1] Elizabeth T Papish,[1] Matthias Zeller.[2], [1]Department of Chemistry, Drexel University, Philadelphia, PA, United States; [2]Department of Chemistry, Youngstown State University, Youngstown, OH, United States.

We have developed a novel route for the synthesis of tris(3-amino-5-methylpyrazolyl)borate ligands that incorporate alkyl amino substituents such as tert-butyl-amino. These ligands are readily transferred to zinc and nickel, providing access to coordinatively unsaturated metal halide complexes supported by a trigonal platform of nitrogen donors. Further functionalization is planned by substituting the metal bound halide using a salt elimination approach, through the treatment with various nucleophiles and bases. It is anticipated that unusual metal complexes can be stabilized by the second coordination sphere influences from the alkyl amino substituents and the unique electronic properties of this new ligand.

17. Artificial Photosynthesis- Photocatalyzed Conversion of CO_2 to CH_4 by Visible Light

Edward G Look,[1] Harry D Gafney,[1] Nicholas F Borrelli.[2], [1]Department of Chemistry and Biochemistry, Queens College, CUNY, Flushing, NY, United States; [2]Sullivan Park, Corning, Inc, Corning, NY, United States.

Photocatalytic reduction of CO_2 to CH_4 occurs in nanoporous Vycor glass doped with tungsten oxides with coadsorbed water providing the hydrogen and reducing equivalents. The energetics of CO_2 reduction suggest that it can driven by visible and near-IR light. However, the absorption characteristics of the monoclinic and orthorhombic WO_3 formed in polished Vycor samples limit absorption, hence photocatalytic activity, to $\leq$350-nm light. In unpolished nanoporous Vycor, the photochromic form of tungsten oxide forms. It contains both W^{5+} and W^{6+} thereby giving rise to intervalence charge transfer and/or polaron absorption occurring in the visible and extending into the near-IR. Excitation of the photochromic oxide with light of $\geq$437 nm drives the conversion with CH_4 evolution occurring with a quantum efficiency of $2\pm1 \times 10^{-4}$. Formation of the different oxides is attributed to a competition between oxidation and aggregation that is determined by structural differences between the interior and exterior volumes of the nanoporous Vycor.

Physical Chemistry

Sponsor: Division of Physical Chemistry
Organizer: Cecil Dybowski

18. Theoretical analysis of the molecular dynamics of ionic liquids

Mark N. Kobrak., Department of Chemistry, Brooklyn College of CUNY, Brooklyn, NY, United States.

Room-temperature ionic liquids, salts that are molten at ambient temperature, are a recently-discovered class of materials of growing technological interest. But many questions remain about the nature of their inter-ion interactions, and how their chemical structure affects their microscopic dynamics. We take a chemical physics approach, and show that relatively simple electrostatic principles can be used to interpret their behavior.

19. Hole mobility for thin-film organic molecular solids in the presence of defects or surface adsorbates: Theory and implications for gas detection

Matthew L Rossi, Karl Sohlberg., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

Improved chemical sensors have the potential to improve national security through simplified detection of explosive agents. Existing sensors generally utilize spectrophotometric methods, which can require bulky instrumentation. A possible alternative it to use changes to hole mobility in a thin-film organic material upon exposure to an analyte gas as the basis for detection. We report a computational procedure for predicting changes to mobility in the presence of an adsorbate. The method is based on an implementation of Marcus hop rate theory. The adsorbate is treated as a defect and the relation between defect density and mobility is studied. We have characterized simple oligoacene species, (especially naphthalene and pentacene) and for validation, the unrelated species a,w-dihexylquaterthiophene (DH4T), a molecule proposed for use in molecular electronics due to observed mobility characteristics. Our results are consistent with published studies of the relationship between mobility and defect density and yield insight into the electronic structure characteristics that render a material suitable for use as a probe of the presence of an adsorbate.

20. Substitution effect on the charge mobility of metal free phthalocyanine

Choongkeun Lee, Karl Sohlberg., Chemistry, Drexel University, Philadelphia, PA, United States.

Charge mobility is the one of the most important parameters to characterize a charge conducting organic materials. Usually, in a molecular crystal, charge mobility is assumed to be approximated by Marcus-Huss theory. There are two parameters that can, in theory the reorganization energy and the coupling matrix element, be used to control the mobility. A substitution is a good way to change the two parameters at the same time. We have employed electronic structure methods to describe the effect of substitution on charge mobility in phthalocyanine, which is the one of the discotic(disk like) materials of interest for use in organic electronic devices. The predicted mobility of a substituted phthalocyanine is found to be more strongly depended on the coupling matrix element than on the reorganization energy. The details of the effect of substitution on charge mobility will be presented.

21. Inhibition of histidine ammonia lyase by 8-methoxypsoralen and psoralen oxidized photo-products

John T Reilly, Trista T Tryner, Kyle A Troester, Dominick A Vitale, Tiffiany T Risher., Department of Chemistry and Physics, Coastal Carolina University, Conway, South Carolina, United States.

The effect of 8-methoxyposralan-UVA therapy on the catalysis of histidine to trans-urocanic acid by histidine ammonia lyase (HAL, EC 4.3.1.3) was examined using an enzymatic assay from Sigma-Aldrich where the growth of the trans-urocanic acid peak at 277 nm was monitored. A Rayonet Photochemical Mini Reactor (Model RMR-600) equipped with eight, 3500 angstrom light sources and a custom UVA filter (Model S-BAL3 2.9 mm), from the Solar Light Company, were used to expose various reaction mixtures to broadband UVA light and UVA/UBV light. A UV-Vis spectrophotometer (Model Shimadzu UV 2540) with a temperature-controlled cell holder (Model TCC240) was used to monitor the growth of the trans-urocanic peak. Results of dark-binding experiments of 8-methoxypasoralen in denatured ethanol indicate no inhibition of enzyme activity due to ethanol but non-competitive inhibition due to 8-methoxypsoralen. The effects of pre-irradiated 8-methopxypsoralen, with both broadband UVA and UVA/UVB, indicate that inhibition was due to psoralen-oxidized-photoproducts. Inhibition of HAL was found when exposed to broadband UVA/UVB but not when exposed to broadband UVA.

22. Thermochemical Characterization of Biodiesel Fuels Synthesized from Various Oil Feedstocks

Michael Bell, **Marc L Richard**., Chemistry Program, The Richard Stockton College of New Jersey, Pomona, NJ, United States.

iodiesel fuels were synthesized by means of transesterification in the presence of an alkali catalyst. Four different vegetable oil feedstocks were used for this study: soybean, olive, peanut, and waste peanut oils. Thermochemical properties including phase transition temperatures and heats of combustion were measured. The cloud points of the synthesized fuels were measured using differential scanning calorimetry. Heats of combustion were measured using bomb calorimetry. Biodiesel derived from peanut oil has a higher calorific value than that of biodiesel derived from waste peanut oil as well as olive oil biodiesel. The heat of combustion of peanut oil biodiesel was 34.69 ± 0.16 kJ/ml compared to waste peanut oil and olive oil biodiesels with heats of combustion of 34.34 ± 0.07 kJ/ml and 34.21 ± 0.23 kJ/ml respectively. On average the biodiesel fuels synthesized in this work produced a heat of combustion 14% less than that of literature values for petroleum diesel fuel and a cloud point 24°C higher.

23. Effects of viscosity on phase separation of liquid mixtures with a critical point of miscibility

Filomena Califano., Chemistry and Physics, St. Francis College, Brooklyn, NY, United States.

After quenching a high-viscosity partially miscible critical liquid mixture to a temperature far below the critical point, it was observed the formation of rapidly coalescing droplets, whose size grew linearly with time, indicating that phase separation process is driven by convection. As predicted by the diffuse interface model, this experimental work showed that the viscosity did not have any effect on the growth rate and the speed of the nucleating droplets. Eventually, when the droplets size reached its critical length, they started to sediment and separated by gravity. At this point, the viscosity influenced the settling speed and the total separation time.

24. Structural and size effects in reactions of CO on O- and NO- covered Ir

Wenhua Chen, Robert A Bartynski., Department of Physics and Astronomy, and Laboratory for Surface Modification, Rutgers, The State University of New Jersey, Piscataway, NJ, United States.

Temperature programmed desorption (TPD) has been used to investigate reactions of CO on planar Ir(210) and nano-faceted Ir(210) with tailored facet size (5-14nm) in the absence and presence of pre-adsorbed O or NO. TPD spectra of CO from planar and faceted Ir(210) are similar. However, TPD spectra of CO2 from CO on the two surfaces pre-covered by O or NO exhibit substantial differences: the onset CO2 desorption temperature is ~100K lower on planar Ir(210) than on faceted Ir(210) at low O coverage or low NO exposure, indicating that planar Ir(210) is more active than faceted Ir(210) for CO oxidation. Moreover, measurements show that faceted Ir(210) with smaller facet size is more active than that with larger facet size. This is the first observation of nanoscale size effects in oxidation of CO by NO on an unsupported catalyst with well-defined surface structure and controlled size. In contrast, no evidence has been found for size effects in the oxidation of CO by O on the same faceted Ir(210) (5-14nm). Our results demonstrate that faceted Ir(210) is a novel nanoscale model catalyst for exploring size effects in surface chemistry in the absence of any support material and without changes in catalyst morphology induced by the changes in its size: two effects that are common to supported catalysts. This work is supported by the US Department of Energy, Office of Basic Energy Sciences (Grant No. DE-FG02-93ER14331).

25. Time evolution of an electron in a simple system

Hae-Won Kim,[1] Karl Sohlberg.[2], [1]Deaprtment of Chemistry, Penn State Abington, Abington, PA, United States; [2]Department of Chemistry, Drexel University, Philadelphia, PA, United States.

We are studying the time evolution of an electron in a two state oscillation system. We can follow the flow of charge for a localized electron in a time-dependent wavefunction by observing how the AO expansion coefficients evolve in time. We are interested in the probability that a particular orbital has been occupied at least once between time t=0 and time t=t. Standard methods give a result that is vanishingly small as the sampling time-step goes to zero, which is not a satisfactory result. We use conditional probability to explore alternative interpretations. We start by considering a simpler analogous problem and apply the result to a two state oscillation system.

26. New empirically corrected AM1 method: Accurately and efficiently modeling supermolecular complexes

Michael Foster, Karl Solhberg., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

Modeling systems that are governed by van der Waals (dispersion) interactions using empirically corrected DFT methods is becoming increasingly popular due to the promise of CCSD(T) level accuracy at the computational cost of DFT. Although, DFT methods are computationally efficient in comparison

to the CCSD(T) method, currently, structural optimizations using DFT methods are generally only feasible for systems of less than a few hundred atoms. In order to model much larger systems, empirically corrected semi-empirical methods appear to be an attractive alternative. As with most common DFT methods, the popular semi-empirical methods (e.g. AM1) also do not model long-range dispersion, (and therefore an empirical correction term is desirable) but this is not their only shortcoming. For weakly interacting systems, hydrogen bonding also poses a concern. AM1-D+, a new empirically corrected AM1 method, achieves significant improvements in these areas by utilizes two empirical correction terms, one for dispersion and one for hydrogen bonding interactions. AM1-D+ has been tested on the popular S22 database, achieving kilocalorie accuracy based on root mean square error. This represents a significant improvement over the AM1 method itself (RMSE = 8.5 kcal/mol). AM1-D+ also improves over the previously reported AM1-D method (RMSE = 1.23 kcal/mol), and does so with substantially less parameterization and without modification of the original AM1 parameters. This new method allows supermolecular complexes to be accurately and efficiently investigated.

27. Synthesis, physical characterization, and toxicity studies of a series of room temperature ionic liquids based on 1-methylimidazole

Evgenia Gasumova, **Bradley Zale**, **Hueanh Tran**, **Marc L Richard**., Chemistry Program, The Richard Stockton College of New Jersey, Pomona, NJ, United States.

Interest in room temperature ionic liquids has steadily increased over the past several years. These materials are seen as possible replacements for volatile organic solvents in an effort to be more "green". A series of room temperature ionic liquids have been synthesized using 1-methylimidazole and various alkyl halides. The liquids have been characterized to determine viscosity and thermal stability. The toxicity of the synthesized materials has been evaluated by exposing radish seeds to various concentrations of ionic liquids and measuring growth over several days.

As expected, the longer alklyl chain length leads to increased viscosity yet has little effect on the thermal stability. The ionic liquids inhibit growth in radish seeds, with the longer alkyl chain length having a larger degree of toxicity. These results call into question the "green" label which has been attached somewhat universally to ionic liquids.

Organic Chemistry I

Sponsor: Division of Organic Chemistry

28. Effects of cis and trans Isomers of alpha-Linolenic Acid on the Formation Kinetics of Cyclic Fatty Acid Monomers

Amélie Desmarais,[1] Jean-Louis Sébédio,[2] Joseph Arul,[1] **Paul Angers**.[1], [1]Food Science and Nutrition, Université Laval, Quebec City, Québec, Canada; [2]Unité de Nutrition Humaine, Institut National de la Recherche Agronomique (INRA), Clermont-Ferrand, France.

Cyclic fatty acid monomers (CFAM) are formed at low levels in edible fats and oils during thermal processing operations such as frying or refining, and inevitably become part of the diet. However, the kinetics involved in their formation is not well known. The objective of the present study was to evaluate the kinetic effects of *cis* and *trans* isomers on cyclization reactions involved in the degradation of alpha-linolenic acid (Ln). Geometrical isomers of Ln were obtained from all-*cis* Ln by nitric acid treatment which promoted the formation of mono- and di-*trans* isomers. These were separated by families of isomers using silver nitrate-silica gel chromatography. All-*cis* Ln and mono and di-*trans* isomers were heat treated at 275°C in hexadecane for periods from 2 to 24 h, and CFAM formation was monitored by GC and GC-MS. The results show that the presence of a single *trans* double bond at C9 or at C15 results in the formation of CFAM at an accelerated rate, compared to the corresponding

cis isomers, resulting in the formation of higher levels of CFAM over shorter time periods. This work suggests that the use of polyunsaturated vegetable oils over extended periods for thermal processing of food may result in the formation of CFAM, in particular if mono *trans* isomers are present in the oil.

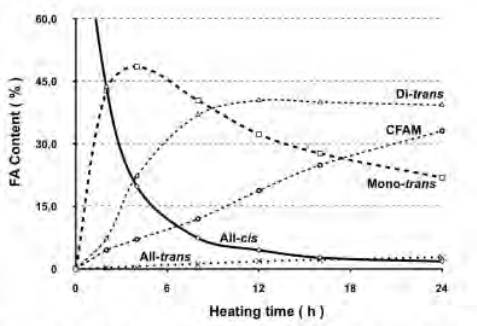
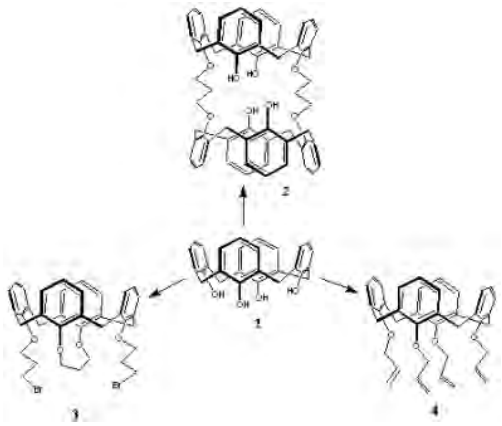


Figure 1. Cyclic fatty acid monomer (CFAM), and mono- and di-*trans* isomer formation during heat-treatment at 275˚C of alpha-linolenic acid (all *cis*).

29. Synthesis of Calixarenes Functionalized at the Lower Rim as Potential Host Compounds

Shimelis T Hailu, Paul F Hudrlik, Anne M Hudrlik., Department of Chemistry, Howard University, Washington, DC, United States.

In the course of a program to synthesize molecular capsules, the synthetic intermediates were investigated to explore their potential use as complexing agents or host compounds for various guests. Calixarene **1** was treated with 1,3-dibromopropane using different bases and solvents. Bridged calixarene **3** was isolated from the reaction of calixarene **1** and K_2CO_3 in CH_3CN with excess 1,3-dibromopropane at reflux. (In addition, the expected 26,28-bis(3-bromopropoxy)-25,27-dihydroxycalix[4]arene (**5**) was observed.) When the reaction was run using a smaller amount of 1,3-dibromopropane, biscalixarene **2** and calixarene **5** were isolated. On the other hand, treatment of calixarene **1** with 1,3-dibromopropane in DMF in the presence of NaH produced calixarene **4** in which four allyl groups have been introduced onto the lower rim. In considering the mechanism of this interesting reaction, an elimination reaction is apparently favored over a substitution reaction. These compounds were analyzed by IR, ^{1}H NMR, ^{13}C NMR, and MALDI-TOF MS to assign their structures. In addition, the structure of the allylcalixarene **4** was confirmed by an independent synthesis from calixarene **1** and allyl bromide, whereas for bridged calixarene **3**, an X-ray structure was obtained. It shows the bridged calixarene compound **3** has a flattened cone conformation. The conformation is apparently fixed by a three-carbon bridge linking the distal phenolic oxygens. Biscalixarene **2**, in which two calixarene units are linked by two $CH_2CH_2CH_2$ bridges, has free binding sites, and has potential applications as a complexing agent.

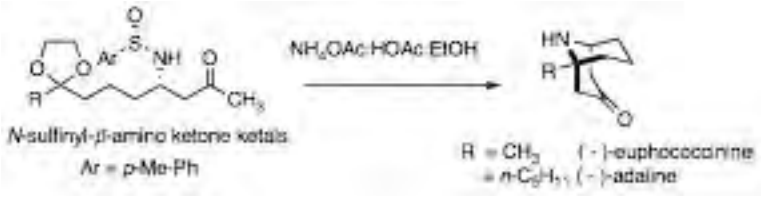


30. Cascade cyclization of acyclic N -sulfinyl b -amino ketone ketals

Franklin A. Davis, **Ram Edupuganti**., Department of Chemistry, Temple University, Philadelphia, PA, United States.

The 9-azabicyclo[3.3.1]nonane ring skeleton, a homologue of the medicinally important tropane skeleton, is common to several insect- and plant-derived alkaloids. For the asymmetric synthesis of substituted tropinones, we recently introduced acyclic *N*-sulfinyl *b*-amino ketone ketals as novel building blocks.[1,2] When the acyclic *N*-sulfinyl *b*-amino ketone ketals are subjected to NH_4OAc:HOAc buffer solution, afforded homotropanones (-)-euphococcinine and (-)-adaline [figure1] *via* biosynthetic imine intermediate.[3]

[1]Davis, F. A.; Theddu, N.; Gaspari, P. M. *Org. Lett.* **2009**, *11*, 1647. [2]Davis, F. A. *J., Org. Chem.* **2006**, *71*, 8993. [3]Davis, F. A.; Edupuganti, R. *Org. Lett.* **2010**, *12*, 848.



31. New synthetic method for 5'-capped oligoribonucleotides

Elizabeth Veliath, Barbara L. Gaffney, Roger A. Jones., Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, NJ, United States.

Capped RNA has a unique 5'-end structure containing a terminal N7-methylated guanosine that is joined via a triphosphate bridge to the 5'-OH of all eukaryotic mRNAs. This structure plays a vital role in regulating RNA maturation, processing, transport and translation, but capped RNA is extremely difficult to synthesize chemically due to its instability.[1] A new protection strategy will be reported that uses a lipophilic dimethoxytrityl (DMT) group at the N2 of the N7-methylated guanine activated intermediate. The DMT group allows separation of the GDP intermediate from the excess phosphate during the reverse-phase purification of the capping reagent. Additionally, the lipophilic DMT group increases the final capping reagent intermediate's solubility in organic solvents which facilitates the coupling reaction; and more importantly, allows efficient purification of the final capped RNA on reverse phase HPLC. This new method has been used to synthesize and purify the unmodified cap structure m^7GpppG, the individual diastereomers of the a thiophosphate analog m^7Gppp(s)G, and mixed sequences of m^7Gppp-(2'-OMe-GAUGC)$_2$ and m^7Gppp-(2'-OMe-GUAUC)$_4$.

(1) Mikkola, S., Salomaki, S., Zhang, Z., Maki, E., Lonnberg, H. *Current Organic Chemistry* **2005**, *9*, 999-1022.

32. New route to g,d-unsaturated nitro compounds via [3,3]-sigmatropic rearrangement of O-Allyl nitronic esters

Alma Pipic, Peter Wade., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

O-allyl nitronic esters, readily obtained from tin(IV)-catalyzed Diels-Alder reaction, undergo thermal (20-90°C) rearrangement to g,d-unsaturated nitro compounds via [3,3]-sigmatropic rearrangement. The O-allyl nitronic ester rearrangement provides stereocontrolled access to diastereomeric 1,2,3,4,4a,5,6,7-octahydro-5-nitronaphthalene derivatives. Thermal isomerization of one cis isomer to a trans-2-nitro-3-phenyl products was observed at higher temperatures (150°C). The rearrangement products are also readily obtained through a direct Diels-Alder reaction, which results in a

mixture of diastereoisomers. The difficulty in separating diastereoisomers is avoided by selectively rearranging nitronic esters to corresponding nitro compounds. This is a newly discovered rearrangement mechanism of nitronic esters, and it has been successfully applied to two systems

33. Surfactant modified carbon nanotubes: Effect of surfactant and surfactant content on electrical conductivity

Juliet Hahn., Department of Chemistry & Biochemistry, University of Delaware, Newark, DE, United States.

Thin films of carbon nanotubes modified by a number of surfactants are being investigated for electrical conductivity. The effect of the surfactant on electrical conductivity is being investigated. The amount of surfactants in surfactant modified carbon nanotubes on electrical conductivity is also being investigated. A number of spectroscopic techniques including FTNMR, FTIR, UV-Vis spectra are being used to develop a method to quantify the amount of surfactants in the carbon nanotube thin films. Potential applications of the carbon nanotube thin films are solar energy collectors, and new electrical materials.

34. Skin cancer reaction in a test tube: Solvent effect on the photodimerization of a derivative of thymine

Juliet Hahn., Department of Chemistry & Biochemistry, University of Delaware, Newark, DE, United States.

Orotic acid photodimerization is being used to model the photodimerization reaction implicated in skin cancer. Orotic acid, a derivative of uracil/thymine, is a stand alone DNA base unlinked by sugars and phosphates. The photodimerization reaction in a number of solvents is being used to investigate the Õ stacking vs. hydrogen bonding effect on the photodimer stereoisomer generated. The photodimerization reaction was followed kinetically in a number of solvents using NMR. A fundamental understanding of why certain fragments of DNA are especially prone to photodimerization resulting in skin cancer may lead to a differnt approach to preventing skin cancer.

35. Aromatic ring strain and carbon 13 NMR

Donald D Clarke,[1] James Foresman.[2], [1]Department of Chemistry, Fordham University, New York, NY, United States; [2]Department of Physical Sciences, York College of Pennsylvania, York, PA, United States.

Carbon 13 nmr signals are usually assigned using additivity rules. That this method fails in strained systems is well established for aliphatic compounds. We observed a failure in the aromatic system 2-nitroaniline which we attempted to explain as due to H bonding. However this was ruled out because its N,N-dimethyl derivative showed a similar anomaly. More recently we found that 2-aminoacetophenone showed the same type of anomaly, i.e. signals at C-4 and C-6 were reversed over the predictions from additivity rules. This suggested that the phenomenon was due to strong electron withdrawal properties of nitro and acetyl groups. To test this idea further, 2-cyanoaniline [anthranilonitrile] was examined and unlike the first two compounds found to fit the additivity rule. Since the CN group is not only strongly electron withdrawing but also has very low steric requirements we concluded that the results with 2-nitroaniline and 2-acetylaniline and not with anthranilonitrile must be due to steric effects. A classic example of anomalous aromatic substitution is the Mills-Nixon effect (1930). 5-Hydroxyindan gave an opposite substitution pattern as compared to the analogous 6-membered tetrahydronaphthol derivative. They explained their result as due to the favoring of one Kekule structure over another. Pauling said this explanation contradicted quantum chemical calculations and blamed it on strain in the phenyl ring of indan. This topic has been discussed over the ensuing decades with experimentalists and theoreticians disagreeing sharply. Recently Stanger developed a theoretical justification for Mills and Nixon's observations and renamed it Strain Induced Bond

Localization [SIBL]. We observed that the C13 nmr spectrum of 5-indanol showed the same type of deviation from additivity rules as does 2-nitroaniline when our experimental data was compared with assignments in the Japanese database [SDBS]. 5-Methoxy and 5-nitroindan behaved similarly. Indan itself also gave results contrary to the assignments in SDBS. In all of these cases calculations of C13 chemical shifts using Gaussian agreed with experimental conclusions arrived at by 2D nmr. Supported in part by a research grant from the Fordham University Research Council and by an NSF grant for a 300 MHz nmr spectrometer.

36. Efficient Synthesis of Vinyl allene and Its Application to Carbocycles

Subin Choi, **Su-sung Oh**, Phil Ho Lee., Chemistry, Kangwon National University, Chuncheon, Kangwon-do, Republic of Korea.

Because allene is a very interesting compound having a hybrid character of C-C double and triple bond, vinyl allenes have been recognized as versatile building blocks in organic synthesis. In particular, vinyl allenes take part in not only the Diels-Alder reaction as the 1,3-diene moiety but also transition metal-catalyzed organic reactions, affording efficient synthetic methods for complex ring compounds. However, because it is not easy to effectively prepare a variety of vinyl allenes, its application to organic reactions has been limited despite the potential of vinyl allenes in organic synthesis. Although vinyl allenes were used in the Diels-Alder reactions, development of synthetic method of cyclic compounds having *exo*-methylene group is still required due to its utility in synthesis of natural products with biological activities. Recently, we have demonstrated that cyclic compounds having *exo*-methylene group were selectively produced through the Diels-Alder reaction of vinyl allene with various dienophile in good to excellent yields.

37. Nucleomistry video lectures: Humorous internet presentations teaching nuclear chemistry

Isaac Shomer., Nucleomistry Research Institute, Arlington, Virginia, United States.

Presented here is an overview of the "Nucleomistry" video lecture series. These videos explain various concepts in nuclear chemistry, such as atomic structure, radioactivity, and the nuclear shell theory in a manner that is intended to be humorous. Nucleomistry lectures include minimal mathematics and a heavy use of analogies, and are intended to be understood by a wide range of audiences. Many of the analogies used to explain said concepts are to popular culture. For example, the rapper Kanye West is lampooned in an explanation of beta decay in Nucleomistry Lecture 7.

Lectures range from about 10 to about 40 minutes in length, with the median length being about 20 minutes. Also included in the nucleomistry lecture series is a song parody of "Part of Your World" from Disney's "The Little Mermaid" extolling the promise of nuclear fusion as a source of energy.

The Nucleomistry lecture series may be found at the following web address: http://www.scivee.tv/user/9658

38. Regio-selective electrophilic fluorination of pyridine derivatives with SelectfluorTM

Daniel Smith,[1] Jianqing Li,[1] Bang-Chi Chen,[2] John Kadow,[1] Balu Balasubramanian,[2] Nicholas Meanwell,[1] Joel C. Barrish.[2], [1]Department of Chemistry, Bristol-Myers Squibb, Wallingford, CT, United States; [2]Department of Chemistry, Bristol-Myers Squibb, Princeton, NJ, United States.

Fluorinated pyridines are important intermediates for many bioactive compounds. In this poster, we wish to present a convenient regioselective electrophilic fluorination of 2-hydroxy pyridine derivatives using SelectfluorTM and its application for the synthesis of 4-fluoro-7-bromo-6-azaindole, a key intermediate of HIV drug candidates.

39. Study of student learning in a conductivity lab using real world samples

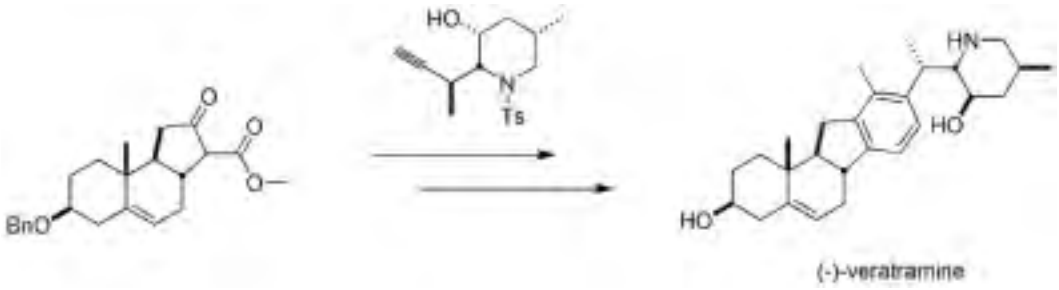
James C Rieben Jr., Daniel B. King., Chemistry, Drexel University, Philadelphia, Pennsylvania, United States.

When designing a laboratory experiment, it is important to consider the content that is to be taught, as well as how that content is to be presented to the student. The effects of both prior knowledge (i.e., does the student know the expected result) and relevance (i.e., how the topic can be applied to the student's everyday life) have been studied for a group of over 600 students performing a conductivity experiment in a general chemistry course. Four experimental variants were employed in an attempt to yield a quantifiable measurement of the effects of both relevance and prior knowledge on student learning. Initial results have shown that by using relevant samples the students show a higher amount of content learning that reinforces their correct ideas and corrects their misconceptions. With the removal of prior knowledge, there is a noticeable difference seen in the students' ability to answer one evaluation question.

40. Towards the total synthesis of (-)-veratramine

James F. Berry, Peter W. DeMatteo, Douglass F. Taber., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

The *Veratrum* alkaloids are a class of compounds isolated from the liliaceous plants of the family Melanthiaceae, native to North America and Europe. Veratramine is a member of this family whose challenging structural framework makes it an attractive target for total synthesis. Veratramine has been investigated for its inhibition of the cardioacceleration response to adrenaline. It is also currently being investigated for its inhibitory role of the hedgehog (Hh) pathway. Several malignant cancers propagate through this pathway, including basal cell carcinoma, pancreatic and prostate cancer. A tricyclic beta keto ester intermediate can be coupled with a functionalized alkyne, and after a few additional transformations, will afford (-)-veratramine.



41. Progress toward the synthesis of a functional Bis-peptide Oligomer that mimics Carbonic Anhydrase

Sharad Gupta, Christian E Schafmeister., Department of chemistry, Temple University, Philadelphia, PA, United States.

Proteins, 'The nanomachines of nature' are the finest illustration of 'bottom-up' assembly. The efficiency and versatility of this natural assembly process is astonishing. However, it is extremely difficult to emulate nature and chemically assemble protein size macromolecules. The biggest hurdle being 'The Folding Problem': For a protein to attain its native state, the linear peptide chain must fold into a specific 3-dimensional shape.

The Schafmeister research group is working towards a unique way to simplify this problem: Interconnect constituent amino acids of a peptide chain with two amide bonds instead of one found in nature. This ladder-like arrangement restricts the conformational flexibility of individual amino acids to a

large extent which in turn drastically reduces the number of allowed conformations for an oligomer. We believe that this new approach will be a quick and effective alternative for the design and testing of new functional macromolecules.

In this poster presentation we illustrate the design of and the progress made towards the synthesis of a bis-peptide oligomer mimicking the Carbonic Anhydrase enzyme's active site. This functionalized oligomer carries three derivatized imidazole groups mounted on a bis-peptide scaffold which are directed along the three tetrahedral coordination sites of a zinc cation. We expect this methodology to be generally applicable and serve as a blueprint for the future development of the synthetic mimics of active sites for other metalloenzymes.

Science Teachers (K-12) Luncheon

42. What is National Lab Day?

Tom Lane., Dow Corning, United States.

National Lab Day is more than just a day. It's a nationwide initiative to build local communities of support that will foster ongoing collaborations among volunteers, students and educators. In the first week of May, 2010 we will celebrate this collaboration with National Lab Day activities across the country.

And as we go out into our communities to create new relationships, to help put a public face—a human face, if you will—on chemistry, as a chemistry ambassador.

Biological Chemistry II

43. Cloning and expression of a putative ligand gated ion channel from Nostoc punctiforme and its extramembranous domain

Stephanie Reichardt, Barry S Selinsky., Department of Chemistry, Villanova University, Villanova, PA, United States.

Ligand gated ion channels (LGICs), also known as Cys-loop receptors, are a superfamily of transmembrane proteins that mediate synaptic signaling in eukaryotic nervous systems. They function as ion selective channels that open in response to the binding of major neurotransmitters. Recent sequence profile searches of various genomes have determined the existence of homologous LGICs in several bacterial species (Tasneem, A., et al. Identification of the prokaryotic ligand-gated ion channels and their implications for the mechanisms and origins of animal Cys-loop ion channels. Genome Biology 6(1):R4 (2004)). Conservation patterns in the four transmembrane spanning helices and the ligand binding domain suggest that bacterial and eukaryotic receptors share general functional and mechanistic properties. In fact, x-ray structures of the cyanobacterial species *Erwinia chrysanthemi* and *Gloeobactor violaceus* propose a novel gating system for LGICs, which involves a change in tilt-forming helices causing channel opening (Hilf, R.J.C., Dutzler, R. Structure of a potentially open state of a proton-activated pentameric ligand-gated ion channel. Nature 457:115-118 (2009)). Here we present the cloning and expression of a putative LGIC homolog and its N-terminal extramembranous domain from *Nostoc punctiforme*. The target gene sequence from the *Nostoc punctiforme* genome was successfully cloned into the expression vectors, MBP-27b and pETpHSUL. These vectors contain maltose binding protein and small ubiquitin related modifier, respectively, and a His-tag for protein purification. The MBP-fusion protein proved to be membrane-associated based on fractionation studies; however the SUMO-fusion protein expressed from the pETpHSUL construct was localized to the periplasmic fraction. Extraction and solubilization of the membrane protein was only successful with

1% SDS, suggesting improper folding and insertion. The N-terminal extramembranous domain expressed to the periplasm is currently being purified by affinity chromatography on a His-select nickel column. Following protein purification, it will be structurally and functionally characterized giving further insight into LGIC family.

44. Allosteric regulation of dynamic, dissociating homo-oligomeric enzymes

Trevor Selwood, Eileen K. Jaffe., Fox Chase Cancer Center, Philadelphia, PA, United States.

The observation that homo-oligomeric protein assemblies can participate in dynamic association/dissociation equilibria under native conditions is well documented. There are many examples of quaternary structure equilibria that are influenced by a covalent modification event. Other quaternary structure equilibria are influenced by non-covalent ligand binding; these are the topic of this poster. In some dynamic equilibria, the dissociated state can have alternate conformations which dictate assembly to functionally distinct alternate oligomers. This property is novel to the class of proteins we have termed morpheeins (Jaffe, *TiBS* **30**:490-7, 2005). The unique and defining characteristics of morpheeins are 1) that different assemblies have different functions and 2) that interchange of alternate oligomeric forms requires dissociation of higher order oligomers to allow conformational change in the dissociated state. The requirement for oligomer dissociation distinguishes the morpheein model of allosteric control from the classical Monod, Wyman, Changeux and Koshland, Nemethy, Filmer models. This presentation follows the evolution of ideas about how homo-oligomeric equilibria can relate to allosteric regulation. The oligomeric equilibria characteristic of morpheeins are compared and contrasted with related phenomena such as the quasi-equivalence of virus coat proteins and the formation of amyloid. We present a rationale for identifying proteins that may function as morpheeins and present a family of proteins for which published data suggests the possible use of the morpheein model for allosteric regulation. Our purpose is to stimulate analysis of homo-oligomeric proteins as possible morpheeins with a view to establishing the potential generality of this model for allostery.

45. Effects of Amino Acid Sequence on Structure, Membrane Binding, and Activity of an Antimicrobial Peptide

Lubov Arotsky, Laura Hagens, Gregory A. Caputo., Department of Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States.

Antimicrobial peptides (AMPs) are short, amphiphilic peptides found as part of the innate immune system of most higher organisms. These peptides exhibit highly selective, broad spectrum activity against many strains of bacteria while having no effect on host cells. The proposed mechanism of action of these peptides involves binding and permeabilizing bacterial cell membranes bringing about cell death. We investigated the effects of amino acid substitutions on the membrane binding behavior of a naturally derived AMP, C18G. Specifically, the effects of altering the cationic moieties in this peptide by replacing the naturally occurring Lysine residues with Arginine or Histidine were investigated using fluorescence and circular dichroism spectroscopy. Acrylamide quenching was also performed to confirm how the peptide oriented in the lipid membrane. The effects of these substitutions on bacterial membrane permeabilization was also monitored. The dependence of charge-charge interactions on the initial membrane binding event was confirmed using mixtures of zwitterionic/anionic lipids as well as alterations of environmental pH.

46. Characterization of an unusual beta-hydroxybutyrate dehydrogenase from the parasite Trypanosoma brucei

Tina D Shah, **Kathryn Capasso**, Meghan Hickey, Jennifer Palenchar., Department of Chemistry, Villanova University, Villanova, PA, United States.

There are many unusual features of energy metabolism in African trypanosomes, the unicellular eukaryotic parasites responsible for African Sleeping Sickness. For example, several of the glycolytic enzymes are compartmentalized and are regulated uniquely. We have identified an unusual trypanosomal b-hydroxybutyrate dehydrogenase (HBDH), an enzyme involved in the production of ketone bodies. This enzyme, which catalyzes the reversible NADH-dependent conversion of acetoacetate to hydroxybutyrate, closely resembles bacterial forms of the enzyme. Furthermore, unlike its homologs in higher eukaryotes, the trypanosome enzyme appears not to be a membrane protein. We have cloned this enzyme from *Trypanosoma brucei* genomic DNA, overexpressed soluble protein in *E. coli*, and have purified active enzyme to approximate homogeneity. Potential substrates have been tested, the kinetic parameters for the substrates have been determined, and cofactor preference has been examined for the trypanosomal b-hydroxybutyrate dehydrogenase. Examination of the oligomeric state of this enzyme is underway.

47. Functional Amino Acid Navigator

Jason K Cargill, Sal Gomez, Peter Palenchar., Chemistry, Rutgers University, Camden, NJ, United States.

The purpose of Functional Amino Acid Navigator (FAN) is to create a database that captures information about how enzymes function with respect to interacting with small molecules and critical amino acids involved in catalysis, and then use that database to address questions related to how enzymes function and genome annotation. FAN will give a detailed picture of enzyme interactions with small molecules at the atomic level. The data in FAN is gathered from primary published literature about how specific enzymes function. The database itself will also contain direct quotes and references from the primary published material that can be accessed through a search function. Information can also be added to FAN by the outside individuals after registration. Data is entered into FAN using the data entry form. The objective of the data entry form is to gather the relevant information with respect to the protein, reaction, and interactions so that it can be searched and used later.

The search function in FAN is still growing. As of now users can select data by enzyme commission number, molecule ID, protein sequence, interaction description ID, amino acids involved in interactions, atoms involved in interactions, and Pubmed ID. The relevant interactions are selected, and the data is output.

When inputting data, FAN utilizes an ontology to describe how enzymes interact with small molecules (e.g. substrates and allosteric effectors). This is based on the existing biochemical language used to describe such interactions. FAN will also analyze BLAST protein sequence alignments to help ensure correct protein annotation by identifying amino acids for which FAN contains a function and determining if they are conserved based on the BLAST alignment.

As of now, FAN contains information covering over a dozen enzyme commission numbers and more than a hundred interactions already in place.

48. Synthesis of Stercobilin and its Deuterated Isotopomer: ESI and MS/MS of a Potential Autism Biomarker

Troy Wood,[2] Amber F Charlebois,[1] **Gregory F Pirrone**.[1], [1]Department of Chemistry and Pharmaceutical Sciences, Fairleigh Dickinson University, Madison, New Jersey, United States; [2]Department of Chemistry, SUNY University at Buffalo, Buffalo, New York, United States.

INTRODUCTION

Autism spectrum disorders (ASD) now affects as many as 1 in 91 newborns in the United States, yet its etiology remains elusive. ASD diagnosis is made through a battery of psychological evaluations, but a biochemical means for ASD diagnosis has not been developed. Hence, there is great interest in establishing the existence of an individual or suite of biomarkers that may be validated for ASD diagnosis. Recently, we used LC-MS/MS to establish that the compound stercobilin, the combined end product of action upon bilirubin by human and bacterial metabolism, is depleted to an average of 33% in urinary levels of ASD subjects vs. control children. For quantitation, a suitable isotopomer is needed to accurately establish urinary stercobilin levels.

METHODS

Stercobilin was synthesized from the metabolite bilirubin and analyzed with nuclear magnetic resonance and electrospray ionization (ESI)-MS and tandem mass spectrometry. Bilirubin was dissolved in glacial acetic acid and hydrogenated using a palladium catalyst. The intermediate was aerated, extracted into chloroform and allowed to evaporate. The resulting product was analyzed by ESI-MS on an ion trap mass spectrometer as well as nuclear magnetic resonance. Deuterated stercobilin was prepared and analyzed via the methods described above, with the exception of utilizing deuterum instead of hydrogen.

PRELIMINARY DATA

Using bilirubin as a starting material, ESI-MS indicated the presence of the (M+H) + peak at m/z 595, which is consistent with stercobilin. MS/MS of the m/z 595 peak indicates the production of two major fragment ions at m/z 470 and 345 that are attributed to stercobilin. For the deuterated sample, ESI-MS indicates the presence of an isotopic envelope, peaking at m/z 599, indicating the average incorporation of four deuterium atoms into stercobilin during synthesis. Interestingly, minimal nozzle-slimmer dissociation of the deuterated isotopomer in the ESI source indicates that the peak at m/z 470 shifts by only 2 amu, suggesting that two of the sites of deuteration, on average, come from the loss of one of the terminal pyrrole rings. Likewise, the peak at m/z 345 does not exhibit a mass shift, showing that the loss of the other terminal pyrrole ring accounts for the other two sites of deuteration; thus, the inner two pyrrole rings, including the carboxylic acid side-chains, are not labeled by deuterium during the synthetic procedure.

NOVEL ASPECT

Novel Aspect: ESI-MS/MS and NMR confirm synthesis of deuterated stercobilin isotopomer to serve as internal standard for urinary stercobilin, an autism biomarker.

49. Structure-function studies of the putative protease TM0727 from Thermotoga maritima

James D Berstler, Thomas L Selby., Chemistry, Bucknell University, Lewisburg, PA, United States.

This study focused on the structure-function relationship of the putative protease TM0727 from *Thermotoga maritima*. The enzyme is annotated as a modulator of DNA gyrase and classified as belonging to the U62 protease family. The x-ray structure of this enzyme at 1.95 Å resolution demonstrated that the 48 kDa protein reveals a novel fold, but no active site amino acids that support the enzyme's ability to function as a protease could be identified. We have produced and isolated the enzyme from

E. coli in two fractions using metal affinity and ion exchange chromatography for the purpose of performing kinetic assays and biophysical studies. Our kinetic assays have yet to provide conclusive evidence of proteolysis activity. Fluorescence and other biophysical measurements are currently being performed to probe conformational changes and study the properties of the two fractions that have been isolated to better understand their structural and/or functional differences.

50. Effects of Ionizable Amino Acids in the Hydrophobic Core of Model Transmembrane a-helices

David Bauer, Benjamin Nixon, Gregory A. Caputo., Department of Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States.

It is estimated that transmembrane (TM) proteins comprise approximately 33% of naturally occurring proteins. These natural membrane proteins typically use a-helices to traverse the hydrophobic interior of the lipid membrane in which they are imbedded. Short, synthetic peptides have proven a good experimental model system to investigate the biophysical properties of TM a-helices. The effects of hydrophilic substitutions on poly-leucine peptides inserted into lipid vesicles were studied. Incorporation of a di-lysine (KK) or a di-ornithine (OO) motif into the hydrophobic portion of peptides are of interest as these amino acids carry a cationic group in the side chain which should be excluded from the nonpolar bilayer core in the protonated state. Tryptophan fluorescence was used to study the behavior and topography of these membrane bound peptides. Peptide orientation and topography was assayed by monitoring fluorescence emission spectrum properties (peak shifts, barycenter, and FWHM). Fluorescence quenching by acrylamide, located in the aqueous milieu, and 10-doxylnonadecance, located within the hydrophobic core of the membrane, were compared to determine tryptophan depth, which relates to peptide orientation. Differences between the effects on peptide orientation by KK and OO substitutions on membrane bound peptides are correlated with amino acid side chain structure. Circular Dichroism spectroscopy confirmed that the peptides retain the a-helical secondary structure under all pH and lipid conditions. The dependence on peptide:lipid ratio and pH are currently being studied to determine the effects of KK and OO motifs on oligomerization and topography.

51. Chemoenzymatic synthesis of conjugate polysialic acid vaccines

Pumtiwitt C. McCarthy, Sylvester L. Mosley, Rina Saksena, Dwight C. Peterson, Justine Vionnet, Willie F. Vann., Laboratory of Bacterial Polysaccharides, Center for Biologics Evaluation and Research, U.S. Food and Drug Administration, Bethesda, MD, United States.

Current vaccine therapy against the bacteria that cause most cases of meningitis, namely *Haemophilus influenzae*, *Streptococcus pneumoniae*, and *Neisseria meningitidis*, target the acidic capsular polysaccharides located on the outer surface of these pathogens. Glycoconjugate vaccines, which contain these polysaccharides chemically attached to a carrier protein, are a powerful tool in combating the disease. These glycoconjugate vaccines are more effective than those based on polysaccharide alone. However, the exact relationship between glycoconjugate structure and the protective antibody response produced has yet to be fully characterized. The chemical methods commonly used in the conjugation process can often lead to heterogeneous mixtures making it difficult to establish the mechanism of action. The overall goal of this project is to develop new ways to create rationally designed vaccines for which the structure-immunopotency relationship can be determined more readily. Here we describe our initial efforts in producing a serologically active glycoconjugate by chemoenzymatic methods. We have prepared a glycoconjugate of bovine serum albumin (BSA) and polysialic acid using chemoenzymatic synthesis. We synthesized a modified lactoside acceptor as a substrate for the bifunctional transferase from *Camplyobacter jejuni* (CST II). The product of this reaction was sialylated with the polysialyltransferase from *Neisseria meningitidis* C (NmC) to yield polysialic acid derivatives with a conjugatable azide as the aglycon. The "click" chemistry method of 1,3 cycloaddition was then performed with alkynyl-modified BSA generating polysialylated-BSA.

This resulting glycoconjugate was shown to be immunoreactive to a monoclonal antibody specific for NmC polysialic acid. Our initial data suggest that chemoenzymatic synthesis may be a new and viable method for future development of meningococcal vaccines.

Chemical Education

Sponsor: Division of Chemical Education
Organizer/Presider: Andrea Martin

52. Using POGIL in the laboratory

Frank J. Creegan., Department of Chemistry, Washington College, Chestertown, MD, United States.

Process-Oriented Guided Inquiry Learning (POGIL) is a classroom and laboratory environment in which students are actively engaged in mastering course content and in developing essential skills by working in self-managed groups on guided inquiry activities. In the classroom these activities take the form of worksheets (ChemActivities) that are composed of data sets (models), which are followed by a series of carefully scaffolded critical thinking questions that guide the students to explore and explain the data so as to develop an understanding of, or to invent, the underpinning chemical concepts. Refinement of the developed theories is achieved by answering a set of additional questions or problems devoted to the application of the concept to new situations. This three-stage learning cycle approach (Exploration – Concept Invention – Application) is also used in the POGIL laboratory where student-generated data are analyzed for trends and patterns. Students, working in self-managed groups, obtain these data by performing experiments and/or making measurements in response to a focus question (Question of the Day) posed by the instructor. Concepts to be developed in the lab have not been previously or fully introduced in the lecture or classroom setting and cannot be completely developed or understood without the use of data pooled from within and/or across lab sections. The use of this student-centered approach in the laboratory will constitute the bulk of this presentation. Data that show improvement in learning will also be presented. Opportunities for joining the growing network of POGIL practitioners via the POGIL Project will be described.

53. Freshman Summer Research Experience

Andrea E Martin, **Louise M Liable-Sands**, Loyd Bastin, Shirley Fischer-Drowos., Department of Chemistry, Widener University, Chester, PA, United States.

With the support of a faculty development grant, two Widener University chemistry majors were provided a stipend to carry out research in the summer following their freshman year. During the summer of 2009, the students worked on several research projects. The students were exposed to a variety of techniques and instrumentation including standard reaction techniques, air sensitive methods, nitrogen-line methods, protein isolation, thin layer and column chromatography, gel electrophoresis, IR spectroscopy, ion chromatography, and NMR spectroscopy. Despite not having taken organic chemistry, they successfully synthesized a macrocyclic ligand and prepared new complexes with various transition metals and isolated several protein extracts from carrots and tested their ability to reduce carbonyl groups. The students kept weekly journals describing their experience. We conclude that with appropriate supervision, freshmen can gain confidence and skills through summer research, which may aid in recruiting and improve retention in the major. This presentation will focus on the planning and organization of the summer experience in addition to presenting some of the student perspectives.

54. Molecular oxygen in organic chemistry

Parvathi S. Murthy., Chemistry and Biochemistry, Georgian Court University, Lakewood, NJ, United States.

Oxidation reactions of organic compounds are a very significant component of the Organic Chemistry course curriculum. It includes reactions brought about by common transition metal compounds as oxidants, predicting the products of oxidation for each class of compounds and the complex mechanism of these oxidation reactions. Although molecular oxygen is an abundantly available and an environmentally benign oxidant, extensively used in biological oxidations, it has relatively few applications in synthetic chemistry and consequently has not been significant in Organic Chemistry course curriculum. This presentation highlights extending the curriculum to incorporate the mechanism of activation of molecular oxygen for oxidation of organic compounds using simple, non-enzymatic, biomimetic reactions.

55. Clicker use in general chemistry: Who uses them and is there a benefit?

Daniel B King., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

Personal response devices (or "clickers") have grown increasingly common in large enrollment freshman-level science courses, such as general chemistry. They are used for a variety of purposes, including taking attendance and providing feedback for the students and faculty member about student understanding. Sometimes points are awarded for their use, either just for answering the question or for getting the question right. In this talk, results will be presented from three years of clicker use in a large enrollment (>200 students) general chemistry classroom. Because only one or two lecture sections (out of 5) use clickers each term, there are no points associated with clicker use. Clickers are provided by the faculty member, so the decision to use the devices is not monetary. Usage statistics will be presented as a function of gender and academic major. Clicker use is compared to exam average and overall course grade. In general, students who use clickers on a regular basis perform better in the course. Scores on a chemistry-based placement exam suggest that active clicker users consist of both students with strong and weak prior chemistry knowledge.

56. Spoken Polymer

Thomas E Twardowski, Nadine McHenry., Department of Chemical Engineering, Widener University, Chester, PA, United States.

An innovative approach to teaching introductory polymer science and engineering as a new language was considered. The class was designed around the theory that engineering communication draws from a language substantially separate from conversational language. By teaching the students the fundamentals of that language along with the appropriate technical content early acquisition of rigorous physical knowledge could be achieved.

Two content-rigorous engineering classes have been taught using a language format with polymer grammar, vocabulary and practical discussion units. The target demographic was pre-engineering and introductory engineering and technical students at the university level, particularly students without the traditional math- chemistry- physics training cycle.

A new pedagogy was required, including complete word definitions, novel technical grammar, the specific roles of symbols and self-correction. The approach was applied twice to teach introductory polymer science to student bodies with mixed preparation levels, resulting in performance substantially equivalent to traditional polymers courses taught at the college junior level. The language concept improved student scientific communication skills, problem-solving ability, especially learning from context, and in general accelerated learning. In particular, the students could express practical knowledge in written form.

57. Baiting the hook: The Chemistry of Beer

Roger Barth., Department of Chemistry, West Chester University, West Chester, Pennsylvania, United States.

Chemistry is not high on the list of potential elective courses for most non-science students. The features need to attract these students include avoiding stoichiometry and other arithmetic, an easy-going grading policy, and a theme that has intrinsic interest to them. By and large, chemistry has a reputation of lacking each of these three features.

Chemistry of Beer is a three credit course with no laboratory designed to attract and appeal to all students. It is coupled with a short, inexpensive, well-illustrated textbook. The course covers the steps in brewing, beer ingredients, chemistry basics, water chemistry, organic chemistry, carbohydrate chemistry, enzyme action, alcoholic fermentation, testing and measuring in the brewing process, beer packaging (including the manufacture of glass and aluminum), and many other topics. Chemical bookkeeping is not covered; the mole is not mentioned. Nonetheless, that material covered includes at least as much descriptive chemistry as the entire General Chemistry sequence.

The first offering of the course was in fall, 2009. Students enjoyed the class and did well in it. Fifty-seven students completed the course. There were 13 A's, 30 B's, 10 C's, 2 D's and 2 F's. Grades were based on tests and quizzes in a word bank format. An informal, unsigned survey gave students the opportunity to indicate whether they preferred more or less of topics and aspects of the course. The average of all responses for all items was 58% more of, 28% less of, and 14% blank. Formal student ratings are being processed and will be presented.

The course is being given for the second time at its full capacity of 75 students. The productivity, which is the ratio of credits generated to faculty work load hours, is at least three times the department average. In addition to bringing chemistry to a wide range of students who would not have considered it as an option, the Chemistry of Beer brings a substantial economic benefit to the chemistry department.

58. Student test scores in math computation in some mid-Atlantic states and school districts and the implications for chemistry instruction

Eric Nelson., Retired Instructor, United States.

In problem solving at all levels, cognitive scientists emphasize the importance of "automaticity in the fundamentals" as a factor in overcoming inherent limitations in the "working memory" where problems are solved.

Solving calculations is a focus of initial chemistry courses. Math computation is a background skill that students are often assumed to have acquired in classes prior to chemistry. Is that assumption valid for the current generation of students?

This paper will present trends in available test score data for students in some mid-Atlantic states and school districts since the widespread K-12 adoption of "NCTM-standard" math textbooks in the early 1990's. Overall, these data show a substantial decline in student math computation skills. Data for states and localities will be presented in which scores in math computation both increased and decreased, and curriculum differences that may have contributed to those trends will be noted.

The opportunities for those concerned with science education to voice their views on state K-12 standards for math computation that impact student learning in the physical sciences will also be reviewed

59. Fundamental chemical demonstrations

Michael A. Stemniski., Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States.

Classroom chemical demonstrations are used to reinforce theoretical concepts. Demonstrations are also used to inspire, motivate, and entertain students of all grade levels. Chemical experiments can arouse the curiosity of young people to further explore the world of science through education. This presentation will consist of a series of simple demonstrations that can be performed for the benefit of all students. The experiments will range from simple color changes to phase changes to controlled combustions. Some specific experiments that will be included are various methanol cannons, an orange juice clock, dry ice and liquid nitrogen demonstrations, an ammonia fountain, blue bottle reactions, clock reactions, hydrogen peroxide decompositions, nitrocellulose, and others. The equipment, chemicals, and solutions needed to perform these exercises will be documented and suggestions for their safe implementation will be presented.

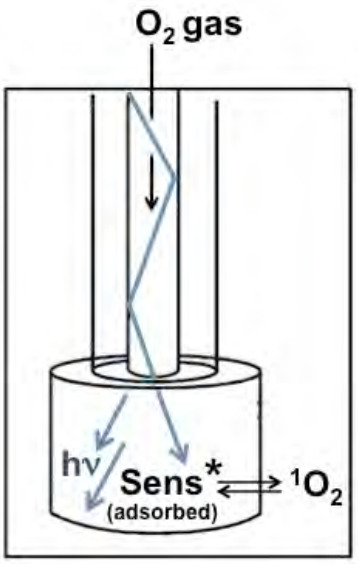
Organic Chemistry II

Sponsor: Division of Organic Chemistry

60. Portable device based on a fiber-optic singlet-oxygen [$^1O_2$ (^1d_g)] generator (FOSG)

David Aebisher, Matibur Zamadar, Adaickapillai Mahendran, Goutam Ghosh, Catherine McEntee, **Alexander Greer**., Chemistry, Brooklyn College of the City University of New York, Brooklyn, NY, United States.

Traditionally, type II heterogeneous photooxidations produce singlet oxygen via external irradiations with a supply of ground-state oxygen from bulk solution. A potential improvement is reported here with a hollow-core fi;ber optic device (oxygen-flowing, porous photosensitizer-end capped configuration) where singlet oxygen is delivered through the fi;ber tip. Steady-state concentrations of singlet oxygen were estimated in the vicinity around the probe tip by *N*-benzoyl-DL-methionine trapping. The device is portable and the $^1O_2$–generating tip is maneuverable, which opened the door to disinfectant studies. We find complete *E. coli* inactivation when the probe tip was introduced into 0.1-mL aqueous samples of 4.4×10^7 cells.



61. Metalla-Cope rearrangements: Bridging organic and inorganic chemistry

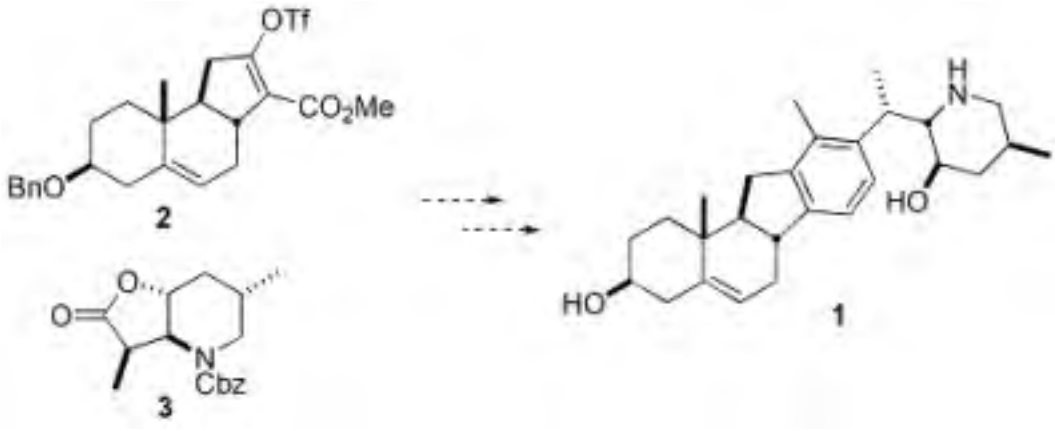
Edyta Greer, Roald Hoffmann., Natural Sciences, Baruch College of the City University of New York, New York, NY, United States.

Density functional theory calculations were performed to explore both concerted chairlike and boatlike as well as stepwise mechanisms of the Cope rearrangement of two hypothetical metalladienes. An osma-1,5-hexadiene was designed by substituting CH_2 in 1,5-hexadiene by its isolobal analogue, 16-electron $Os(PH_3)_4$. The energy of activation corresponding to the rearrangement of osma-1,5-hexadiene involving the chairlike saddle point was computed as 37.4 kcal/mol, 3.9 kcal/mol above the energy barrier of the parent 1,5-hexadiene calculated with the same method and basis set, and was 4.5 kcal/mol below that of the boatlike pathway. In another isolobal replacement, the CH in 1,5-hexadiene was substituted by a 15-electron $Re(PH_3)_3$ fragment. In this case, the chairlike rearrangement of the rhenia-1,5-hexadiene had an E_a value of 23.0 kcal/mol, 10.8 kcal/mol less than the energy barrier of the parent 1,5-hexadiene calculated at the same level of theory. The ring inversion of the chair and osma-chair diradical intermediates of the stepwise reaction pathway were also examined and were found in both cases to proceed through a very flat potential energy surface involving twist intermediates.

62. Progress Towards the Total Synthesis of (-) Veratramine

Douglass F. Taber, James F. Berry, **Peter W. DeMatteo**., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

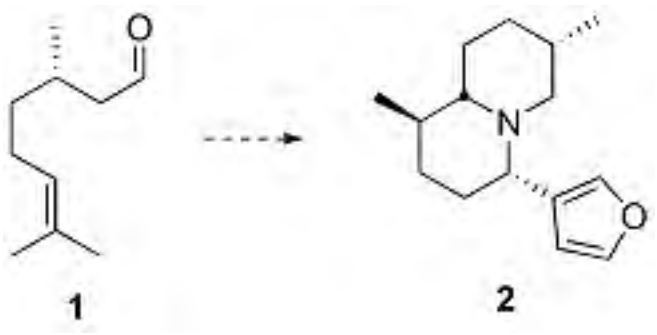
Over the past decade, the Hedgehog (Hh) pathway has come to light as a promising chemotherapeutic target for inoperable carcinomas. Veratramine (**1**) has high inhibition of Hh. We propose a convergent total synthesis of **1** from chirons **2** and **3**, and will detail our more recent steps towards its conclusion.



63. The Total Synthesis of (-) Deoxynupharidine

Douglass F. Taber, **Peter W. DeMatteo**, **Patrick J. Straney**., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

(-) Deoxynupharidine (**2**) is an aquatic alkaloid isolated from the water lily. We have recently developed a methodology that grants facile access to *cis*-2,5 disubstituted piperidine rings such as the northern ring of **2**. A concise diastereoselective synthesis from (-) citronellal (**1**) will be presented.



64. Allylic Substitution versus Suzuki Cross-Coupling: Capitalizing on Chemoselectivity with Bifunctional Substrates

Mahmud M. Hussain, Byeong-Seon Kim, Nusrah Hussain, Patrick J. Walsh., Department of Chemistry, University of Pennsylvania, Philadelphia, PA, United States.

Bifunctional reagents that contain a vinyl boronate ester embedded in an allylic acetate have been prepared. Given the choice between the allylic acetate and a vinylboronate ester, under neutral conditions with amine nucleophiles, palladium preferentially reacts at the allylic acetate to give the allylic substitution product. Subsequent addition of aryl bromide and base results in a Suzuki cross-coupling to afford (*E*)-trisubstituted allylic amines. We have developed orthogonal reaction conditions wherein this chemoselectivity can now be reversed by addition of base to allow Suzuki cross-coupling to be performed *in the presence of the allylic acetate functionality.* The chemoselectivity is remarkable considering the same Pd catalyst can be used to effect allylic substitution or vinylic cross-coupling reactions selectively and interchangeably despite the differences in reaction mechanism. Full use of selective reactivity of our bifunctional reagents is expected to have a high impact on organic synthesis.

65. Olefin and fullerene sulfurations with thiozone (S_3). A theoretical study

Alvaro Castillo, Alexander Greer., Chemistry Department, The City University of New York, Brooklyn College and The Graduate Center, Brooklyn, NY, United States.

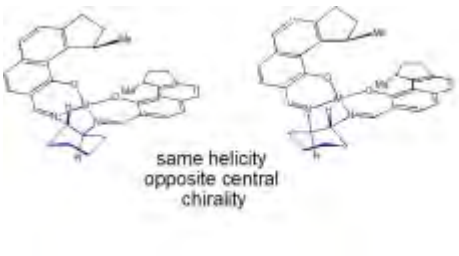
Thiozone, S_3, has been proposed as an intermediate in the atmospheric chemistry of Venus, the mechanism of cytotoxicity of the natural product varacin, the decomposition of disulfur monoxide or norbornanetrithiolanes, and in molten sulfur. A DFT study was conducted, which suggest that S_3 is best described by a zwitterionic, not a biradical, structure. The addition of S_3 to ethylene and to C_{60} occurred as expected, at the double-bond and [6,6] position respectively resulting in the production of C_{ethane}-S or C_{60}-S bonds. The 1,2,3-trithiolane structure was found as a stable intermediate in both cases. Pathways to thiosulfine or dithiirane were found to be very high in energy. The computations also point to a high-energy process in converting trithiolane to episulfide and the diatomic sulfur intermediate, S_2. Sulfurations with thiozone are predicted to provide a facile route to ethylene or fullerene adducts containing the trisulfane moiety.

66. Examining the role of helicity in salen catalysis

James N Plampin III, Joseph M Fox., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

Chiral salen catalysts have become ubiquitous in asymmetric synthesis, but much debate still centers on the mechanism of asymmetric induction. Specifically, it is unclear whether ligand helicity plays a role in asymmetric induction. Described is a new class of catalysts that separate the contributions of backbone chirality and helical chirality in salen catalysts. The structures are shown in the figure below. These structures have will have the same sense of abs. helicity as controlled by the chiral end

groups. However, structures**[figure1]**1 and 2 differ in the abs. stereochemistry of the diamine in the backbone. These complexes will allow us to directly test the role that helicity plays in asymmetric induction.



67. Synthesis, Characterization, Stability, and Antiproliferative Activity of a New PEGylated Benzopolysulfane, 4-$CH_3(OCH_2CH_2)_3NHC(O)$-C_6H_4-1,2-S_5

Adaickapillai Mahendran,[1] Angela Vuong,[1] David Aebisher,[1] Yaqiong Gong,[2] Robert Bittman,[2] Gilbert Arthur,[3] Akira Kawamura,[4] Alexander Greer.[1], [1]Department of Chemistry, Brooklyn College and Graduate Center of The City University of New York, Brooklyn, New York, United States; [2]Department of Chemistry and Biochemistry, Queens College and Graduate Center of The City University of New York, Flushing, New York, United States; [3]Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, Manitoba, Canada; [4]Department of Chemistry, Hunter College and Graduate Center of The City University of New York, New York, New York, United States.

A benzopentathiepin was synthesized with a PEG group attached through an amide bond and examined for stability, water solubility, and antitumor activity. The presence of the PEG group improved water solubility by 50-fold compared to the unsubstituted benzopolysulfane, $C_6H_4S_5$, based on intrinsic solubility measurements. The PEG conjugated benzopentathiepin had IC_{50} values 1.2-5.8 times lower than the parent "unsubstituted" benzopentathiepin against four human tumor cell lines PC3 (prostate), DU145 (prostrate), MDA-MB-231 (breast), and Jurkat (T-cell leukemia). Complete cell killing was observed for the PEG polysulfane with 4 μM for PC3 and DU145 cells, and with 12 μM for MDA-MB-231 cells. The results suggest that solubilization of the polysulfur linkage is a key parameter to the success of this compound as a drug lead.

68. Copper-free Sonogashira coupling of aryl bromides and chlorides using highly active Pd catalysts in API development

Hongbo Li, Thomas Colact., Johnson Matthey Catalysts, West Deptford, NJ, United States.

Over the last decade, there have been significant advancements in Pd based cross coupling catalysis for various C-C and C-heteroatom transformations. As a continuation of these developments, Johnson Matthey has been successful in developing several examples of phosphine based Pd(II), Pd(I) and Pd(0) catalysts for various transformations in pharmaceutical processes.

Although copper mediated palladium catalyzed synthesis is widely practiced for the Sonogashira reaction to construct a $C(sp^2)$– C(sp) bond, the use of CuI introduces another variable to the catalytic system and often creates the potential for contaminating of the API. In addition, Cu is mostly suited to the coupling of aryl iodides. In this study, we describe the synthesis of new palladium-phosphine complexes and demonstrated their use as highly active catalysts for *copper-free* Sonogashira coupling of aryl/heteroaryl- bromides and chlorides with aliphatic and aromatic acetylenes with excellent yield under milder conditions. Details of the work, which includes reaction conditions, such as choice of the base, solvent and additives will be presented.

69. Synthesis of PABA derivatives: The Fischer Esterification reaction revisited, Part IV: An adventurous Pathway for teaching and learning research through Organic Synthesis!

Nagarajan Vasumathi,[1] Kristin Shirey,[1] Thai Huynh,[1] Caterina Lazaroni.[2], [1]Department of Physical and Earth Sciences, Jacksonville State University, Jacksonville, AL, United States; [2]Physical and Earth Sciences, Jacksonville State University, Jacksonville, AL, United States.

Esters of p-aminobenzoic acid are well known for their analgesic and anti inflammatory properties. There are different methods known for the synthesis of esters. The commonly exploited Fischer Esterification method is known to be a tedious method and give poor yields since it is an equilibrium reaction. However, this method involves less toxic, less expensive chemicals and more environmentally friendly procedure. Our research group, using Dean-Stark apparatus as a tool with specific modifications in the procedure, successfully synthesized Butamben, the butyl ester of PABA, known for its neuropathic pain-relieving properties in about 99 % yield with maximum purity[1]. Applying this method, we synthesized isoamyl and octyl esters of PABA with maximum purity in moderate yields[2]. An important observation made was each synthesis required some modification in the method as we changed the alcohol counterpart. Reaction of PABA with cyclohexanol formed a mixture of cyclohexyl ester and a dicyclohexyl derivative. With an attempt to synthesize selectively the monoalkyl ester or the dialkyl derivative, we repeated the reaction of PABA with cyclohexanol using different catalysts. Both homogeneous and heterogeneous catalysts such as PTS, Sulfuric acid, $BF_3.Et_2O$ and anhydrous Ferric sulfate were found to be inactive towards the esterification process[3]. However, with anhydrous copper chloride and copper chloride monohydrate or dihydrate catalysts, some unexpected observations were made and different products other than the anticipated esters were formed. The preliminary results have shown the formation of PABA-copper metal complexes instead of the anticipated ester. The reactions were repeated using different solvents and heating at different temperature conditions using both anhydrous $CuCl_2$ and $CuCl_2.2H_2O$. In all cases two distinguishable solid crystals, dark purple and green in color were isolated. The method of synthesis, isolation, purification and characterization by various spectroscopic methods is discussed. Further exploration to study the effect of zeolite catalysts on the reaction is also underway.

References

Nagarajan Vasumathi, Haley Booker and Christopher Goodwin, "Synthesis of Butamben: The Fischer Esterification Reaction Revisited – Part I", paper submitted to ***The Missouri Journal of Undergraduate Chemical Research***, November, 2009.

Nagarajan Vasumathi, Kristin Shirey, Haley Booker and Meriem Zettili, "Syntheses and characterization of some Aliphatic Esters of PABA: The Fischer Esterification reaction revisited – Part II", Abstract, ***Annual Biomedical Research Conference for Minority Students (ABRCMS)***, p 196, # C51, 2008.

70. Effect of nonionic co-surfactants on corrosion inhibition effect of cationic gemini surfactant in acid medium

Dourna Asefi,[1] Mokhtar Arami,[2] Niyaz Mohammad Mahmoodi.[3], [1]Polymer Engineering, Islamic Azad University South Branch of Tehran, Iran (Islamic Republic of); [2]Textile Engineering, Amirkabir University of Technology, Iran (Islamic Republic of); [3]Environmental Research, Institute for Color Science and Technology, Iran (Islamic Republic of).

The effect of chain length compatibility on corrosion inhibition effect of mixed inhibitor systems of cationic gemini surfactant, l,4-butan-bis(Dodecyl Dimethyl Ammonium Bromide) (designated as 12-4-12) with nonionic co-surfactants, C_7OH (1-heptanol), $C_{12}OH$ (1-dodecanol) and $C_{15}OH$ (1-pentadecanol), on low carbon steel in acid medium was studied using weight loss, open circuit potential (OCP) and electrochemical impedance spectroscopy (EIS) measurements. Data represented that the

corrosion rate decreased by increasing surfactant concentration. In addition, less chain length difference causes more compatibility and inhibition on behavior of surfactant and co-surfactant mixture. Increasing of inhibition efficiency for $C_{12}OH$ + gemini surfactant was more than other mixtures.

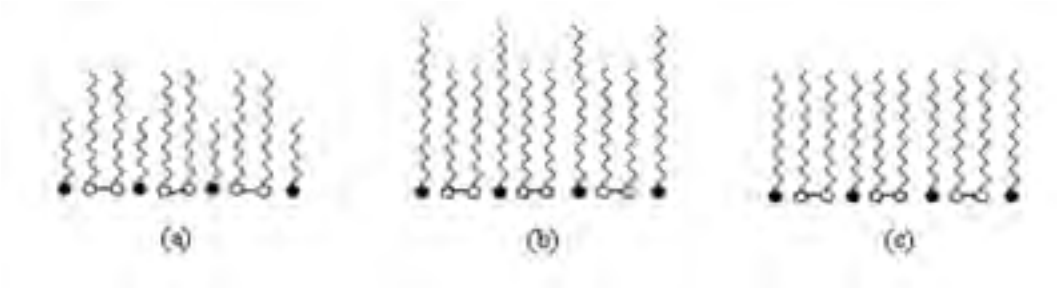


Figure. Three modes for orientation of surfactant and co-surfactant molecules on metal surface. Chain length of co-surfactant molecules are (a) shorter than, (b) longer than, (c) equal to the chain length of surfactant molecules.

ACS Undergraduate Research Symposium - I

Sponsor: American Chemical Society
Organizer/Presider: Narmada Gunawardena

Session Overview: Posters may be set up any time between 8:00 - 8:30. The symposium provides an excellent opportunity for undergraduate chemistry students to present the results of their research. Presenters should be by their posters from 8:30 - 10:00.

71. Quantitative determination of gallic acid in commercial tea and juice beverages using HPLC

Christine Casas, Soraya Svoronos, Pedro Irigoyen, Paris Svoronos., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

Gallic acid, a polyphenolic compound, is known for its antioxidant properties. The content of gallic acid in various brands of beverages is measured and compared using High Pressure Liquid Chromatography (HPLC). Analyzed samples include commercial bottled teas as well as grape and pomegranate juices. The advantages and disadvantages of this method are presented with emphasis on the potential interference of other compounds present in these beverages.

72. Determination of the total phenol content in commercial bottled beverages via the Folin-Ciocalteau Micromethod

Kyu-Ree (Katie) Lee, Soraya Svoronos, Pedro Irigoyen, Paris Svoronos., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

The total phenol content in beverages such as bottled teas as well as grape and pomegranate juices was determined using the Folin-Ciocalteau Micromethod. According to the experimental procedure the total quantity of phenolics is measured by their oxidation to a blue colored product when treated with the Folin-Ciocalteau reagent in basic medium. The oxidized phenols' concentration is measured spectrophotometrically using Beer's law at 755 nm. The advantages of this method as well as possible interferences from other compounds that are present in the beverages are discussed.

73. Probing the interaction of gold nanoparticles with nanofibers of polyaniline and its analogs

Bhawanie Persaud,[1] David M. Sarno,[1] Mathew M. Maye.[2], [1]Department of Chemistry, Queensborough Community College of CUNY, Bayside, NY, United States; [2]Department of Chemistry, Syracuse University, Syracuse, NY, United States.

Polyaniline (PAni) nanofibers and gold nanoparticles (Au-NP's) are both of interest for nanoscale electronics. PAni nanofibers have been combined with Au-NP's of varying sizes (20-90nm with citrate or ascorbate shells) to create nanocomposites which may find use in a multi-component sensor material. UV-Vis was used to probe the interaction of the two materials by titrating the polymer into an aqueous solution of the NP's. It was observed that the characteristic spectrum of the Au-NP's was considerably red-shifted as the amount of polymer increased, which we believe corresponds to an increase in the uptake of the NP's by the polymer. This effect was seen whether the polymer was in its doped or dedoped form. Scanning electron microscopy of dried samples shows that Au-NP's are deposited onto the PAni nanofibers with little evidence of free particles. Notably, neither nanomaterial suffers any structural change when mixed together to form the composite. Preliminary studies on the influence of sulfonic acid substituents on the polymer backbone show that the NP's do not deposit very well and instead tend to aggregate together. It is thought that this is due to an electrostatic repulsion between the shell of the NP's and the polymer backbone which are both negatively charged. An investigation into this phenomenon using positively charged Au-NP's is underway.

74. Temperature effect of alcohols on refractive index measured by a laser pointer

Ernest Choi, Esther Yang, Jun H Shin., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

Refractive index is one of well-known analytical technique to identify compound, however, it is rarely adopted to the undergraduate laboratory curriculum because a proper and easy to approach setup for the experiment is not fully developed yet. Recently we have developed a simple, accurate and inexpensive system for a refractive index experiment using a laser pointer. The setup was very easy to use and was very accurate for single and binary solvent systems. The laser pointer method has been further applied to measure the temperature effect on the refractive index of alcohol compounds such as n-propanol, n-butanol and ethylene glycol.

75. Refractive index of hydrocarbons at various temperatures measured by a laser pointer

Esther Yang, Ernest Choi, Jun H Shin., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

We have developed a simple, accurate and inexpensive system for a refractive index experiment using a laser pointer. With the system we could measure the refractive index of organic liquids and their mixtures accurately. The laser pointer system was further applied to investigate the temperature effect on the refractive index of hydrocarbons (non-polar compounds) such as cyclohexane, heptane and toluene.

76. Ring-contraction of 3 H -1-benzazepine to 1,2-diarylquinoline

Sasan Karimi,[1] **Prakash Prasad**.[2], [1]Department of Chemistry, Queensborough Community College, Bayside, New York, United States; [2]Department of Chemistry and Biochemistry, Queens College of CUNY, Flushing, New York, United States.

Quinolines, like benzazepines, are pharmacologically active heterocycles that are potential antibacterial and antimalarial agents. Attempted free-radical bromination of the allylic position of 3*H*-1-benzazepine with NBS led to an unusual ring-contraction reaction, giving rise to 1,2-diphenylquinoline in good yields. We have found that several other 2,4-diarylbenzazepines also undergoes ring-contraction to give 1,2-diarylquinolines in synthetically useful yields. Similar reactions have been previously observed for conversion of 3*H*-azepines to pyridine derivatives, and 1*H*-benzazepines to isoquinoline derivatives. Investigations are ongoing to deduce this intriguing mechanistic transformation.

77. Detection of nitrofuran metabolites in imported shrimp: An internship experience at the Food and Drug Administration

Timothy Fitzgerald,[1] LeRae Graham,[2] Paris Svoronos,[1] Michael Fazio.[2], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]158-15 Liberty Avenue, Food and Drug Administration Regional Office, Jamaica, NY, United States.

The process of the tandem liquid chromatography-mass spectrometry method for the detection of nitrofuran metabolites in shrimp is described. A main concern with shrimp is the threat that they have been treated with nitrofuran antibiotics that are known human carcinogens. Testing for the nitrofuran tissue-bound antibiotic metabolites was done to the part per billion sensitivity level using both liquid chromatography and mass spectrometry after extracting about 0.2mL of proteins from a 2-gram shrimp sample. The process has three phases of preparation before the sample is analyzed by the chromatograph and mass spectrometer. These are compositing, derivitization and extracting. A recently improved method can be completed by one analyst in one day.

78. Antibiotic resistance and chemical profiling of actinomycetes in New York soils.

Krisna Sricharoon, Ruth Lee, Monica Rivera, Monica Trujillo, Mangala Tawde., Department of Biological Sciences and Geology, Queensborough Community College, Bayside, NY, United States.

Actinomycetes are Gram positive bacteria with a high GC content and are well- known producers of secondary metabolites. We have put together a collection of about 60 Actinomycetes strains isolated from New York State park soils. The whole collection is being analyzed and characterized for antimicrobial activity. All strains have been tested for their capacity to produce antimicrobial compounds active against *Staphylococcus aureus and Escherichia coli*, Gram positive and Gram negative bacteria respectively. We have also characterized the TLC profile of the strains analyzing their secondary metabolite production in solid soy flour mannitol media. Their antibiotic resistance profile is also being characterized which includes 5 commercial antibiotics of clinical use.

79. Determination of the ionization constant of weak carboxylic acids using microscale freezing point depression measurements

Parsa Sharifi,[1] Gopal Subramaniam,[2] Pedro Irigoyen,[1] Paris Svoronos.[1], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Department of Chemistry and Biochemistry, Queens College, Flushing, NY, United States.

Freezing point depression is a colligative property that depends only on the number of particles present but not on the nature of the particles. The freezing point of a substance (the solvent) is lowered (depressed) when another compound (the solute) is added, resulting in a mixture (the solution). The van't Hoff Factor (*i*), is a measurevof the solute's degree of dissociation. Microscale freezing point

measurements allowed the calculation of the ionization constant (K_a) of five weak acids (maleic, malonic, dichloroacetic, trichloroacetic and oxalic acids) at approximately 0°C. The experimental set up enabled the measurement of solutions that involved quantitites as low as 0.1g of the solute in 4g of water.

80. Computational studies of methylcobalamin binding to aminoacids in solution

Jerry Kouloumbes, Jordan Verdis., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

It has been proposed that the oral bioavailability of methylcobalamin increases in the presence of aminoacids. In this study the binding of methylcobalamin to lysine and glutamic acid in solution is investigated computationally with ab initio and molecular dynamics methods in an effort to substantiate these claims.

81. Preparation of poly(o-toluidine) as porous micron-scale spheres

Mauricio Murillo, David M. Sarno., Department of Chemistry, Queensborough Community College of CUNY, Bayside, NY, United States.

Polyaniline is among the most studied and useful conducting polymers because of its facile synthesis, environmental stability, and simple acid/base-doping/dedoping chemistry. By modifying a method known to produce uniform nanofibers of polyaniline and its derivatives, we have found that methyl-substituted aniline, poly(o-toluidine), can be obtained as highly porous micron-scale spheres. Interestingly, this morphology does not appear to be native to the polymer as synthesized. Rather, it is achieved via the post-synthetic workup during which a highly concentrated precipitate of the polymer in aqueous acidic solution is rapidly deprotonated with an excess of ammonium hydroxide. Further, the morphology of the final material can be altered by diluting the precipitate with water prior to its exposure to base. Scanning electron microscopy shows that at the highest polymer concentrations, deprotonation typically produces porous spheres of varying size which are fused together into very large particles. They often appear fragmented or damaged. As the concentration decreases, discrete whole spheres become the primary morphology. With sufficient dilution, spheres are completely replaced by clusters of much smaller irregularly-shaped particles. An investigation of the formation of the different morphologies is ongoing. Reproducible porous structures may find application to the encapsulation of other smaller particles, leading to novel hybrid materials.

82. Determination of a solute's molecular weight using microscale freezing point depression measurements

Shiran Zhavian, Pedro Irigoyen, Paris Svoronos., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

Freezing point depression measurements of a solution is a standard method in the determination of the molecular weight of a solute. However this undergraduate procedure usually requires large quantities of both the solute and solvent whose K_f value must be considerably high. A new improved method has been designed and implemented using quantities as low as 0.1g of the non-ionizable solute and 4g of the solvent. Solute-solvent combinations include solid-solid, solid-liquid, liquid-solid and liquid-liquid cases, with accuracies of $\pm$ 2 amu units for the molecular weight of the solute.

83. Determination of acid and base concentrations using a laser pointer: Refractive index vs. concentration

Rebecca Cho, Esther Yang, Jun H Shin., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

Refractive index is one of well-known analyticaltechnique to identify a liquid compound. We developed a new system using a laser pointer to measure the refractive index of various liquids and solutions, and found that there was a good relationship between the refractive index and various types of concentration such as %volume, %mass, molarity and density. We further applied this laser pointer system to determine the concentrations of acid and base solutions such as HCl and NaOH.

84. Determination of chlorine residual in water by the DPD method.

Grace Song,[1] Sophia Mezina,[2] Panayiotis Meleties,[3] Paris Svoronos.[1], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Bureau of Wastewater Treatment, New York City Department Environmental Protection, Wards Island, NY, United States; [3]Office of Academic Affairs-Math and Science Division, York College, Jamaica, NY, United States.

The purpose of chlorinating polluted waters by the New York City Division of Environmental Protection (DEP) is to primarily destroy or deactivate disease-producing microorganisms. A secondary benefit, particularly in treating drinking water, is the overall water quality improvement that results from the reaction of chlorine with ammonia, iron, manganese, sulfide, and some organic substances. However, chlorination may also produce adverse effects as it potentially forms chloroorganics which harm some aquatic life. To carry out the primary purpose of chlorination while minimizing any adverse effects, it is vital that proper testing procedures be used with an understanding of the limitations of this analytical determination. To evaluate the chlorine residual, the DPD method is used under neutral pH conditions. Testing the chlorine residual indicates to the chemist the effectiveness of chlorine addition. A minimal reading of 0.2 ppm ensures that enough chlorine has been added to kill off all microorganisms. The description and analysis of this procedure will be presented.

85. Effect of Carnitine and Co-Enzyme Q10 on Astrocyte Mitochondria

Jose Zhagnay, Regina Sullivan, Marisa Cotrina., Department of Biology, Queensborough Community College, Bayside, NY, United States.

Carnitine and Co-enzyme Q10 (CoQ10) are two naturally occurring substances with important mitochondrial functions. Carnitine transports lipids into mitochondria for oxidation and energy production. It is also responsible for transporting toxic compounds out of the mitochondria. CoQ10 is directly involved in cellular respiration. As heart and liver have some of the highest energy demands, carnitine and CoQ10 are two supplements commonly prescribed to improve muscle performance and energy levels in a variety of disorders like ischemia, heart disease, cancer and osteoporosis. Little is known about the effects of these two compounds in another organ with high metabolism - the brain. The objective of this work is to test whether carnitine and CoQ10 can improve mitochondrial integrity and cell survival of astrocytes, the main brain cell type involved in survival and metabolic support of neurons. To this end, we will subject primary astrocytes from mice brain in culture to a non-lethal insult of hydrogen peroxide. Using an epifluorescence microscope, we will evaluate 1) cell death with the cell-impermeable fluorescent indicator Hoechst (which only labels nuclei of dying cells) and 2) mitochondrial integrity with the fluorescent indicator MitoTracker, which labels mitochondria in active, living cells. Last, we will test whether carnitine and CoQ10 have an additive effect when both compounds are administered together. These experiments will help evaluate if carnitine and CoQ10 have any therapeutic potential against neurodegeneration.

86. The effect of outdoor smoking on an indoor environment: A Brookhaven National Laboratories experience.

Christine Casas,[1] John Heiser.[2], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Environmental Research & Technology Division, Brookhaven National Laboratories, Upton, NY, United States.

The objective of the winter research Mini-Semester at Brookhaven National Laboratories in Upton, NY is to introduce students to the importance of scientific research and the practical application of the various disciplines of science. My experience dealt with the study of the effect of outdoor smoking on an indoor environment. Several air quality testing devices were placed in various locations within one of the newer buildings on campus and then perfluorocarbon tracers (PFT) were released into the atmosphere at the three designated smoking areas outside the building. Half the devices were then collected within twelve hours and the other half after twenty-four hours. Once collected, the samples were brought into the Environmental Sciences Department to be analyzed using an automatic electron capture gas chromatograph and determine if and when the tracers reached the interior of the building. Initial results of several trials indicated that the tracers were detected indoors rather quickly and in relatively high concentrations.

87. Analysis of milk for fat, protein, and lactose Authors Waddah Guneid , Bruce Montalbano, Joe Iorio, Irina Rutenberg,

Waddah Guneid, Irina Rutenburg, Pedro Irigoyen, Bruce Montalbano, Joseph Iorio, TianChun Xu., Chemistry, Queensborough Community College, Bayside, New York, United States.

Milk is one of the most common items in human diet, at least in the USA. Milk provides proteins, carbohydrates, fats as well as other essential nutrients. We have been investigating various methods available in the literature for separation and characterization of milk components to choose the simplest and safest ones. our objective is to modify and supplement these methods for incorporation into laboratory chemistry courses for Allied Health Professions and Consumers- giving these students the opportunity to learn and practice various basic techniques of analytical chemistry.

88. A summer internship at the DEP: An application of what I learned in class to the real world.

Kyu-Ree (Katie) Lee,[1] Panayiotis Meleties,[2] Sophia Mezina,[3] Paris Svoronos.[1], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Office of Academic affairs-Math and Science Division, York College, Jamaica, NY, United States; [3]Owls Head Park, New York City Department Environmental Protection, Brooklyn, NY, United States.

Through an ATE grant that included York College and four CUNY community colleges, students have the opportunity to engage in a ten-week internship at the D.E.P. (Department of Environmental Protection) located at the Owl's Head Lab for the Waste Water Treatment facility in New York City. The experience involved applications learned in the General Chemistry course. Water samples were first composed from different facilities, such as Owl's Head, Jamaica and 26 Ward . The temperature was then measured for each sample contained in a Nalgene bottle ranging between 0° -6° Celsius for preservation purposes; with the pH buffered around pH=7. In addition titrimetric and gravimetric analyses were performed to measure the concentration of the chloride anion. The nature of the water that was processed at the lab is wastewater that comes from streams located at Prospect Park and the Verrazano Bridge.

89. DNA Isolation and phosphate detection: An undergraduate chemistry experiment

Noor Sardar, Jordan Verdis., Department of Chemistry, Queensborough Community College of CUNY, Bayside, NY, United States.

An experimental procedure has been developed in which DNA from strawberries is isolated and characterized as a phosphate ester macromolecule using only general purpose chemicals, glassware and instrumentation found in the typical undergraduate organic chemistry laboratory. The use of costly electrophoresis equipment, specialized glassware or hazardous dyes is avoided. Two versions of the procedure are presented, one to fit into a single laboratory session and one requiring two sessions. The experiment is suitable for entry-level organic chemistry students.

90. Analysis Of Antibiotic Induced Evolutionary Changes In E.coli .

Elana Santos, Omid Khalpari, Nidhi Gadura., Department of Biology, Queensborough Community College, Bayside, New York, United States.

This study is designed to look at microbial evolutionary changes in *E. coli* brought about using a controlled dosage of the antibiotic ciprofloxacin as the selective pressure. The evolutionary changes were studied using bioinformatics. Wildtype (drug sensitive) *E. coli* was grown in a medium containing a low concentration of ciprofloxacin in order to keep the population stable over the course of several hundred generations. Ciprofloxacin is a type of quinolone antibiotic that binds to and interferes with the function of topoisomerases. Gyrase is a type of topoisomerase, an essential enzyme that unwinds DNA during replication. Mutations in genes *GyrA* or *GyrB* can prevent DNA replication. We used PCR to amplify both of these genes and analyze their sequences to reveal if long term exposure to ciprofloxacin has induced any mutations. Various drug resistant strains will also be isolated, the *GyrA* and *GyrB* DNA sequenced and analyzed to look for mutations.

91. Optimizing Plant cell walls for Biofuels: Role of carbohydrate binding proteins in wall polymer assembly

Ahsan Waqar,[1] Desigan Kumaran,[2] Mangala Tawde,[1] Paul Freimuth.[2], [1]Department of Biological Sciences and Geology, Queensborough Community College, Bayside, New York, United States; [2]Biology Department, Brookhaven National laboratory, Upton, New York, United States.

Cellulose, a linear polymer of glucose subunits, comprises ~30% of the mass of plant cell walls. To produce biofuels from plant biomass, the cellulose must first by separated from other carbohydrate and non-carbohydrate polymers with which it is tightly assembled. A better understanding of the mechanisms of cell wall polymer assembly would provide important insights for development of more efficient separation methods, or alternatively for development of transgenic plants that produce cell walls that are optimized for biofuels processing. Plant cell walls contain >300 different carbohydrate-active protein species predicted to function in the assembly of cellulose and other polymers into tightly cross- linked networks. We are expressing these proteins in bacterial hosts to determine their biochemical mechanisms. Here we show the results of our studies on a carbohydrate binding protein (CBP-1) from the model plant *Arabidopsis thaliana*.

92. Creating a structure based searchable database for FDA approved chemotherapy drugs using KnowItAll®

Ghada J. Alabed, Jordan Wheatley, Malcom J. D'Souza., Department of Chemistry, Wesley College, Dover, DE, United States.

The process by which new chemotherapy drugs are discovered, tested *in vitro*, subjected to patient's trials, and finally brought to market, is a long, enormously costly and time consuming process. In general an average of 15 years at a cost of over 800 million dollars is required to introduce a mar-

ketable chemotherapy drug that is accepted by the FDA. Recently many *in-vitro* and *in-silico* techniques targeting the identification of "structure activity relationship" (SAR properties) have been developed for early identification and subsequent disqualification of misfit chemical compounds to help researchers improve time-consumption, and cost effectiveness for the development of new chemotherapy drugs. The latter *in-silico* method encompasses computerized testing of millions of searchable candidate chemical compounds using commercially available tools such as the KnowItAll® platform. The absorption, distribution, metabolism, excretion and toxicology (ADME/Tox), along with other pharmacokinetic parameters are usually reported in long wordy non-searchable PDF files at the FDA website. The aim of this study is to extract the relevant information from the printed drug packets and to create a chemical-structure based (SAR relevant) searchable database for FDA approved chemotherapy drugs using KnowItAll®. Subsequently, we will study the accuracy of predicting pharmacokinetic properties of chemotherapy drugs using this newly developed "FDA Chemotherapy Drug Database". The database will include the 3D chemical structures of the drugs, and ADME/Tox predictive properties could eventually serve as a customizable *in-silico* tool for screening chemotherapy drug candidates early in the process ultimately expediting the development and testing of new drugs.

93. Copper Surface-Mediated Toxicity Correlates With Memebrane Lipid Peroxidation In E.coli .

Rachel Hammer, Nidhi Gadura., Department of Biology, Queensborough Community College, Bayside, New York, United States.

The mechanism(s) by which copper alloy surfaces kill microorganisms is still largely unclear. The aim of our project is to determine the relationship between exposure to copper alloy surfaces or copper ions, lipid peroxidation, and killing of *Escherichia coli*. We also determined the relationship between membrane lipid peroxidation and plasma membrane structural integrity in *Escherichia coli*. Quantitative dilutions series were performed to test for bacterial cell death. Our results indicate a biphasic killing curve when *E.coli* is exposed to copper chips. TBARS assay was used to measure the lipid peroxidation levels. The bacterial killing rate upon exposure to copper surface also correlates with increased lipid peroxidation levels.

94. Is food labeled "Organic" in our supermarkets "Genetically Modified"?

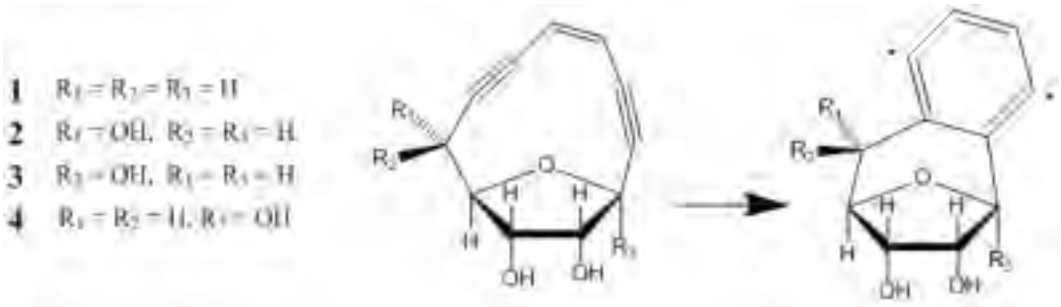
Athanasia Pavlou, Nidhi Gadura., Department of Biology, Queensborough Community College, Bayside, New York, United States.

Tomatoes, soybeans, and corn were among the first genetically modified food products approved by US agencies in the 1990s. Since then food biotechnology continues to grow rapidly. This has also led to a lot of ethical debates on what should be done about genetically modified foods. Proper labeling is very important for consumers. We decided to test food products from the supermarket that marked "organic" and compared them to regular food. Since plants are usually modified using viruses like CaMV, in our study we used primers specific to genetically modified food to reveal the truth in food labeling.

95. Computational studies of the Bergman reaction in substituted oxabicyclo[7.2.1]dodecaenediynes

Sahar Refua, Jordan Verdis., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

Geometries for the starting material and the Bergman reaction product of four substituted bicyclic dodecaenediyne compounds **1-4** have been calculated. In addition, transition state geometries have been determined by a potential energy scan of the reaction coordinate. The relevant geometries and reaction activation energies will be presented.



96. Reactivity of tris (trimethyl silyl) phosphate(TMSP): Synthesis of the bisphosphonate derivatives of b-alanine

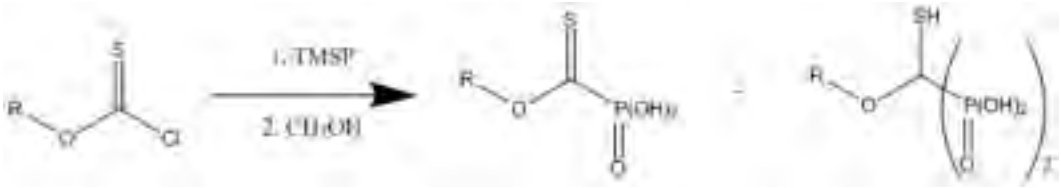
Anibal Davalos-Morinigo, Luis Vargas., Department of Chemistry, Queensborough Community College, Bayside, Ny, United States.

Bisphosphonates (BP) are well known for their affinity to bone tissue, were they inhibit osteoclast activity. They are often the drug of choice in the treatment of bone resorption diseases, such as osteonecrosis of the jaw while encouraging osteoclasts to undergo apoptosis. The synthesis of the corresponding bisphosphonate derivative of b-alanine (an endogenous b-amino acid) using tris (trimethylsilyl) phosphate(TMSP) under different conditions and is described. The identification of the product is analyzed spectroscopically.

97. Computational and experimental studies of the reaction of aryl chlorothionoformates with tris(trimethylsilyl)phosphite

Byung-Min Shin, Tresa Ambooken, Luis Vargas, Jordan Verdis., Department of Chemistry, Queensborough Community College, Bayside, NY, United States.

It is known that chloroformate esters react with tris(trimethylsilyl)phosphite (TMSP) to form alkoxycarbonylphosphonic acids after methanolysis, but the reaction does not continue to the diphosphonic acid adduct. This work presents the corresponding thiocarbonyl reactions using alkyl and aryl chlorothionoformates and explores the electrostatic factors affecting their reactivity on the basis of ab initio computations with a view to predicting the viability of other methylenediphosphonic acid derivatives.



98. Formation of [Tris(3-trimethoxysilylpropyl) Isocynurate] (TTPI) capped Palladium Nanoparticles onto Single-Walled Carbon Nanotubes

Esther Ahn, Chi Kwan Wong, Eunchul Kim, Moni Chauhan, Tirandai Hemraj-Benny., Department of Chemistry, Queensborough Community College, Bayside, New York, United States.

The integration of one-dimensional nanotubes with zero-dimensional nanoparticles (NPs) to form hybrid structures have shown to have great potential applications. In this study, we investigated the growth of palladium nanoparticles (PdNPs) onto raw, pristine single-walled carbon nanotubes (SWNTs). A "bottom-up" approach, which involves the formation of the metal nanoparticles directly onto the carbon nanotube surfaces, was considered since this method may render better systems for applications in electronic and sensor fields. In a one pot synthetic procedure Tris(3-trimethoxysilylpropyl) Isocynurate (TTPI) was treated with Palladium acetate and SWNT resulting in the decoration of SWNT with Pd. The process is straightforward and does not require functionalization of carbon

nanotubes. The SWNT-Pd NP hybrid system was characterized by High Resolution Transmission Electron microscopy (HR-TEM), Energy Dispersive X-ray Spectroscopy (EDX), UV-Vis and Infrared Spectroscopy.

99. Antimicrobial activity of Nano Silver versus Silver Salts

Ruth Lee,[2] **Eunchul Kim**,[1] Moni Chauhan,[1] Mangala Tawde.[2], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Department of Biology, Queensborough Community College, Bayside, NY, United States.

Ag nano particles were synthesized in a one-step process by the reaction of silver nitrate, [Tris(3-trimethoxysilylpropyl) isocyanourate] TTPI, and trioctyl amine. The reaction was monitored via UV-Vis spectra and the particles were analyzed by SEM and TEM. The nano Ag particles and different silver salts were then tested for antimicrobial activity against a Gram positive bacterium *Staphylococcus aureus,* a Gram negative bacterium *Escherichia coli* and a *Saccharomyces cerevisiae, a* representative of fungi*. E. coli* was selected as a bacterial indicator since it is a Gram negative bacterium with high lipid content in its cell wall. Various concentrations of nano Silver and silver salts were tested on selected microorganisms for growth inhibition/death using Kirby-Baur method and broth killing assay. The Minimal Inhibitory Concentration (MIC) for the Ag nano particles was determined by these and other standard methods. We aim to determine the mode of action of antibacterial effect of silver nano on bacterial membrane components. We are also preparing nano silver in TTPI gels that will be tested against target bacteria.

100. Determination of Caffeine Content in Energy Drinks by High Pressure Liquid Chromatography.

Xiaomei Ye, TianChun Xu, Pedro Irigoyen., Department of Chemistry, Queensborough Community College of CUNY, Bayside, NY, United States.

High pressure liquid chromatography (HPLC) has been successfully used to determine the concentration of caffeine in various energy drinks. The correlation between these measurements and those associated with different coffee drinks is highlighted. Partial conclusions will investigate the possibility of whether the surge in energy by the drinker is caused by the vitamins and amino acids in the drink or a caffeine boost. The stepwise procedure for this experimental analysis and drawbacks will be presented.

101. Analyzing commercial discharges for various pollutants: A DEP industrial pre-treatment program internship.

Gerasimos Kouloumbes,[1] Faye Jacques,[2] Panayiotis Meleties,[3] Paris Svoronos.[1], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Bureau of Wastewater Treatment, New York City Department Environmental Protection, Wards Island, NY, United States; [3]Office of Academic Affairs-Math and Science Division, York College, Jamaica, NY, United States.

The DEP Industrial Pretreatment Program (IPP) is a federally authorized program by the Clean Water Act of 1971 that works to control commercial discharges by requiring industries targeted by federal and local pretreatment regulations to remove specific toxins from their wastewater before it is released into the City's sewer system. IPP helps to protect the sewers, the wastewater treatment plants and the City's receiving waters. By collaboration with several community colleges in NYC, including Queensborough Community College, interns are assigned to various sectors including IPP. Interns would accompany IPP technicians into the field, analyzing commercial discharges for several infractions including harmful biological agents, chemical pollutants such as cyanide, high chlorine levels, high lead and mercury content, and irregular pH levels. All procedures and testing follow New York State and Federal guidelines.

102. Analysis of Holistic Fish Based Dry Dog Food for Heavy Metals Using X-ray Fluorescence Spectrophotometry

Andre Smithson, Pedro Irigoyen, Irina Rutenburg, TianChun Xu., Chemistry, Queensborough Community College of CUNY, Bayside, NY, United States.

During the last decades the holistic approach to human health, medical care, nutrition, and life style in general had gained tremendous popularity and extended from human life style to their pets in every aspect of their life as well. Veterinarians offer acupuncture, massage, and herbs instead of medications. It has already been for a while that all pets' foods are fortified with vitamins and minerals, but lately the additional trend of elimination of all unhealthy ingredients became very strong. It is difficult to create vegetarian food for dogs and cats – thus companies offer alternative to standard chicken and beef, or even lamb and turkey proteins. These alternative proteins being buffalo, elk, venison, rabbit, kangaroo, pheasant, duck, and finally fish. Health officials have been warning consumers about the hazard of having too much fish in human diet due to the possibility of relatively high concentrations of heavy metals in sea food – as the result of contamination of ocean water with various pollutants. We are interested to investigate the possibility of the presence of heavy metals in the holistic fish based dry dog food – using X-ray Fluorescence Spectrophotometry. We compare the fish based food with other holistic as well as standard foods (supermarket brands). We also compare our results with the EPA standards for heavy metals in drinking water and FDA standards for heavy metals in human food.

103. Importance of Linear Free Energy Relationships LFERs in studying solvolytic behavior in Thio- and Thionocarbonyl Esters

Brian Mahon., Department of Chemistry, Wesley College, Dover, DE, United States.

Many thio-and thiocarbonyl esters are used as precursors to prepare low molecular weight protease inhibitors that can be effective anti-HIV agents or uselfull AIDS ttreatments. These compounds have also proven to be effective as pro-drugs against the microbial infection, Pneumocystis carinii pneumonia and have other potential for their anti-Hepatitis B virus activiy. The specific rates of solvolysis of methyl and isopropyl chlorothioformate, and 4-fluorophenyl chlorothionoformate have been analyzed and compared using the extended Grunwald-Winstein equation. Previous research from our laboratories has shown that solvolysis occurs at the C=O or C=S group via a stepwise addition-elimination pathway in the more nucleophillic solvents. We acknowledge the NIH NCRR INBRE grant 2 p20 RR016472-09 for reaserch support.

104. Kinetic Evaluation of s -Isobutyl Chlorothioformate

Matthew McAneny, Malcolm D'Souza., chemistry, Wesley College, Dover, Delaware, United States.

Thiochloroformate esters are often used as intermediates in the synthesis of novel pro-drugs that are activated by the organism by means of natural biochemical processes. As a result there has been significant interest in their hydrolysis, alcoholysis, and aminolysis processes, as such reactions are useful models for enzymatic mechanisms.

The effects of solvent variation of the available specific rates of solvolysis of *s*-isobutyl chloroformate, are analyzed in terms of the extended Grunwald-Winstein equation using the N_T scale of solvent nucleophilicity (S-methyldibenzothiophenium ion) combined with a Y_{Cl} scale based on 1-adamantyl chloride solvolysis. Previous studies found that alkyl or phenyl chlorothioformates solvolyze in the more nucleophilic solvents by an addition-elimination mechanism with the addition step being rate-determining and in the highly ionizing solvents, the mechanism is unimolecular.

105. High pressure synthesis of water splitting oxynitrides

Parsa Sharifi,[1] William Woerner,[2] Lars Ehm.[3], [1]Department of Chemistry, Queensborough Community College, Bayside, NY, United States; [2]Department of Giosciences, Stony Brook University, Stony Brook, NY, United States; [3]Mineral Physics Institute, Stony Brook University, Stony Brook, NY, United States.

While hydrogen is a potential "green" energy source, obtaining hydrogen through conventional processes consumes large amounts of energy. Solar water splitting on semi-conductive surfaces might be an economic way of producing hydrogen. A promising class of materials for solar water splitting are oxynitrides, $A_{1-x}B_xO_{2-y}N_y$ (A=metal, B=transition metal, 0£x£1, y£1). The water splitting properties of oxynitrides are amplified by increasing the amounts of nitrogen. Incorporation of nitrogen can be increased in the crystal structure through the utilization of high pressure synthesis. We performed the synthesis of oxynitrides in a piston cylinder apparatus. The initial reagents were GaN and TiO2 in a stoichiometric ratio of 1:1. The runs were performed at 9.3 Kbar and at 1473K. The synthesis products were characterized by x-ray powdered diffraction and electron microprobe analysis. Through optical microscopy, three distinct phases could be identified. No total conversion of the initial reagents to the targeted $GaTiO_2N$ oxynitride occurred. Optimization of pressure and temperature parameters for the high pressure synthesis is needed. Further analysis, to be conducted after the conclusion of this summer session, using x-ray powdered diffraction and microprobe analysis is needed to qualitatively and quantitavely identify the phases.

106. Bacterial metabolism of ionic liquid-pretreated lignocellulose: production of biofuels

Firmause Payen,[1] Samanta Boursiquot,[1] Sharon I Lall-Ramnarine,[1] Marie Thomas,[2] James F. Wishart.[2], [1]Department of Chemistry, Queensborough Community College, CUNY, Bayside, NY, United States; [2]Department of Chemistry, Brookhaven National Laboratory, Upton, NY, United States.

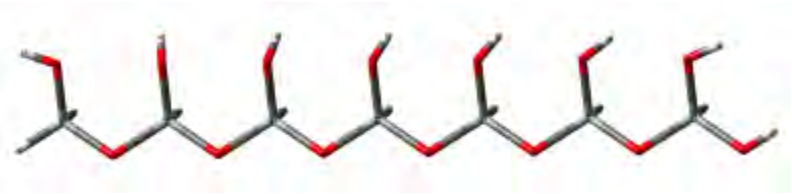
Ionic liquids (ILs) which are compounds that melt below 100 °C. They have a number of attractive properties including non-volatility, high conductivity, good dissolution properties, and the potential to be recyclable. These properties make them popular choices as solvents among researchers in many areas. The goal of this project is to design different types of ILs that can dissolve wood flour to extract the cellulose for the production of biofuels. Halide salts based on N-methylpyrrolidine, 1, 4-diazabicyclo [2.2.2] octane, and 4-dimethylaminopyridine were prepared with hydroxyl group functionalities. These salts were purified and converted to ILs bearing alkyl-phosphate anions. The structures of the salts were confirmed using ^{1}H, ^{13}C, and ^{31}P nuclear magnetic resonance (NMR) spectroscopy. The N-(3-hydroxypropyl)-N-methylpyrrolidinium dibutyl phosphate was used in an attempt to dissolve wood flour. However no dissolution occurred. Unfortunately we could not do more dissolution experiments because the other ILs could not be dried on time. Future work will focus on performing more dissolution experiments with the ILs that were synthesized. Then the cellulose extracted will be broken down to fermentable sugars, which can be fermented with bacteria such as Clostridia Sp to produce ethanol and butanol. This work was supported in part at BNL by the U. S. DOE Office of Basic Office of Basic Energy Sciences under contract # DE-AC02-98CH10886.

107. Si-H bond activation in models of siloxanes – a DFT study

Daniel Sangobanwo, Mihaela Diana Bojin., Chemistry, Queensborough Community College, CUNY, Bayside, NY, United States.

Siloxanes are polymers containing Si-O bonds. Recent studies point out that their functionalization could enhance their physical and chemical properties, and thus enrich their potential applications. A typical pathway for this process is Si-H bond activation by removing hydrogen atoms either as protons or as hydrides. This is achieved by adjusting reaction conditions and the groups attached to each silicon center. We investigate a series of molecular models of polysiloxanes with linear structures. These molecules range from just one silicon center, up to seven silicon atom chains, Si_7O_7 (Figure 1),

by gradually increasing the number of silicon and oxygen atoms. The strength of the Si—H bonds is varied by using either electron donating or electron accepting groups, such as NH_2, CF_3, OH, CH_3 and F, to determine the conformation of these silicon polymers. We are using theoretical methods, Density Functional Theory (DFT), B3LYP/6-31+G(d,p), to optimize these structures and perform frequency analyses. We aim to correlate our results with the experimental data obtained by Dr. Moni Chauhan at QCC, and extend our findings to polymer chemistry.



Analytical Chemistry I

108. Imaging of impact modifier dispersion in plastics with an optical microscope

Gunter Moeller, George Papakonstantopoulos., Department of Analytical and Systems Research, Arkema Inc., King of Prussia, Pennsylvania, United States.

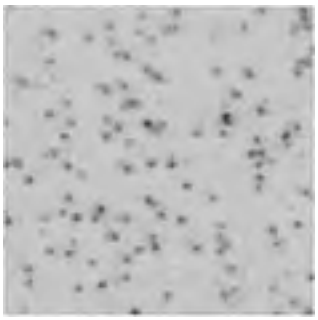
Mechanical, optical, and chemical properties of polymers depend largely on functional fillers such as processing aids, pigments, flame-retardants, and impact modifiers. Besides the chemical nature of the additives, their dispersion quality, average size, and size distribution are crucial for understanding field performance. To determine these parameters rather costly and labor-intensive techniques, such as electron microscopy and atomic force microscopy are commonly used.

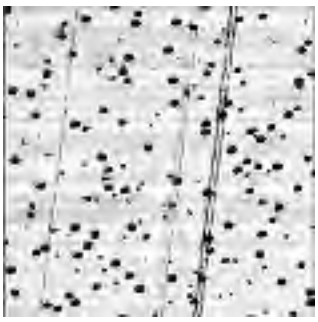
We demonstrate how optical microscopy in combination with image analysis can be used for dispersion analysis in plastics as a cost effective alternative. The study was done using a research grade compound microscope with a high numerical aperture to maximize lateral resolution. Image analysis was done using the ImageJ software.

Refractive index mismatch and particle size are key parameters for the determination of impact modifier dispersion quality with an optical microscope. Particle size analysis results are in very good agreement with AFM results provided proper image analysis tools are used and the particles are large enough. For smaller particles and typical impact modifiers with a multi-modal size distribution and varying particle shapes (agglomerated type versus grow-out) it may not be possible to determine the dispersion quality and degree of agglomeration as accurately as with the AFM method. We show results for nine different impact modifier / matrix systems with varying refractive index contrast and particle sizes, and distributions.

When the material contains larger amounts of other additives such as pigments, flow aids, metallic flakes etc. it is not possible to visualize individual impact modifier particles using the optical method because of optical interference. The method works best for relatively low loadings of impact modifiers.

Optical image (figure 1, upper image) and AFM image (figure 2, bottom image) of a proprietary Arkema impact modifier dispersed in a matrix. The imaged area is 20 mm x 20 mm in both cases.





109. Characterization of degradation pathways of modified therapeutic oligonucleotides using mass sequencing via UPLC MS

Ann M O'Brien,[1] Natalie A Daurio,[2] Anthony M Leone.[1], [1]Merck Co. Inc., West Point, PA, United States; [2]College of Arts & Sciences, Syracuse University, Syracuse, NY, United States.

In 2006 the Nobel Prize in Physiology or Medicine went to Fire and Mello for their work on RNA interference (RNAi). Their discovery of a fundamental mechanism of gene regulation demonstrated that a gene can be silenced via mRNA elimination by short interfering RNA (siRNA). This discovery has stimulated efforts to expand the potential of RNAi in the development of novel genome therapeutics. A more recently published development in the RNAi field by Morrissey *et al* showed significant *in vivo* siRNA stability with the introduction of specific modifications to the RNA sequence, while not reducing its specific silencing activity. Little is known however, on the long term stability or the specific degradation pathways of these modified oligonucleotides.

To be pursued as a viable therapeutic the stability and degradation pathways of these modified oligonucleotides must be characterized. Using multiple forced stress conditions an array of degradation products are generated in an effort to quickly produce entities that might be encountered during the multi-year development of a therapeutic product. For initial studies, two types of forced stress were applied, acid and base. For the acid stress, formic acid (pH3) is added to the modified oligonucleotide and incubated at 65C for several hours. For the base stress, ammonium hydroxide (pH11) is added. Following incubation the solution is adjusted to pH8 to quench the degradation. Ion-pairing, reversed phase UPLC is used to separate the degradation products prior to Q-TOF MS analysis.

110. Multivariate analysis for resolving tryptophan and tyrosine emissions

Carol A. Roach, Sharon L. Neal., Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

Protein emission from the amino acids tryptophan and tyrosine has been extensively studied. The microenvironment sensitivity of tryptophan has led to the development of techniques that sacrifice tyrosine emission in order to gain structural information about the protein. With its low quantum yield (~15%), and overlapped absorption spectrum with tyrosine, much of the tryptophan emission is sacrificed as well. Using multivariate data analysis of emission decay matrices, we have resolved the

emissions and lifetimes of tryptophan and tyrosine simultaneously excited in solution. We propose that this analysis will be useful in the study of single tryptophan proteins as excitation closer to the absorption maximum will result in larger emission signals that may be resolved into the individual contributions of tryptophan and tyrosine.

111. Probing light-harvesting with photo-induced chronoamperometry

Jonas I Goldsmith., Department of Chemistry, Bryn Mawr College, Bryn Mawr, PA, United States.

The single component photocatalytic system based on $Ir(ppy)_2(bpy)(PF_6)$ (where ppy is 2-phenylpyridine and bpy is 2,2′ bipyridine) effects the reduction of water to hydrogen gas without the need for an electron-shuttling catalyst. A crucial step in this process is the reductive quenching of the photoexcited iridium complex to generate a highly active Ir(II) species. To examine this process, photoinduced chronoamperometry (PICA), a variant of traditional potential step chronoamperometry, was employed. In the PICA technique, the potential at a working electrode is held constant and a pulse of light and the concomitant photochemistry stimulated by that pulse is used to effect a rapid change in the composition of the solution. A current transient that decreases with time is the signature of the photochemically generated species being detected at the working electrode. In this work, PICA is used to investigate the effect of light intensity on the production of the reductively quenched iridium species, described above, that is involved in the photocatalytic generation of hydrogen.

112. High pressure direct protein extraction from tissue

Nicholas Sobol, Jennifer Oprihory, Parth Kothiya, Zeineen A. Momin, Naresh Vasani, Vladamir Kachalov, Tiffany Remsen, Faraj Al Qaraghuli, Paul H Pevsner., Department of Pathology, University of Missouri School of Medicine, Columbia, MO, United States.

High pressure direct protein extraction from tissue takes 30 seconds while other separation techniques, can take hours. The Barocycler, a high pressure instrument (Pressure BioSciences Inc., South Easton, MA) was used for these experiments. We hypothesized that any tissue sample such as heart or brain can be put in the instrument and as long as a buffer, ammonium bicarbonate, is added, proteins can be extracted.

Sections of normal and 1-3 Gy irradiated mouse tongue and heart were obtained. They were used for protein extraction and later tandem mass spectrometry LCMS analysis for amino acid sequence and bioinformatics protein identification. The section was immersed in 900 µl of ammonium bicarbonate in a Barocycler pulse tube. The pulse tube was filled with solvent because a fluid void in the pulse tube could result in collapse of the tube and loss of sample while under high pressure. The proteins were extracted with 35,000 psi alternating pressure for about 30 seconds. After the cycles were finished, the protein containing solution was transferred to a microcentrifuge tube. The extracted samples were centrifuged for about 5 minutes then lyophilized to a volume of 50 µl. The samples were run in the LCMS for protein identification.

The LCMS was able to identify proteins from mouse tongue and heart. In the tongue, post 1 Gy, hemoglobin subunit a was identified; post 2 Gy, fatty acid-binding protein adipocyte was identified and post 3 Gy, hemoglobin a chains was identified. Albumin was identified in post 2 and 3 Gy. In the heart, the protein was Actin, alpha cardiac muscle 1 OS=Mus musculus was identified.

The proteins identified with LCMS demonstrated rapid high yield extraction with high pressure and confirmed our hypothesis.

113. Maldi imaging, ims, of tissue field defects in colorectal carcinoma

Tiffany Remsen, Parth Kothiya, Zeineen A. Momin, Naresh Vasani, Vladamir Kachalov, Jafar Imanpour, Siddharth Mathur, Chethana Kanaparthi, Sury Anand, Paul Pevsner., Department of Pathology, University of Missouri School of Medicine, Columbia, MO, United States.

Recently, specimens from two patients, imaging MALDI (IMS) displayed two proteins, gi|119592539 hCG1787564 [Homo sapiens] Mass: 57590 and gi|119592490 hCG2040674 [Homo sapiens] Mass: 108178 in colon adenocarcinoma and normal tissue. This discovery may represent a marker for field cancerization or defect. These alterations result in microsatellite instability, where synchronous and metachronous lesions develop into cancers. Therefore, histopathology could affect therapy by underestimating the extent of metaplastic or malignant disease. We hypothesized that comparing IMS to histopathology would improve the identification of satellite metaplastic.

Specimens were obtained from individuals with colon adencarcinoma and compared to normal colon tissue. Samples were immersed in a solution of dimethyl sulfoxide (DMSO) 2%, glycerol 20%, and ethyl alcohol 78% and stored at 4º C. The mixture cryoprotects the tissue without fixed cross-linking proteins. Cryosections were obtained for IMS, hematoxylin and eosin staining, and protein extraction. A pathologist reviewed each specimen. Proteins were extracted from colon tissue with organic solvent and high pressure using ProteoSolve and a Barocycler (Pressure Biosciences, West Bridgewater, MA). Protein fractions were trypsinized, and peptides studied with LCMS.

Additional proteins were identified in the colon biopsies using Mascot search engine interrogation of the NCBInr and Swiss prot databases.

Variation in polyp proteins in biopsy tissue suggests genetic field differences, which could predict carcinoma developing in these polyps and at other sites in the colon. These findings may alter diagnosis of tumor and require examination of biopsy tissue with histopathology and mass spectrometry for complete diagnosis to exclude malignancy.

114. Maldi and lcms protein biomarkers of ionizing radiation

Tiffany Remsen, Vladamir Kachalov, Parth Kothiya, Zeineen A. Momin, Naresh Vasani, Jason Chouake, Douglas C. Miller, Paul Pevsner., Department of Pathology, University of Missouri School of Medicine, Columbia, MO, United States.

Purpose

The goal of this project was to identify dose-related protein biomarkers of ionizing radiation (IR) with mass spectrometry, specifically, biomarkers of the 2 Gy threshold dose for radiation sickness. This goal was pertinent because a civilian nuclear power plant accident or a terrorist nuclear event on U.S. soil could result in a vast number of casualties. Some of the victims would be hospitalized because of acute signs and symptoms, such as vomiting, burns and pain requiring immediate care. Some victims would appear symptom free, but may have received ³ 2 Gy; total body radiation (TBI). They would develop radiation sickness in the next 6-24 hours. Initial mass spectrometry (MS) experiments demonstrated radiation dose-related albumin and other induced proteins in radiosensitive murine buccal mucosa and tongue tissue.

Methods

Swiss Webster (CFW®) Mice, 25-30 gram were used. Forty mice, 10 control and 30 experimental were used. The animals were, anesthetized with intraperitoneal, ip, ketamine-xylazine (k/x, 80/10 mg/kg), Sigma Aldrich, St. Louis. The animals received TBI as follows: 1 Gy (10 mice), 2 Gy (10 mice) and 3 Gy (10 mice), in groups of five. Sucrose 30%, 5cc was used to clear the vasculature of blood by intracardiac/femoral perfusion under terminal anesthesia. The sucrose protected the tissue

from freezer artifact, disruption of tissue architecture by ice crystals, when the tissue was frozen for cryosection. One-micrometer (μm) serial sections were obtained for histology, IMS, and protein extraction for LCMS.

Results

H&E tissue sections and IMS of post 1 Gy TBI, demonstrated corresponding progressive increases in tissue destruction on the tissue sections and changes in tissue albumin with increasing IR dose. At 2 Gy there was peripheral tissue damage of the spicules on H&E, and AFM images and a corresponding increase in peripheral albumin in the IMS images. At 3 Gy the peripheral tissue damage of the spicules and the central damage of the tongue was severe on the H&E sections. The albumin was now virtually absent in the periphery and concentrated in the center of the IMS image. LCMS studies were performed on trypsin digest protein extracts from normal and post 1, 2 and 3 Gy tongue tissue, and normal and post 2 Gy IR heart tissue. Albumin was demonstrated in the mouse tongue 1 hour post 2 Gy and 3 Gy. LCMS confirmed the finding of Hemoglobin Subunit a in the IMS post 1 Gy; Fatty Acid-Binding Protein Adipocyte in the IMS image post 2 Gy; and Hemoglobin a Chains in the IMS image post 3 Gy. The LCMS protein identified in the normal and post 2 Gy cardiac tissue was identical, Actin, alpha cardiac muscle 1 OS=Mus musculus.

Conclusion

MALDI, IMS, and LCMS identified IR induced dose-related proteins. The identification of these IR dose-related biomarkers is novel. These protein biomarkers of IR could distinguish the 2 Gy threshold dose level for radiation sickness. This study is proof of principle that MALDI and LCMS can identify dose-related protein biomarkers of IR.

115. Maldi imaging and diagnosis of prostate cancer

Tiffany Remsen, Adair Seager, Jonathan Melamed, Paul Pevsner., Department of Pathology, University of Missouri School of Medicine, Columbia, MO, United States.

Abstract

In a previous experiment, prostate samples were obtained to see if we could produce images and identify proteins. We succeeded in using MALDI-imaging (IMS) to identify prostate cancer proteins. The most important proteins were TGFb1, LTGFb and hCG. These can be used for potential biomarkers. For this experiment, more prostate samples, 240 in total, were studied. Finally, we are going to try to run IMS for peptides and MALDI-MSMS to prove these results are not tentative.

Methods

The prostate polyp sections were mounted on target plates where they were put in a methanol bath for 15 minutes and dried in an oven. Then the target plates were put in a xylene bath for 15 minutes and dried in an oven. Matrix and calibrate was pipetted near the tissue while matrix was pipetted on top of the samples. The target plates were put in the oven to dry and run on MALDI for imaging. For MALDI imaging, the system was opened and the cursor was moved to the location of calibrate and the target plate was calibrated. After calibration, the cursor was moved to the tissue sample where the width, height, center x and y were calculated for each prostate. There were 20 prostate samples per coordinate and there were 12 coordinates. The width, height, center x and y were put into the system. The system was set to store all, saved before the run and then fired, to run MALDI imaging. After the run, the data was exported to biomap. Then biomap and the spectrum was opened. The peaks were highlighted which displayed an image. IMS procedure was performed for peptides and MSMS.

Results

Proteins were identified in the prostate biopsies using Mascot search engine interrogation of the NCBInr and Swiss prot databases. The most common proteins found in the majority of samples were hCG, immunoglobulin chain and proteins associated with HIV type 1.

Conclusion

Variation in prostate proteins in biopsy tissue suggests genetic field differences, which could predict carcinoma at these and other sites in the prostate. These findings may alter tumor diagnosis and require examination of biopsy tissue with histopathology and mass spectrometry for complete diagnosis.

116. Application of principal component analysis and two dimensional correlation spectroscopy to investigate drug-polymer miscibility

David Heaps, Alfred Rumondor, Lynne Taylor., Department of Analytical Chemistry, AstraZeneca Pharmaceuticals LP, Wilmington, DE, United States.

Drug-polymer miscibility in a binary mixture may dictate the ability of the system to deliver poorly soluble therapeutic compounds. In this work, principal component analysis (PCA) and two dimensional correlation spectroscopy (2D COS) are used to elucidate results obtained through infrared spectroscopy, powder x-ray diffractometry, and differential scanning calorimetry (DSC). Four model binary systems are chosen, namely felodipine-poly(vinyl pyrrolidone) (PVP), nifedipine-PVP, ketoconazole-PVP, and felodipine-poly(acrylic acid) (PAA). The results obtained shows that through the application of PCA and 2D COS to data collected, the miscibility behavior of these binary systems can be better explained. It is found that felodipine-PVP and nifedipine-PVP clearly formed miscible mixtures, while felodipine-PAA did not form a miscible mixture. Additionally, partial miscibility is observed for ketoconazole-PVP system

Computers in Chemistry

Organizers: Sandeep Patel, Zheng Yang
Sponsor: RCH Solutions

117. Computational alanine scanning with linear scaling semi-empirical quantum mechanical methods

David J Diller,[1] Christine Humblet,[1] Xiaohua Zhang,[2] Lance M Westerhoff.[2], [1]Consultant, East Windsor, NJ, United States; [2]QuantumBio Inc., State College, PA, United States.

Alanine scanning is a powerful experimental tool for understanding the key interactions in protein-protein interfaces. Linear scaling semi-empirical quantum mechanical calculations are now sufficiently fast and robust to allow meaningful calculations on large systems such as proteins, RNA and DNA. In particular, they have proven useful in understanding protein-ligand interactions. Here we ask the question: can these linear scaling quantum mechanical methods developed for protein-ligand scoring be useful for computational alanine scanning? To answer this question, we assembled 15 protein-protein complexes with available crystal structures and sufficient alanine scanning data. In all, the data set contains DDGs for 400 single point alanine mutations of these 15 complexes. We show that with only one adjusted parameter the quantum mechanics based methods out perform both buried accessible surface area and a potential of mean force and compare favorably to a variety of published empirical methods. Finally, we closely examined the outliers in the data set and discuss some of the challenges that arise from this examination.

118. Molecular description of flexibility in an antibody combining Site

Ian F. Thorpe., Department of Chemistry and Biochemistry, University of Maryland, Baltimore County, Baltimore, MD, United States.

Mature antibodies (Abs) specific for virtually any foreign molecule may be produced by affinity maturation of naïve (or germline) Ab. However, the finite number of germline Ab available suggests that, in contrast to mature Ab, germline Ab must be broadly polyspecific so that they are able to recognize a wide range of ligands. Thus, affinity maturation must play a role mediating Ab specificity. One biophysical property that differentiates polyspecificity from specificity is protein flexibility; a flexible combining site is able to adopt a variety of conformations that recognize different foreign molecules (or antigens), while a rigid combining site is locked into a conformation that is specific for a given antigen. Recent studies (Proc. Natl. Acad. Sci. USA 104:8821-8826, 2007) have examined the structural properties that mediate changes in flexibility at four stages of affinity maturation in the 4-4-20 Ab. These studies employed molecular dynamics simulations to reveal a network of residue interactions that mediate the flexibility changes accompanying maturation. The flexibility of the Ab combining sites in these molecular systems was originally measured using 3-pulse photon echo spectroscopy (3PEPS). The present investigation extends this work by providing a concrete link between structural properties of the Ab molecules and features of the spectroscopic measurements used to characterize their flexibility. Results obtained from the simulations indicate that the spectroscopic signal is sensitive to protein dynamics distributed throughout the combining site. Thus, the simulations provide a molecular level interpretation of the changes induced by affinity maturation of the Ab. The results suggest that 3PEPS spectroscopy in combination with molecular dynamics simulations can provide a detailed description of protein dynamics and, in this case, how it is evolved for biological function.

119. Development of the Next Generation of the Shape Signatures Technique for Molecular Shape Comparison

Randy J Zauhar,[1] William J Welsh.[2], [1]Depts of Chemistry & Biochemistry/ Bioinformatics & Computer Science, University of the Sciences, Philadelphia, PA, United States; [2]Department of Pharmacology, University of Medicine & Dentistry of New Jersey, Piscataway, NJ, United States.

The Shape Signatures method is an approach for compactly encoding the shapes of molecules and protein receptor sites. It uses a technique much like *ray-tracing* (a method widely used in computer scene rendering) to explore the volume interior to a ligand's solvent-accessible surface, or the volume exterior to a protein receptor site. Shape Signatures are simply probability distributions derived from the ray-trace, and stored as histograms. They are sensitive to the details of molecular shape (and optionally electrostatic properties), and are rapidly compared - chemical libraries with millions of structures can be scanned in a matter of minutes to assess similarity to a query compound.

The first generation of Shape Signatures was restricted to considering a target molecule as an indivisible unit. While proven effective in a number of drug discovery projects, the original method loses selectivity for molecules that incorporate a significant number of heterogeneous ring systems, as the shape descriptors essentially lump together contributions of independent and dissimilar molecular components. To avoid this consequence, a new generation of the method has been developed that includes the following significant improvements:

Automatic fragment generation: Molecules are now partitioned automatically into component fragments using ring systems as anchors. The ray-trace is decomposed into inter-and intrafragment contributions, as are the Shape Signature descriptors derived from the trace. **Automated mapping of query and target structures:** Molecules being compared have their constituent fragments mapped onto each other in all ways consistent with chemical structure, and with overall scoring derived from the individual fragment-based shape comparisons.

The new approach retains the principle advantage of the original method, namely its focus on shape independent of chemical structure, while still using the underlying chemical bonding as a foundation for decomposing the shape representation in a meaningful way. We expect this will greatly improve the selective power of the method when complicated structures are being compared. Computational details of the new approach will be presented, along with illustrations of its application.

120. CADD methodologies for lead optimization: Recent advances

Richard D Cramer., CSO, Tripos Intl, St. Louis, MO, United States.

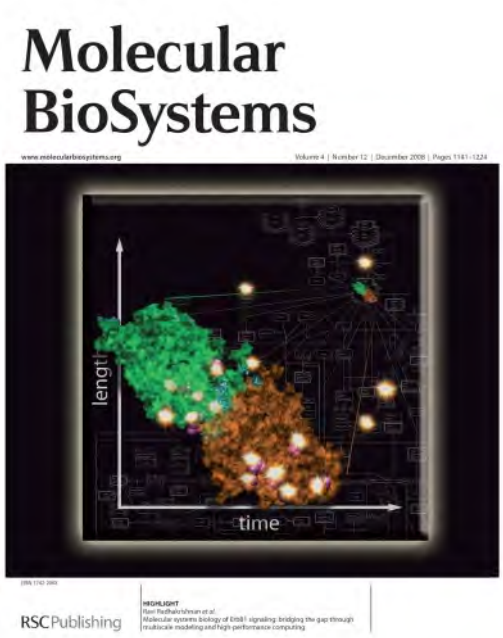
During lead optimization, the candidate structures are very similar, usually differing only by an R-group., and therefore exhibit similar potencies, typically having a variance little more than a log unit. Although "locally-derived" QSAR models are the only CADD approach capable of meaningfully ranking such similar candidates, previous 3D-QSAR approaches have required tedious and somewhat subjective manual structural alignments. However, emerging results from prospective make-and-test applications of the new topomer CoMFA approach, combined with an exceptional ease of use, strongly encourage its beneficial use in any lead optimization project. Its unprecedented "RGVS" capability to identify the most promising novel R-groups from among >10E6 candidates could even be project critical.

Other CADD advances for lead optimization include a docking capability that can be "locally optimized" whenever many experimental structures and/or potencies exist, a multi-criteria optimization function that is readily adaptable to individual project goals and is associated with a project-proven de novo engine.

121. Molecular systems biology through multiscale modeling and high-performance computing

Ravi Radhakrishnan., Department of Bioengineering, University of Pennsylvania, Philadelphia, PA, United States.

We focus on an important cell-signaling pathway whereby the activation of the ErbB family growth factor receptors on the cell membrane lead to important cellular decisions such as cell-proliferation, cell-death, or cell-migration. We employ multiscale simulation approaches to incorporate a molecular context to the signaling pathway involving this receptor to capture how subtle differences in the molecular context of the intracellular environment (e.g., differences in phosphorylation states or closely related mutant proteins can nevertheless translate into crucial differences in the manifestations of the emergent signaling and trafficking responses and cell decisions. Specifically, (1) we employ atomistic models to gain insight into the activation mechanism of the growth factor receptor and how it initiates signaling. (2) We also employ a recently developed a coarse-grained methodology for combining membrane mechanics and dynamics using the time-dependent Ginzburg-Landau (TDGL) formalism together with the stochastic kinetic Monte Carlo (or KMC) based dynamics of curvature inducing proteins for modeling how the receptor endocytosis. Mechanisms (1) and (2) represent activating and deactivating steps in the signaling pathway and a balance between the two is essential for cellular homeostasis. We show how point mutations in the receptor that perturbs a single amino acid position can cause cascading effects of fragility both at the molecular level and at a signaling network level and discuss the mutations in the context of a particular cancer cell line.



A. Shih, J. Purvis, R. Radhakrishnan, Molecular Systems Biology of ErbB1 Signaling: Bridging the Gap through Multiscale Modeling and High-Performance Computing, 2008, Mol. Biosystems. (A Royal Society of Chemistry Journal), 4, 1151-1159. Highlight article. (Pubmed ID: 19396377).

122. Fluctuation dynamics analysis of gp120 envelope protein reveals a topologically based communication network

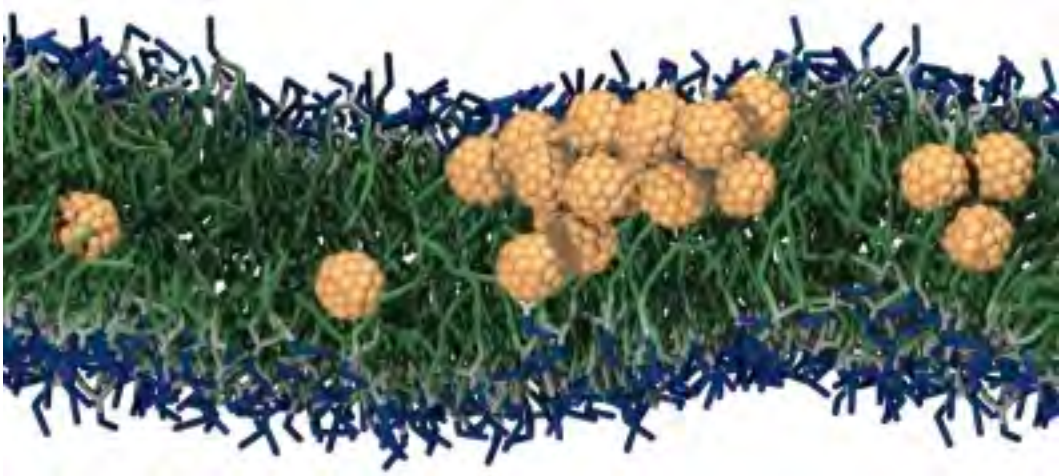
Judith M. LaLonde,[1] Indira Shrivastava.[2], [1]Chemistry, Bryn Mawr College, Bryn Mawr, PA, United States; [2]Department of Computational Biology, School of Medicine, University of Pittsburgh, Pittsburgh, PA, United States.

HIV infection is initiated by binding of the viral glycoprotein gp120, to the cellular receptor CD4. Upon CD4 binding, gp120 undergoes conformational change, permitting binding to the chemokine receptor. Crystal structures of gp120 ternary complex reveal the CD4 bound conformation of gp120. We report here the application of Gaussian Network Model (GNM) to the crystal structures of gp120 bound to CD4 or CD4 mimic and 17b, to study the collective motions of the gp120 core and determine the communication propensities of the residue network. The GNM fluctuation profiles identify residues in the inner domain and outer domain that may facilitate conformational change or stability, respectively. Communication propensities delineate a residue network that is topologically suited for signal propagation from the Phe43 cavity to the chemokine receptor binding site. These results provide a new context for interpreting gp120 core envelope structure-function relationships and may be used to guide structure based drug design.

123. Coarse-grained molecular dynamics simulations of fullerines interacting with lipid bilayers.

Preston Moore,[1] Steven Nielsen,[2] Russel DeVane.[3], [1]Department of Chemistry & Biochemistry, University of the Sciences in Philadelphia (USP), Philadelphia, PA, United States; [2]Department of Chemistry, University of Texas at Dallas, Richardson, TX, United States; [3]Institute for Computational Molecular Science and Department of Chemistry, Temple University, Philadelphia, PA, United States.

We will present our results on the biophysical and physicochemical properties of biological membranes interaction with fullerenes through coarse-grain (CG) molecular modeling. Specifically we ahve developed a transferable coarse grained molecular dynamics potential for proteins, lipids, and carbon based nanomaterials. Specifically, the intermolecular potentials, which are based on Lennard-Jones functional forms, were parametrized and validated using experimental thermodynamic data including surface tension, density and partitioning data. We have applied these CG potential to investigate different factors that affect the solubility of buckyballs (C60) and single-walled carbon nanotubes (SWNTs) while providing access to time and length scales unavailable through fully atomistic methods. Solubility, transfer free energy, and dimerization free energy data for C60 and SWNTs obtained using the proposed models show excellent agreement with experimental and fully atomistic MD data. In particular, cluster analysis of C60 aggregation in a hydrocarbon melt corroborates the force field parameters. The combined results provide a strong basis for applying this model for further large scale MD studies involving C60 and SWNTs.



124. Role of electrostatics in modulating hydrophobic interactions and barriers to hydrophobic assembly

Brad A. Bauer, Sandeep Patel., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

Hydrophobic effects influence a range of physical phenomena ranging from the aggregation and assembly of colloids in water to protein folding. In this work, the interaction of two large-scale hydrophobic plates and water is examined using molecular dynamics (MD) simulations. Various water models, encompassing polarizable and nonpolarizable force fields, are considered and compared. Position dependent profiles of water density, dipole moment, orientation, hydrogen bonding, and free energy of plate-plate interactions are presented. Predictions of critical plate separation distances (suggestive of the onset of drying transitions) are also considered. We expand upon current understanding of hydrophobic interactions and the empirical models used to study them.

125. Binding pocket analysis of seven helical transmembrane proteins: Is sequence identity alone suitable for modeling GPCRs as drug targets?

Vagmita Pabuwal,[1] Zhijun Li.[1,2,3], [1]Department of Chemsitry & Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, United States; [2]Department of Bioinformatics and Computer Science, University of the Sciences in Philadelphia, Philadelphia, PA, United States; [3]Institute for Translational Medicine and Therapeutics, University of Pennsylvania, Philadelphia, PA, United States.

Transmembrane proteins are responsible for various physiological and pathological mechanisms in human body. They account for ~30% of human genome which makes it important to understand their structure function relationship. Seven helical transmembrane proteins including the G-protein coupled receptors (GPCR), accounts for ~26% of current drug target and has proven to be important and lucrative pharmaceutical targets. Analyzing their binding sites would give us better understanding of their function with respect to their structure. Various computational methods have been introduced so far for the binding site comparison of soluble proteins. In current work we compare the binding sites of these seven helical membrane proteins using Cavbase, a software taking into account the physicochemical properties and shape of the side chain residues at the binding site for the comparison of any two binding sites. This study was done on 92 seven helical membrane proteins including bacteriorhodopsin and bovine rhodopsin, squid rhodopsin, $beta_1$ adrenergic, $beta_2$ adrenergic, and adenosine GPCRs. Our study suggests that structure with high sequence identity may have low structural similarity around binding site although these are suppose to be conserved structurally. This implies that we should not rely solely on sequence identity for selecting templates for homology modeling of GPCRs.

126. Molecular Dynamics Simulation of Protein-Carbohydrate Interactions in Hen Egg White Lysozyme Complex Using a Polarizable Force Field

Yang Zhong, Sandeep Patel., Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States.

Lysozyme is a well-studied enzyme that hydrolyzes the b-(1,4)-glycosidic linkage of N-acetyl-D-glucosamine (NAG) oligmer. The active site of hen egg-white lysozyme (HEWL) is believed to consist of six subsites, A-F, which is able to accommodate six sugar residues. To probe the free energetics associated with such binding processes, we present studies exploring the use of polarizable force fields in prediction of binding free energies of complexes of HEWL and NAG oligsaccharides. Thermodynamic integration (TI) and the Bennett acceptance ratio (MBAR) are applied and compared on their performances of computing the free energy changes of HEWL/NAG systems studied.

Nano Science, Technology, & Material Science I

127. Catalyst-free, one-pot synthesis of monodisperse, high-quality PbSe nanorods

Weon-kyu Koh,[1] Adam C Bartnik,[3] Frank W Wise,[3] Christopher B Murray.[1,2], [1]Department of Chemistry, University of Pennsylvania, Philadelphia, PA, United States; [2]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, United States; [3]School of Applied and Engineering Physics, Cornell University, Ithaca, NY, United States.

We report catalyst-free, one-pot synthesis of monodisperse, high-quality PbSe nanorods using a new selenide precursor. As shown in CdSe nanorods, PbSe nanorods also showed liquid crystalline alignment or vertical alignment under controlled evaporation conditions. The growth of nanorods was monitored by TEM and absorption spectroscopy, indicating that oriented attachment could be involved to provide anisotropic PbSe nanostructures. In-plane XRD showed an enhanced (200) peak

for PbSe nanorods, indicating preferred alignment of nanorods on the substrates and their growth along the <100> direction. Absorption and emission spectra, along with lifetime measurements, show the differences between nanoscale PbSe spheres and rods.

128. Hexagonal Nanopillars of Melamine-Cyanuric Acid Complex Prepared by A Crystallization After Mixing on Surfaces (CAMS) Method

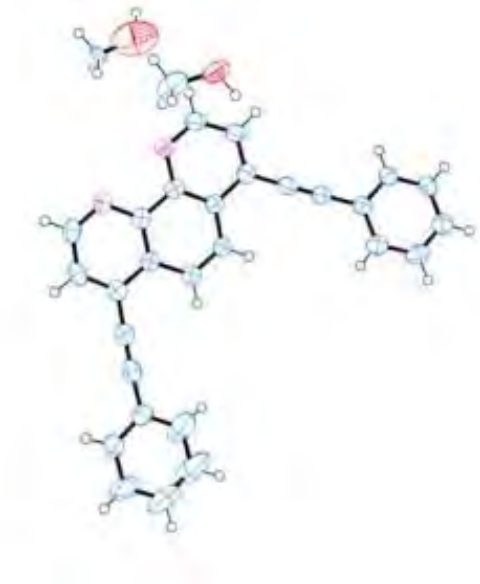
Hai-Feng JI., Chemistry, Drexel University, Philadelphia, PA, United States.

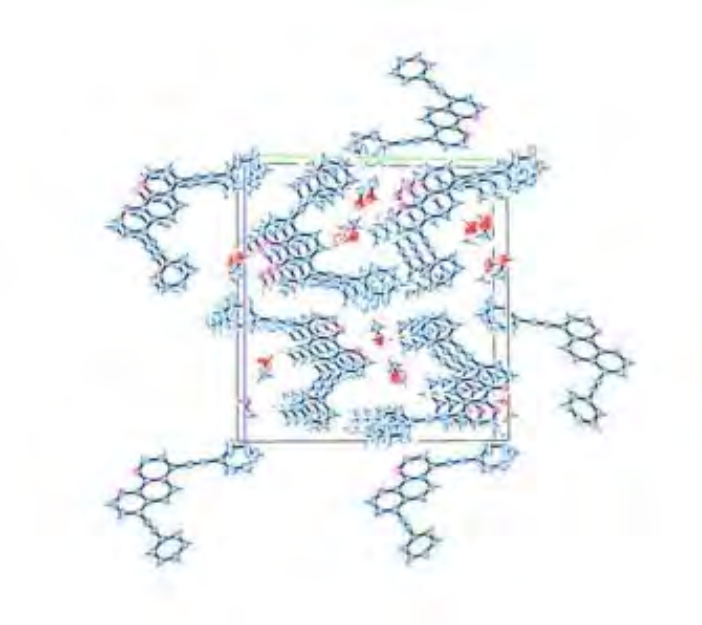
We report a well-defined, organic, hexagonal nanopillar array on gold surface. The array was prepared from a cyanuric acid-melamine complex by mean of a crystallization after mixing on surfaces (CAMS) method. These nanopillars had uniform diameters of 200–400 nm and 1 mm in length. They were well facetted with hexagonal cross-sections. The nanopillars had a crystalline structure, and the pillars exhibited a layered texture in the longitudinal direction. The CAMS method described herein provides an unprecedented control of nanometer-scale structures and represents a simple but significant advance in the functionality of building blocks for nanoscience and nanotechnology. We expect that the present results open up many opportunities in developing well-defined nanofilms on surfaces and we are exploring whether the CAMS method can be used to grow a variety of nanostructure arrays that are self-assembled from organic, inorganic, and organic-inorganic hybrid materials. If so, the CAMS method could offer wide opportunities for technological applications due to the capability of large-scale fabrication of nanometer-sized systems with controllable morphologies and properties. These studies are driven by the technological relevance of nanostructures on surfaces from perspectives such as surface coatings, nanosensors, nanoelectronics, and heterogeneous catalysis.

129. Synthesis and properties of conjugation extended phenanthrolines

Hyungsock Suh, Dominick J Casadonte, Jr., Chemistry, Texas Tech University, Lubbock, TX, United States.

Several conjugation-extended 1,10-phenanthrolines were synthesized via a modified Sonogashira coupling reaction. The 4 and 7 positions of the phenanthroline were linked with ethynyl moieties. [figure1] The crystal structures indicate that the phenanthrolines form p-stacked network.[figure2] The luminescence properties exibit a significant red shift from non-substituted 1,10-phenanthroline. The development of new luminescent materials via complexation using Cu(I) and triphenylphosphine and through polymerization of the mononuclear Cu(I) complexes will be discussed.





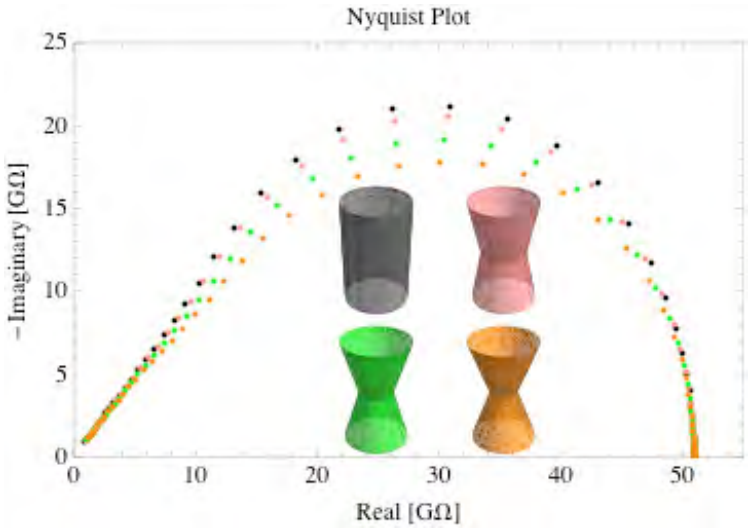
130. Novel patterned protein assay to measure differential extracellular matrix protein affinities for cellular attachment and axonal outgrowth

William Theilacker,[1] Amy Styer,[1] Dianna Willis,[2] Holt Bui,[1] Jeffery L. Twiss,[2] Thomas P. Beebe.[1], [1]Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States; [2]Alfred I. DuPont Hospital for Children, Nemours Biomedical Research, Wilmington, DE, United States.

Cellular preference for extracellular matrix (ECM) proteins was assayed on patterned surfaces presenting two ECM proteins that compete for cell attachment and proliferation. Micro-contact printing (mCP) techniques and reactive surface chemistry were used to modify glass substrates with alternating 40-mm-wide lanes of fibronectin and laminin. The spatial distribution and morphology of the substrate-bound proteins were measured by fluorescence imaging and surface-sensitive techniques including Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS), X-ray Photoelectron Spectroscopy (XPS) and Tapping Mode Atomic Force Microscopy (TM-AFM). The biological activity of the substrate-bound proteins were probed with domain-specific monoclonal antibodies and measured by a fluorescence-based ELISA. Attachment and outgrowth of neuron-like pheochromocytoma (PC12) cells on striped substrates were analyzed up to 4 days. At each time point, three patterned samples were fixed and immunostained prior to fluorescence imaging. Images were analyzed for the number of cells attached to each protein region and the number and length of neurite extensions. Results indicate for PC12 cells, an approximately equal number of cells on fibronectin and laminin stripes after 24 hours in cell culture. However, from 48 hours to 96 hours, the number of cells on laminin versus fibronectin continually increased. By 96 hours, 80 percent of the PC12 cells were attached to laminin versus fibronectin.

131. Using electrochemical impedance spectroscopy to determine the geometry of radially symmetric nano-channels

Michael J Vitarelli, David S Talaga., Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, New Jersey, United States.



Here we use electrochemical impedance spectroscopy to determine the geometry of radially symmetric nano-channels. Employing a modified transmission line arrangement of resistors and capacitors, we develop a new equivalent circuit complex impedance function that includes the effects of capacitive double layers inside the nano-channels as well as the influence of varying nano-channel radius.

We then evaluate the high and low frequency limits of the function and show that it correctly reduces to the electrolyte resistance in the zero frequency limit, and to zero in the infinite frequency limit. We also show that for the case of a constant radius channel our impedance function reduces to a form analogous to the finite length Warburg impedance. We then evaluate how the impedance frequency spectrum will change with different nano-channel aspect ratios and different degrees of constriction at the channel center.

We measured the impedance frequency spectrum of a nano-capillary array membrane at varying concentrations of electrolyte to separate the bulk circuit behavior from the nano-channel behavior. We used our nano-channel function in an equivalent circuit model that also included the contributions from the membrane capacitances and the measurement apparatus. This model was used to globally fit the data at the different conductivities to determine the nano-channel geometry. The resulting values matched well with the known geometries of the nano-capillaries. The systematic variation with conductivity of the nano environment of the channels was systematically different than that of the bulk elements and allowed separation of the nano-channel contribution from the other signals in the system. Thus, our model allows for easy shape and surface characterization of nano-channels and can easily be employed in various environments.

132. Characterization of natural fiber welded biopolymer composites

Zane A Fayos,[1] Luke M Haverhals,[1] Hadley M Sulpizio,[1] W Matthew Reichert,[1] Matthew P Foley,[1] Hugh C De Long,[2] Paul C Trulove.[1], [1]Department of Chemistry, United States Naval Academy, Annapolis, MD, United States; [2]Mathematics, Information and Life Sciences Directorate, Air Force Office of Scientific Research, Arlington, VA, United States.

Ionic liquids are effective solvents for the dissolution of biopolymers such as cellulose and silk. Resent work in our laboratory has shown that robust biopolymer based structures may be created without full dissolution of the material by a method we call "Natural Fiber Welding." This process allows the generation of novel natural fiber structures while maintaining much of the material in its native state. Consequently, natural fiber welding enables the preservation of many of the desirable properties of natural biopolymers while allowing for new configurations. Examples of the natural fiber welding process will be discussed with a focus on the characterization of the structural alteration. We will present results for the micro-scale analysis of materials generated by natural fiber welding using a variety of spectroscopic and imaging methods. These results will be framed within the context of macroscopic property observations (i.e., material strength as probed by tensile and ballistics testing) so as to inform the ongoing development of processing methods and techniques.

133. Particle reformation in small anisotropic silver nanocolloids

Stuart T. Gentry, Mark W. Bezpalko., Department of Chemistry and Biochemistry, La Salle University, Philadelphia, PA, United States.

Silver nanocolloids having high-aspect-ratio triangular prismatic morphologies (plate thicknesses less than 10nm and edge lengths over 100nm) have been shown to remain stable over multiple months. By contrast, nanoprism particles made with the same chemical components and plate thicknesses but with edge lengths less than 30nm lose their prismatic morphologies over a short number of hours. We will compare several possible instability mechanisms that may be present in the system. While particle aggregation cannot be ignored, the data are not consistent with a simple flocculation or coagulation process. Instead, we will focus on a discussion of Ostwald ripening versus internal restructuring of the particles in these nanoparticle systems. We will also address environmental factors that can affect the restructuring process

134. Characterization of Tethered Bilayer Lipid Membranes (tBLMs) with Unsaturated Lipidic Anchor Molecules with Comparison to tBLMs with Saturated Lipidic Anchors

David J Vanderah,[1] Gintaras Valincius,[2] Frank Heinrich,[3,4] Rima Butvytyte,[2] Prabhanshu Shekhar,[4] Gediminas Niaura,[2] Vlada Voiciuk.[2], [1]Biochemical Science Division, National Institute of Standards & Technology, Gaithersburg, MD, United States; [2]Institute of Biochemistry, Vilnius, Lithuania; [3]Center for Neutron Research, National Institute Of Standards & Technology, Gaithersburg, MD, United States; [4]Department of Physics, Carnegie Mellon University, Pittsburgh, PA, United States.

Self-assembly of 1-thialipidic molecules [$HS(CH_2CH_2O)_6CH_2CH(OR)CH_2(OR)$, where R = long hydrophobic carbon chains] and b-mercaptoethanol followed by rapid solvent exchange of a lipid/ethanol solution (ethanol ® water) afford tethered bilayer lipid membranes (tBLMs) that are anchored to but decoupled from the underlying substrate (Au). The anchoring 1-thialipidic molecules with the lipids of the second step complete the inner leaflet whereas the outer leaflet consists solely of the lipids used in the solvent exchange step. Here we report the characterization of tBLMs prepared using a 1-thialipidic molecule with unsaturated alkyl chains [R = oleoyl, $(CH_2)_8CH=CH(CH_2)_7CH_3$] using electrochemical impedance spectroscopy, neutron reflectometry, spectroscopic ellipsometry, atomic force microscopy, and infrared spectroscopy. Our data is presented in comparison to previous tBLMs where R = alkyl, i.e., no double bond, and discussed as to the comparative insulating properties and disorder. Enhanced disorder generally results in greater bilayer fluidity, a desirable property of the reconstitution and study of integral membrane proteins.

135. Highly stabilized nanoparticles fuctionalized with GdDTPASH as magnetic resonance imaging contrast agent

Talha S Siddiqui,[1] Lindsay K Hill,[2] Youssef Zaim Wadghiri,[2] Marc A Walters.[1], [1]Chemistry, New York University, New York, NY, United States; [2]Radiology, New York University Langone Medical Center, New York, NY, United States.

Magnavist™ a complex of diethylenetriaminepentaacetic acid (DTPA) and Gd^{3+} 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 thiol linkage (DTPASH). The resulting contrast agent, GdDTPASH, was bound to Ag and Au nanoparticles. The construct was further stabilized in buffered solution with the addition of a thiolated PEG chain. The ligand, its Ln complex and thiolated PEG were characterized by ^{1}H and ^{13}C NMR spectroscopy, electrospray ionization mass spectrometry (ESI-MS) and IR spectroscopy. The highly stabilized nanoparticle construct delivers a high payload of Gd compelex and is an effective T_1 brightening agent. The production of this type of construct opens the way for engineered multimodal MRI contrast agents.

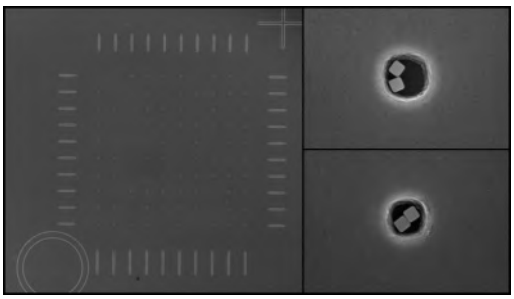
136. Surface-enhanced Raman spectroscopy with silver nanocube dimers: Experiment and calculations

Seung Yong Lee,[1] Jane E Cornett,[1] Garrett S Lang,[2] Ling Hung,[2] Isaak D Mayergoyz,[2,3] Oded Rabin.[1,3], [1]Department of Materials Science & Engineering, University of Maryland, College Park, MD, United States; [2]Department of Electrical & Computer Engineering, University of Maryland, College Park, MD, United States; [3]Center for Applied Electromagnetics, University of Maryland, College Park, MD, United States.

Surface-enhanced Raman spectroscopy (SERS) is a powerful technique for ultra-high sensitivity chemical analysis. In this technique, plasmonic structures in the vicinity of the analyte interact with the incoming and scattered radiation. They can amplify the EM field intensity by many orders of magnitude in the near-field, and lead to larger Raman signal intensities in the far-field. We present a bottom-up approach to study the relationship between SERS and configurations of silver nanocube (AgNC) dimers.

Monodispersed AgNCs were synthesized via a modified polyol reduction protocol. The AgNCs formed ordered arrays of plasmonic structures by directed self-assembly on patterned silicon substrates [figure 1]. When a thiol monolayer was deposited on the surface of the AgNCs, a wide range of SERS enhancement values were recorded due to variations in the configuration of the dimers from site to site. The AgNC dimers used in the SERS measurements were analyzed by SEM in order to correlate the SERS intensities with their configurations. We generated a database of AgNC dimers. All the dimers were sorted into three categories based on the relative orientation of the nanocubes: We defined dimers where a face of a cube neighbors a face of the other cube as FF dimers, dimers where a face neighbors an edge as FE dimers, and dimers where an edge neighbors an edge as EE dimers. Our analysis shows that the distribution of enhancement factors of the three types of dimers can be modeled successfully by the Weibull distribution. The Weibull distribution shape parameter for the FF dimer category is the highest, indicating that the enhancement factor of FF dimers shows the broadest distribution. When the maximum SERS signal in each type of dimer is compared, that of an EE dimer was found to be the highest, but the Weibull distribution scale parameter of EE dimers is twice lower than that of the FE dimers; i.e. the enhancement factor of FE dimers is higher, on average, than that of EE dimers. Numerical calculation of plasmon resonance frequencies and enhancement factors for the three types of dimers reveals the plasmon resonance dependence on the inter-particle gap. FF dimers achieve the highest enhancement factor, but the enhancement values of this category are the most sensitive to the inter-particle gap, leading to the broad distribution seen in the experimental results. For FE and EE dimers the calculated highest enhancement values are lower than for

FF dimers, but the enhancement is weakly dependent on the gap size. Both the experimental and the calculated distributions point at the FE dimers as the suitable SERS substrate to obtain high and uniform SERS signal enhancements.



137. Characterization of the fractal geometry of SBA-15, and its use as a vanadia oxide support for the partial oxidation of methanol

Thomas M Baldassare, Michael A Smith., Department of Chemical Engineering, Villanova University, Villanova, PA, United States.

The reactivity and selectivity of a vanadia catalyst on a mesoporous silica support is studied using the partial oxidation of methanol to formaldehyde. SBA-15 was used as the support and synthesized using the procedure developed by Zhao et.al. [1] The calcinations of the support were also done at higher temperatures (500, 700, 850 ºC) to vary the porosity of the support. Vanadia oxide catalysts were grafted on the support using a processes researched by the Gary Haller group at Yale [2] as well as a new grafting technique developed at Villanova. The fractal geometry and catalyst structure were thoroughly characterized using N_2-physisorption, X-ray diffraction, small angle X-ray scattering (SAXS), scanning electron microscopy (SEM), and X-ray fluorescence (XRF). The results of a decrease in surface area and a smoothing of the topographical surface of SBA-15 were confirmed using N_2-physisorption.The partial oxidation experiments performed have shown greater catalytic performance when compared to incipient wetness techniques, as well as conversion and selectivity differences due to the changes made to the support porosity.

[1] D. Y. Zhao, Q. S. Huo, J. L. Feng, B. F. Chmelka, G. D. Stucky, J. Am. Chem. Soc. 120 (1998) 6024-6036.

[2] G. Du, S. Lim, M. Pinault, C. Wang, F. Fang, L. Pfefferle, G. L. Haller, J. Catal. 253 (2008) 74-90.

138. Novel fluorescent nanomaterials, via assembly of anionic poly(phenylene vinylene) with lipid vesicles, divalent cations, and/or silica beads

An T Ngo, Pierre Karam, Kai L Lau, Melanie Burger, Jeffrey Quesnel, Gonzalo Cosa., Department of Chemistry, McGill University, Montreal, QC, Canada.

This talk describes novel architectures for fluorescent detection, involving the anionic light-emitting polymer MPS-PPV (poly[5-methoxy-2-(3-sulfopropoxy)-1,4-phenylenevinylene]) in complex with biological molecules (lipids), and/or silica beads. The vesicular encapsulation of light-emitting polymer produced a "liposome beacon" for the detection of fluorescence quenching events at the lipid membrane surface. Divalent cation was furthermore used to modulate interactions between the light-emitting polymer and zwitterionic lipid vesicles. Binding to the lipid vesicles disrupted polymer aggregates, producing enhancement and peak shift in the light-emitting polymer's fluorescence. FRET with a membrane-embedded dye also elucidated the effect of divalent cation in promoting lipid-polymer association. The photophysical effects of silica bead adsorption on the fluorescence of the poly(phenylene vinylene) were investigated via ensemble spectroscopy and single-particle total-

internal-reflection fluorescence microscopy. Our results provide insight towards tuning the sensitivity of fluorescent water-soluble poly(phenylene vinylene)s, contributing to the development of new applications for conjugated polyelectrolytes in fluorescent assays.

139. Determining the mechanical response of propellants for large caliber ammunition

Stephanie M Piraino, Michael Leadore, Melissa Meyer, Rob Lieb., Energetic Materials Science Branch, Army Research Laboratory, Aberdeen Proving Ground, MD, United States.

An important consideration in the design of gun propellants for large caliber ammunition is the mechanical properties of the propellant grains. At the Army Research Laboratory, developmental propellants are tested at high rates in the compressive mode to evaluate the propellant response at various temperatures of interest. Scanning electron microscopy analysis is done in conjunction with mechanical properties testing to fully characterize the samples by probing any micro-structural defects that may affect the propellant's response. Current research will be presented which links the formulation and design of new propellants to the importance of their mechanical behavior.

Polymer, Colloid, and Emulsion Chemistry

Sponsor: Division of Polymer Chemistry

140. Microencapsulation of gentamicin sulphate using chitosan and alginate for time-released drug delivery systems (DDS)

Shakera M Guess, Cherese Winstead., Department of Chemistry, Delaware State University, Dover, Delaware, United States.

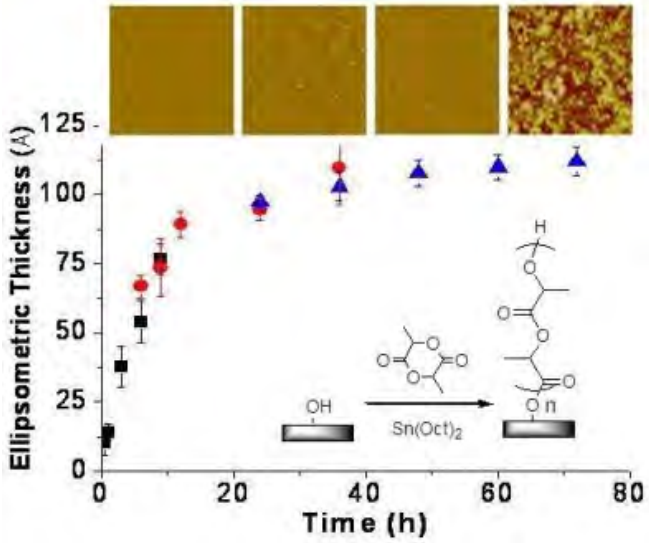
An antibiotic drug delivery system for the cationic and water soluble gentamicin sulphate has been prepared via microencapsulation using chitosan-alginate (CS-AG) polymer carriers. Bovine serum albumin (BSA) and hemoglobin (Hb) was selected as a model proteins for loading efficiency (LE) experiments. The influence of the following variables was investigated: (1) protein concentration; (2) equilibration time; (3) % chitosan coating on the exterior wall; and (4) degree of alginate gelation. Results showed that ionic gelation with 1.5% alginate, 0.8% BSA, and 0.05% chitosan yielded the highest encapsulation efficiency of BSA (100% at 4 hr). Thermal Gravimetric Analysis and Differential Scanning Calorimetry (DSC) of chitosan and alginate showed the thermal stability and characteristic endotherms of the respective biopolymers, but with the formation of an additional endotherm (~ 200°C) and added weight loss occurring at 235°C. FTIR analysis and X-ray diffraction further confirmed this interaction of cationic chitosan and anionic alginate. Contact angle measurements were conducted to determine the surface properties of alginate (45°) and chitosan (65°). Particle Size Analysis (PSA) and distribution of the alginate and chitosan were evidenced through Confocal Laser Scanning Microscopy (CLSM). The size distribution was determined to be (~1 μm) with fluorescence marking using Coomassie brilliant blue R-250 and Nile Red to show confirm presence of the alginate core and chitosan exterior wall.

141. Preparation of Poly(lactic acid) Brush for dynamic surface

Lebo Xu, Chris B. Gorman., Department of Chemistry, North Carolina State University, Raleigh, North Carolina, United States.

Conditions for the efficient production of poly(lactic acid) brushes on a surface were determined. Use of the native hydroxyl group on silica and hydroxyl-terminated thiols on gold worked equally well as an initiator. Various growth temperatures were compared to determine its effect on the growth

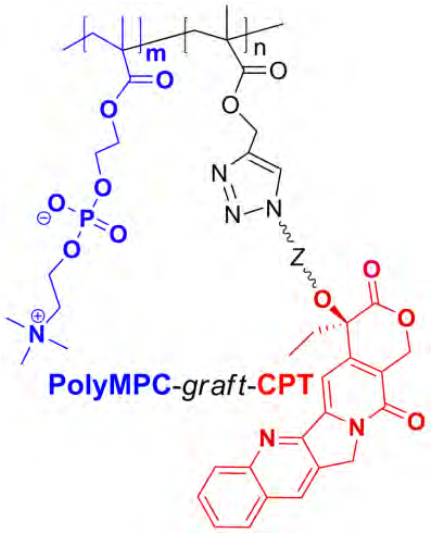
thickness. Running surface polymerization at relatively low temperatures was a practical approach to minimize the polymerization in solution for gave good thickness control. Under optimal conditions, brushes of ca. 10 nm could be grown in ca. 20 h, with good reproducibility.



142. Synthesis of conjugates of camptothecin and phosphorycholine polymers for cancer therapeutics

Xiangji Chen, Samantha McRae, Sangram Parelkar, Todd Emrick., Department of Polymer Science & Engineering, University of Massachusetts, Amherst, Amherst, MA, United States.

Novel polymer-drug conjugates, consisting of zwitterionic poly(methacryloyloxyethyl phosphorylcholine) (polyMPC) as the polymer component, and camptothecin (CPT) as the drug, were prepared by a one-pot ATRP-"click" conjugation strategy. This polymerization/conjugation method gave novel polyMPC structures with multiple copies of the drug pendent to the zwitterionic polymer chain. PolyMPC-*graft*-CPT conjugates were prepared with high weight percent drug loading (up to 14 percent CPT) and different molecular polymer molecular weights (up to ~50 kDa). The polyMPC-CPT conjugates showed excellent solubility in pure water (> 250 mg/mL). Light scattering studies on the polyMPC-CPT conjugates indicated the formation of polymer unimers, with diameters in the range of ~10 nm or less, in which the hydrophobic CPT moieties on a single chain collapse and are shielded by the hydrophilic polyMPC backbone. The linkage chemistry chosen between the polyMPC backbone and the pendent drugs proved critically important for drug release in the presence of different media and at different pH values. The toxicity of the polymer-drug conjugates was examined in cell culture against breast (MCF7), ovarian (OVCAR-3) and colorectal (COLO 205) cancer cell lines, giving IC50 values for the polymer-drug conjugates that are higher than native CPT alone, since toxicity of CPT sets in only following liberation from the polymer chain.



143. Drug elution kinetics and structure of absorbable matrix coatings

Srilekha Sarkar Das, Martin K McDermott, Anne D Lucas, Timothy E Cargal, Lakir Patel, David M Saylor, Dinesh V Patwardhan., Division of Chemistry and Materials Science, US FDA/CDRH/OSEL, Silver Spring, MD, United States.

An important area of modern medical research is drug delivery from biodegradable polymer coatings. *In vivo*, site-specific release of a therapeutic drug is commonly controlled by incorporating the drug with a solid polymer matrix. Typically, drug aggregates form in situ as the solvent evaporates from a cast drug-polymer solution. In this work, we probe the impact of polymer chemistry and solvent evaporation rate on drug structure in and the subsequent elution from a biodegradable polymer matrix. Coatings made from solutions of tetracycline (TC) and two different copolymer ratios of poly(lactic-glycolic-acid) (PLGA) were formed at two different solvent evaporation rates. This study relates the composite drug microstructure to the release kinetics of TC during the first two days of soaking. The results suggest that polymer chemistry affects the rate of water absorption and drug dissolution which in turn alters the rate of TC release during the early stages of drug elution.

144. Synthesis and characterization of metal loaded plastic and liquid scintillator composites of cobalt benzne dithiolate, tetra phenyl butadine and poly(tegdma)

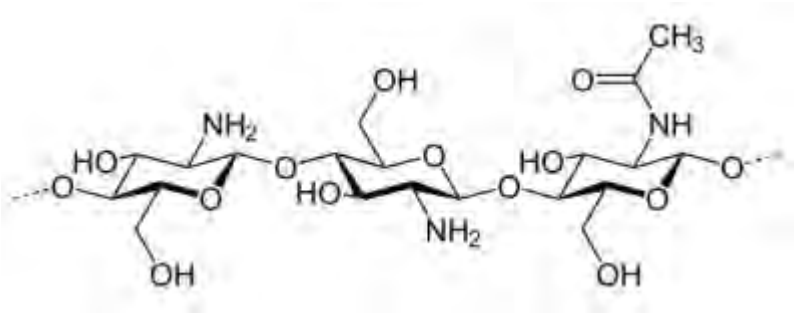
DEVIN M MCKELVEY, **Kristin R Jones**, **Brittney Wass**, Mohit P Patel, Susan Jansen Varnum., Chemistry, Temple University, Philadelphia, PA, United States.

Novel scintillating materials for neutron detection were fabricated by using the radical polymerization for plastic based scintillator. For comparison purposes water based liquid scintillator was also prepared in the absence of the polymer. Scintillators were constructed using a wavelength shifter, TPB (Tetra Phenyl Butadiene) and benzene dithiolate metal cobalt complexes doped into both liquid and cross-linked-polymer matrices. Characterization of the liquid scintillator was accomplished using UV-VIS spectroscopy, Spectrofluorometer and Fourier Transform Infrared spectroscopy. Two different polymerization methods were followed for preparing plastic scintillator composites. First, TEGDMA (Triethylene Glycol Dimethacrylate) monomers were doped with TPB/cobalt complexes and radical polymerization was initiated with benzoyl peroxide, second, "Accelerated-Promoted Free Living Radical Polymerization" of TEGDMA monomer was initiated by AIBN/TEMPO. The poly(TEGDMA) scintillators were characterized using TGA (Thermogravimetric Analysis) and FTIR-ATR (Fourier Transform Infrared - Attenuated Total Reflectance).

145. Modifying Chitosan for biomedical purposes

Elza Chu, Alexander Sidorenko., Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, United States.

Chitosan is the deacetylated form of chitin, composed of *b*-(1-4)-linked D-glucosamine and N-acetyl-D-glucosamine units, which is a primary component of anthropod exoskeletons. Alongside its abundance, chitosan is also non-toxic, biocompatible and biodegradable. It has already been put to use for biomedical purposes where it enhances wound healing properties in dressings, drug delivery and anti-tumor agents[1]. Although chitosan has many desirable characteristics, it is very hydrophobic which lengthens the time required for it to degrade *in vivo*. Past research demonstrates that chemical modification of chitosan does not change its underlying frame, hence, allowing it to maintain its original properties while also rendering it newer, and more controlled properties[2]. It also shows that chitosan when used as a medium can support other chemicals or cells to survive[3].



The objective of this project is to design an amphiphilic derivative of chitosan which can be used for orthopedic applications. The main focus of this project is to produce a phosphorylated and an alkylated chitosan derivative; the former rendering it hydrophilic properties, while the latter amplifying hydrophobic properties. Once this is accomplished, an appropriate combination of both syntheses will be constructed to provide an amphiphilic chitosan derivative which can attract calcium ions to solidify once *in vivo*, as well as sustain its shape in a largely aqueous environment. The modified chitosan materials are characterized using IR and NMR spectroscopy.

Approximately 550,000 joint replacement surgeries are performed in U.S.A. every year; and according to the 73rd Annual meeting of the American Academy of Orthopedic Surgeons (AAOS), the demand for such surgeries will increase by 673% by the year 2030[4]. Therefore, the implementation of chitosan derived bone implants will not only reduce surgical costs for patients, but also make it more accessible to patients living in third-world and developing countries where health care is less advanced. This will also allow the orthopedic industry to stimulate the economy by recycling unused byproducts of the seafood industry and conserving other resources like titanium, stainless steel and cobalt-chromium alloys[5].

References

[1]Kim I. Y.; Seo S. J.; Moon H.S.; Yoo M. K.; Park I. Y.; Kim B. C.; Cho C. S. Review: Chitosan and its derivatives for tissue engineering applications. *Biotech. Adv*. 2008, 26, 1-21.

[2]Rinaudo M. Review: Main properties and current applications of some polysaccharides as biomaterials. *Polym. Int*. 2008, 57, 397-430.

[3]Wu T.; Nan K. H.; Chen J. D.; et al. A new bone repair scaffold combined with chitosan/hydroxyapatite and sustained releasing icariin. *Chinese Sci. Bull*. 2009, 54, 2953-2961.

[4]Orthopedic Surgery. http://www.orthopaedic-surgeries.com/statistics_surgery.htm (accessed Oct 20, 2009).

[5]Frost & Sullivan. Research and Markets. *Orthopedic Implant Market- Living in a Material World*. http://www.researchandmarkets.com/reports/463829 (accessed Oct 20, 2009).

ACS Undergraduate Research Symposium - II

Organizers: Narmada Gunawardena, Andrea Martin

Session Overview: Posters may be set up around 10:00. The symposium provides an excellent opportunity for undergraduate chemistry students to present the results of their research. Presenters should be by their posters from 10:15 - 11:45.

146. Detection of PSA antigen on carbon nanotubes using fluorescence microscopy

Seo-Young Kwon, Amos M Mugweru., Department of Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States.

The detection of prostate-specific antigen (PSA) attached to multi-walled carbon nanotubes (MWCNT) has been described. Antibodies specific to PSA were first covalently bound to MWCNT. The MWCNT modified with the antibody was then incubated in a solution containing PSA. The MWCNT containing the PSA were then placed in another solution containing a fluorescence labeled secondary antibody. The carbon nanotube modification was followed using FTIR and fluorescence microscopy. Fluorescence microscopy images positively indentified of PSA in our test solution. Results discussed indicate MWNT/antibody conjugates using fluorescence microscopy may provide a novel method of monitoring PSA levels.

147. Time-dependent DFT studies of the photoluminescence of amine-decorated 1-D CuCN chains

Jasprina L Ming,[1] Craig A Bayse,[1] Robert D Pike.[2], [1]Department of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA, United States; [2]Department of Chemistry, College of William and Mary, Williamsburg, VA, United States.

Solid copper(I) cyanide is made up of extended one-dimensional CuCN chains with interesting photoluminscent properties. Recent work by our group has shown that the UV spectrum of CuCN may be attributed to Laporte-allowed excitations from occupied to unoccupied p-type molecular orbitals (MOs). The emission spectrum is attributed to relaxation from an excited state triplet with a bent structure due to distortions that remove degeneracies in the partially occupied MOs of the linear triplet. Decoration of CuCN with aliphatic and aromatic amines leads to substantial changes in the structural and photophysical properties of the material including shifts in lmax for both the excitation and emission spectra. We have extended our study of CuCN to examine the relative stability of various structural motifs of decorated CuCN (zig-zag, helical, and figure 8) using truncated CuCN chains optimized at the DFT(BLYP) level. Time-dependent DFT (TD-DFT) studies on the optimized structures of these model compounds reveal that excitations are generally consistent with the unsubstituted chains with important differences due to the motif, stoichiometry and type of ligand.

148. Theoretical investigation of the gas-phase polymerization of ethylene by the chromium hydroxide cation ($CrOH^+$)

Patrick O'Kane, Timothy J Dudley., Department of Chemistry, Villanova University, Villanova, PA, United States.

The mechanism of gas-phase ethylene polymerization by $CrOH^+$ is examined computationally at the UB3LYP/6-31G(d) level of theory. The potential energies for the ethylene, ethylidene, and vinyl complexes, which can be formed when a single ethylene reacts with $CrOH^+$, were examined. A second ethylene molecule was then introduced in to the system and it was found that the overall stability of the complex increases when a second ethylene is bound to the chromium. The potential energy surfaces for several possible polymerization pathways and termination of polymerization were characterized. It has been found that the hydroxide group bound to the chromium may play a role in aiding hydride shifts that occur during the polymerization.

149. Investigating a tandem cyclization-coupling reaction between o-ethynylbenzoic acids with p-iodoanisole as part of an approach to the Aristolactam alkaloids

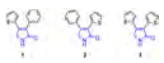
David M. Degan, **Erin T. Pelkey**., Department of Chemistry, Hobart and William Smith Colleges, Geneva, NY, United States.

Aristolactams are highly oxygenated phenanthrene and lactam ring containing compounds derived from the plant species Aristolochia that display moderate biological activity, particularly against leukemia cell lines. The key step in our synthetic strategy employs a palladium-catalyzed tandem cyclization-coupling reaction of o-ethynylbenzoic acid **1** with p-iodoanisole. This cyclization-coupling reaction led to a mixture of (*E*)- and (*Z*)-3-arylideneisobenzofuran-1-ones **2** and **3**. Interestingly, treatment of major product **2** with hypervalent iodine reagent PIFA led to formation of **3** via a novel isomerization. Progress towards the synthesis of the aristolactams from **3** will be presented.

150. Convergent method towards thiophene substituted 3-pyrrolin-2-ones

Jacob P. MacDonald, Jessica G. Greger, **Erin T. Pelkey**., Department of Chemistry, Hobart and William Smith Colleges, Geneva, NY, United States.

We have developed a convergent methodology to 1,2-diaryl-1-nitroalkenes, and subsequently, 3,4-diaryl-3-pyrrolin-2-ones. This communication is focused on the synthesis of the thiophene-substituted 3-pyrroln-2-one targets **1**-**3**. 3,4-Diaryl-3-pyrrolin-2-ones are an important class of molecules that have demonstrated biological activity including pain reduction, anti-inflammatory, and anti-cancer. Herein, we report our progress towards synthesizing novel 3,4-diaryl-3-pyrrolin-2-ones that contain thiophene side chains. Thiophene rings were chosen as part of our investigation into novel heterocyclic analogs as thiophenes are often incorporated into novel pharmaceutical analogs for biological evaluation.



151. Synthesis of a Macrocyclic Ligand and a New Copper Complex

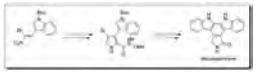
Erika D Druckenmiller, **Brittney L Offenbacker**, Andrea E Martin, Louise M Liable-Sands., Department of Chemistry, Widener University, Chester, PA, United States.

As part of a freshman summer research experience, the macrocyclic ligand 1,4,7,12,15,18-hexaazacyclodocosane was prepared, using a modification of a published synthesis. New complexes of this ligand with $CuCl_2$, $NiCl_2$, and $CoCl_2$ were prepared. The copper and cobalt salts precipitated readily, while the nickel complex is highly soluble and has resisted characterization. The dicopper(II) complex was characterized by single-crystal x-ray diffraction; the molecule has an inversion center with the ligand adopting an s-shaped configuration and the coppers each bound to three nitrogens and two chloride ions in a square pyramidal geometry.

152. Synthetic approach to staurosporinone utilizing pyrrole Weinreb amides

Jessica G. Greger, Jacob P. MacDonald, **Erin T. Pelkey**., Department of Chemistry, Hobart and William Smith Colleges, Geneva, NY, United States.

The following research seeks to improve upon methods for preparing biologically active 3,4-disubstituted-3-pyrrolin-2-ones. Specifically, a convergent methodology to pyrrole Weinreb amides and subsequently 3-pyrrolin-2-ones was developed. Key steps include a cross-coupling reaction of a-bromonitrostryrenes giving 1,2-diaryl-1-nitroalkenes and the subsequent cyclocondensation of the latter with isocyanides giving pyrrole Weinreb amides. Progress towards the synthesis of staurosporinone, a protein kinase C (PKC) inhibitor, will be highlighted.



153. Thermodynamic investigation of $LiNTF_2$ dissolution in ionic liquids

Angelo Andriola, Lei Yu., Department of Chemistry and Biochemistry, Rowan University, Glassboro, New Jersey, United States.

Ionic liquids (ILs) have recently become the focus of an always growing interest due to many of their remarkable properties. These unique characteristics include negligible vapor pressures, low melting points, non-flammability, good solvents to many organic and inorganic chemicals, and finally high ionic conductivity. These properties make ILs candidates for numerous applications, most importantly here as the electrolyte solution in electrochemical processes and in lithium batteries. There is no doubt that the Li / Li-ion batteries which are inherently bonded with the element of lithium have many advantages, such as very high energy density or capacity, low self-discharge rate and high voltage. The major drawback of Li / Li^+ batteries is their safety concern due to the use of organic solvents in the electrolyte solution. Owing to the negligible-volatility and non-flammability of ILs, the long-life and safety are significant advantages when ILs are used as electrolytes. In our experimentation, the interaction of Li^+ salts and IL solutions have been observed by means of a constant pressure calorimeter to provide qualitative data about their interactions. The goal of the overall experiment is to produce favorable properties as electrolyte solutions, coupled with reproducible results. These expectations will be obtained by measuring the enthalpy of dissolution of the Li^+/IL solutions. Several variables will be manipulated one at a time during experimentation such as the Li^+ salt, the IL solution, and the concentration of the solution as well.

154. Synthesis and characterization of magnetic nanoparticles for drug delivery applications

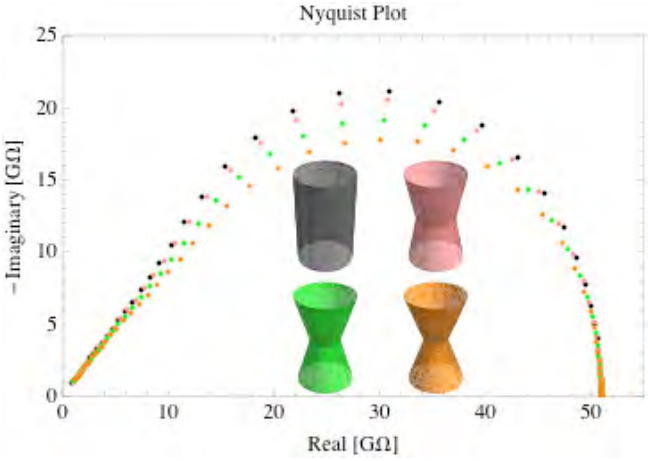
John Kong, Amos Mugweru., Department of Chemistry & Biochemistry, Rowan University, Glassboro, NJ, United States.

The search for new drug delivery systems is key in the fight against many diseases. In this work manganese-based magnetic nanoparticles ($La_xSr_{1-x}MnO_3$), were prepared by using reverse micelle method for potential use as drug carriers. The nanoparticles after synthesis were analyzed using powder X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM). Drug molecules were attached to these nanoparticles by first modifying with an amino group containing silica coating. The nanoparticles with attached drug molecules were characterized using Fourier Transform Infrared (FTIR) spectroscopy, and Raman spectroscopy.

155. Ferrocenium trifluoroborate: An unexpected product

Paul F. Smith, Joseph J. Grzybowski., Department of Chemistry, Gettysburg College, Gettysburg, PA, United States.

The cyclic voltammetry of ferroceneboronic acid reveals what appears to be a perfectly reversible redox couple with an $E_{1/2}$ centered at 475 mV (vs the saturated Ag/AgCl reference electrode). However, exhaustive electrolytic oxidation of a solution of ferroceneboronic acid generates an unexpected species that has a redox potential 350 mV more cathodic than that observed for ferroceneboronic acid. The production of this new species is dependent on the supporting electrolyte, with it appearing in the presence of BF_4^- and PF_6^- salts but not if ClO_4^- salts are used. Chemical oxidation of ferroceneboronic acid with $NOBF_4$ and $NOPF_6$ has shown that this unexpected result is due to a ferrocenium trifluoroborate species. The characterization of this surprising reaction along with its expansion to other boronic acids will be discussed.



156. Self assembled multilayer films of cytochrome C and DNA for bio-activation studies

Marc Iuliucci, Amos Mugweru Mugweru., Department of Chemistry & Biochemistry, Rowan University, Glassboro, United States.

In this work, various electrochemical techniques were used to investigate the behavior of cytochrome c (cyt c) on glassy carbon surface. Films of cytochrome C and polyions, polystyrene sulphonate (PSS) and DNA were constructed on glassy carbon surface and on quart slide by alternate adsorption of a polyanion and cytochrome c. The growth of the layered film was monitored using voltammetric, impedance and spectrophotometric techniques. The catalytic behavior of these sensors in epoxidation reactions will be discussed.

157. Synthesis and characterization of molecular switch containing organic bridging compounds and their effects on the fluorescence process

Thomas J Comey, Ann Lezama, Kenneth Yamaguchi., Department of Chemistry, New Jersey City University, Jersey City, NJ, United States.

Significant interest has been shown in the area of organic bridging compounds, molecular switches and the effects they have on the fluorescence process. We will report on the synthesis and characterization of a family of substituted benzoxazole moiety coupled to various bridged 8-quinolinols. Within this substituted benzoxazole, a proposed molecular switch has been introduced. This switch containing ligand system will be chelated to metals and their luminescent properties studied.

158. Determination of hydrogen peroxide concentration in dental bleaching gel

Kaitlyn Grosso, Ryan Sours., Department of Chemistry, Towson University, Towson, Maryland, United States.

An in-office dental procedure to bleach teeth involves applying a bleaching gel to the patient's teeth for three separate 15-minute intervals. It was questioned whether the three separate 15-minute applications are necessary, or if a single application of the gel for 45 minutes would produce the same results. The latter would reduce the amount of bleaching gel required, the amount of waste produced, and the cost.

Hydrogen peroxide is the active ingredient in many bleaching gels used for this procedure. If the concentration of the hydrogen peroxide in the bleaching gel can be measured before application and after different time intervals from 0 to 45 minutes, it can be determined how much hydrogen peroxide was used for that amount of time. Therefore, the effectiveness of the gel at each time interval can be inferred. Furthermore, it can be resolved whether the three separate 15-minute applications or single 45-minute application has a greater amount of effectiveness, or if their bleaching capabilities are similar.

Several different methods were used to determine hydrogen peroxide concentration. These methods included UV-visible spectrophotometry, potentiometry, titration, and cyclic voltammetry. Standard hydrogen peroxide solutions were used to create successful calibration curves for each method. However, each method failed to provide a reliable peroxide concentration for bleaching gel samples. We suspected that a component of the gel must be adversely interfering with each of the selected methods. Standard addition was performed, but surprisingly also produced unreliable results.

159. Use of multicomponent coupling reactions for the synthesis of lipophilic a-acetoxyamides

Subash C Jonnalagadda, Christopher M Bashian, Joseph R Schafer, Anthony Cirri., Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States.

Multi-component coupling is an extremely important tool in organic/medicinal chemistry towards the synthesis of structurally diverse scaffolds of biological interest. The isocyanide based 3-Component Passerini (3-CP) coupling reaction offers an easy access to a diverse range of peptidomimetic analogs under mild reaction conditions. Low density lipoprotein (LDL) contains about 1500 molecules of cholesterol esters per LDL particle and functions as a main carrier of cholesteryl esters in blood circulation. Several cancers such as malignant human gliomas overexpress LDL receptors, and thus consume high levels of LDL derived cholesteryl esters for the cell membrane biosynthesis. In this regard, we synthesized several lipophilic amides derived from cholesterol and long chain fatty acids via three component Passerini reaction. We hypothesize that these new compounds could have similar physico-chemical characteristics with native cholesteryl and fatty acid esters and consequently may interact well with LDL and replace some or entire cholesteryl ester core of LDL. We also envisage that the reconstituted LDL may utilize the elevated LDL receptor expression for targeted delivery of synthetic compounds to cancer cells. Our synthetic studies in this project will be presented.

160. Synthesis and characterization of spiropyran polymers

Kelechi Chikeka, **Phuong Ha**, Shannon E Stitzel., Department of Chemistry, Towson University, Towson, MD, United States.

The long-term goal of this work is to develop a stable, field-deployable chemical sensor for the detection of metal ions in aqueous systems. While there are numerous sensors to measure thermal or mechanical change in our environment, stable sensors available to monitor *chemical* changes are less common. Stability is an important issue in chemical sensor design, especially for applications such as environmental monitoring and process control, where sensors would ideally be left *in situ* over several weeks, months or even years. Many factors, including biofouling and chemical instability, make the development of such a sensor challenging. One approach to help mitigate such interfering factors is to use spiropyran dyes immobilized in polymer matrixes as sensor platforms.

Spiropyrans are a class of photochromic molecules that can be opened when exposed to ultraviolet light and closed when exposed to white light. Only in the open form will the dye complex with analyte metal ions. Spiropyrans could improve sensor stability for field use because they can be activated for sensing only when necessary for a measurement. By adding photocontrol of the active state of the sensor, an additional protective mechanism may be added to the sensor. Current work is presented on the synthesis and characterization of 3', 3'-Dimethyl-6-nitro-1'-(2-methacryloxyethyl)spiro[2H-1-benzopyran-2,2'-indoline] and spiropyran derivatives with varying carbon chain lengths. The influence of the dye chain length on the amount of dye incorporated into bulk polymer matrixes, and the dye kinetics both in solution and bulk polymers are examine by UV-Visible spectroscopy.

161. Automated Detection of GNRA Tetraloop Prevalence Using 3DNA and Python

Prerana Pradhan,[2] Mauricio Esguerra,[1] Wilma K Olson.[1], [1]Department of Chemistry and Chemical Biology, Rutgers, the State University of New Jersey, Piscataway, New Jersey, United States; [2]Department of Biomedical Engineering, Rutgers, the State University of New Jersey, Piscataway, NJ, United States.

RNA motifs are sequential and structural patterns associated with different levels of RNA organization. One well known example of a structural motif is the GNRA tetraloop, a hairpin loop consisting of the G, N, R, and A bases, where G is guanine, N is any nucleotide, R is a purine, and A is adenosine. The importance of the GNRA motif lies in its appearance in crucial stabilizing interactions with other molecules. For example, the GNRA tetraloop is involved in a loop-receptor interaction with Y-RNA in the HIV-1 packaging signals (Yu *et al*. 2008). 3DNA is a software package utilized for reconstruction and analysis of 3D nucleic acid structures. In order to better understand and detect RNA motifs, we wrote Python scripts to examine the output from 3DNA. The script has been used to identify GNRA tetraloops in the 23S subunit of the ribosomal RNA in *Haloarcula marismortui*, and their corresponding base-step parameters. The program runs through a given 3D structure and collects the locations of the GNRA tetraloops based on a base-step parameter derived seed. Automated detection of RNA motifs allows for better scrutiny of the role of rRNA motifs in ribosomal properties. The script can be modified for detections of other RNA motifs, as well as for identification of new structural motifs.

Yu E. T., Hawkins A., Eaton J., Fabris D."MS3D structural elucidation of the HIV-1 packaging signal." *Proc Natl. Acad. Sci., USA*. 2008; 105(34): 12248 - 12253.

162. Effect of the ionic liquid 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide on small peptide structure

Karson Schmidt, Leigh Murray, Michael Noss, Jia Huang, **Michelle R Bunagan**., Department of Chemistry, The College of New Jersey, Ewing, NJ, United States.

Ionic liquids have become materials of great interest to the chemical field due to their unique and useful properties. With regard to biomolecules, they have been found to stabilize and solubilize proteins, prevent aggregation, and serve as solvents for long-term storage, although the molecular mechanism by which this is achieved is yet to be fully understood. Using 1-butyl-1-methylpyrrolidinium bis(trifluoromethyl sulfonyl)imide, we observed the effect of neat ionic liquid on the secondary structure of small peptides, including alanine-based helical peptide AKA_2 and b-hairpin TrpZip4. Circular dichroism spectroscopy of AKA_2 in ionic liquid yielded an increasingly negative ellipticity at 222 nm with increasing temperature. However, as temperature increased, the ellipticity of TrpZip4 at 215 nm appeared to decrease. These results are discussed based upon the intra-molecular interactions present in each peptide structure and the resultant inter-molecular interactions formed between the peptide and ionic liquid.

163. Preparation of ionic liquids and their use in electrophilic aromatic substitution reactions with naphthalene and guaiazulene

Ryan Ludwig, Francis C. Mayville., Department of Natural Science - Chemistry, DeSales University, Center Valley, PA, United States.

This investigation will involve the preparation of several ionic liquids containing the 1-hexyl-3-methyl-imidazolium cation coupled to various anion systems. These ionic liquids can be substituted for typical organic solvents and used in the electrophilic aromatic substitution reactions of naphthalene or guaiazulene to produce several interesting analogs. There are many advantages for using these ionic liquids over organic solvents in synthesis reactions. Ionic liquids are recyclable, they can stabilize intermediates better then traditional solvents and the product yield is much higher. The ionic liquids can also be used for synthesis at lower temperatures and are a less toxic alternative to typical organic solvents.

164. Squeeze Flow of Shear Thickening Fluids as a Possible Protective Garment

David E Barlaz,[1] Charles Swanik,[2] Richard Dombrowski,[1] Norman Wagner.[1], [1]Department of Chemical Engineering, University of Delaware, Newark, DE, United States; [2]Department of Health, Nutrition, & Exercise Science, University of Delaware, Newark, DE, United States.

A number of Newtonian fluids, as well as continuously and discontinuously thickening fluids, have been tested under squeeze flow impact conditions to determine viability in a protective garment for hip fracture prevention. The peak force required to fracture a hip bone is approximately 4.1 kN. Fluid plugs were impacted using an Instron drop tower to assess how the various fluids behave under impact conditions similar to that of a human fall. At a speed of 2 m/s, the discontinuously thickening fluids are the only fluid type to offer sufficient protection. In addition, these fluids showed the least sensitivity to changes in sample weight and impact speed. This makes discontinuously thickening fluids a good candidate for impacts with speeds and energies more comparable to a human fall. Testing at higher energies showed a strong inverse trend in peak force versus area fraction of fluid in the pad with effectiveness peaking around 50%. Mathematical simulations of these impacts were developed in tandem with the impact experiments. Squeeze flow models for Newtonian fluids have been successful at predicting the same trends observed experimentally. Future testing will involve a custom built pendulum impactor designed to simulate human falls.

165. Investigation of various effects on gold nanoparticle aggregation

Allison Sturm, **Rodger E. Berg**., Natural Science, DeSales University, Center Valley, PA, United States.

The physical and chemical properties of a substance are size-dependent over a certain size range specific to the substance and properties. When a particle of gold metal is similar in size to wavelengths of visible light, it interacts with light in interesting ways. The color of a gold nanoparticle solution depends on the sizes and shapes of the nanoparticles. When a citrate salt reduces Au(III) ions to Au atoms, the gold nanoparticles experience repulsive charges due to the citrate salt's role as a reducing agent. Some research shows that when adding electrolytes or various ligands to gold colloids, they shield the charges of the gold (Au) nanoparticles, allowing them to aggregate. The effects of several electrolytes and ligands on the formation and aggregation of gold nanoparticles will be investigated. Aggregation of gold nanoparticles could have important functional effects when employing them for real life tasks, such as transport. A thorough understanding of the gold nanoparticles' properties allows for application of these special particles in fields of energy storage, medicine, drug delivery, etc.

166. The extraction and isolation of the active ingredient, resveratrol, from grapes and various red wines

Stephanie A. Lee, **Laura A. Smith**, **Francis C. Mayville**., Natural Science, DeSales University, Center Valley, PA, United States.

The objective of this study is to extract and isolate the active ingredient, resveratrol, from various types of grapes or red wines. Liquid-liquid phase techniques were used to extract the resveratrol from the grape flesh and different red wines, each known to contain the highest amount of the active ingredient. Ultraviolet/Visible (UV/Vis) spectroscopy was used to evaluate and quantify the total amount of resveratrol extracted from each type of grape or wine system. High Performance Liquid Chromatography (HPLC) was used to isolate the active ingredient from the extraction mixtures. The end result will identify the type of grape or wine that contains the highest concentration of resveratrol.

167. Investigation of the effect that different drying methods have on the release mechanism of naproxen from ethyl cellulose/microcrystalline cellulose beads

Julianne Berger, **Jonathan Fura**, **Francis C. Mayville**., Natural Science, DeSales University, Center Valley, PA, United States.

Samples of microcrystalline cellulose, MCC, combined with 5 or 10% ethyl cellulose and 10% naproxen were granulated, extruded and marumerized into dried sustained release beads. These dry beads were then exposed to two different humidity conditions; KNO_3 (high humidity) and LiCl (low humidity). The rate of naproxen release from the MCC/EC bead systems was measured by dissolution methods using a sodium phosphate buffer pH 8.0 as the solvent system. The control for this experiment was the convection oven dried beads. The results observed, based on these dissolution studies and analysis using UV/Vis spectroscopy, suggest that the rate of naproxen release from each MCC/EC bead system, either increases, decreases or follows the same release rate as the control sample. This further suggests that the rate of release of naproxen from each MCC/EC sample depends on the humidity condition the dry bead systems were exposed to.

168. Aerosol preparation of spherical zirconia (ZrO_2) and polymer coated zirconia particles

Alyssa Maltese, **Francis C. Mayville**., Natural Science, DeSales University, Center Valley, PA, United States.

This project was developed to produce uniform spherical polymer particles of zirconia (ZrO_2) through an aerosol reaction method. Once the ZrO_2 particles are produced they will undergo surface coating with an organic system. This surface modification will be studied by FT-IR. Uniform dispersions have many applications such as catalyst, magnetic labels, cell sorting and controlled drug release to mention a few. The simplest way to obtain uniform dispersions is through chemical reactions involving the use of aerosols. In this method, droplets of a reactant are exposed to a vapor of co-reactants yielding a new product. Because of the nature of the process, it is possible to produce finely dispersed powders by extremely rapid chemical processes which would be difficult to control using other techniques.

169. Python Graphical User Interface (GUI) for Control of the Levitated Dipole

David Z Jacome., Department of Applied Science and Technology, Saint Peter's College, Jersey City, New Jersey, United States.

The Levitated Dipole Experiment (LDX) is used to study the confinement properties of plasmas in a magnetic dipole field. In LDX a superconducting coil is levitated for up to 3 hours within a large vacuum chamber to produce the confining dipole field. The plasma experiments take place during this time, with ~ 10 second plasma shots, one shot every ~ 5 min. MDSplus software is used to run the experiment and store the data. The software is currently controlled by command line operations. Since levitation time is limited, its important to maximize efficiency and accuracy of experimental operations. Here, we present a Graphical User Interface (GUI) to efficiently control the operation of the experiment. The need for a GUI that integrates the MDSplus data cycle, cell access control, and routine experimental parameter controls is necessary. The GUI program provides a simple method for monitoring and setting experiment parameters. Python is used as the primary language to run the commands. A program called XRCed distributed by wxPython works as a visual tool.

170. Characterization of self-assembled monolayer on gold electrode in ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate

An D Le, Lei Yu., Department of Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States.

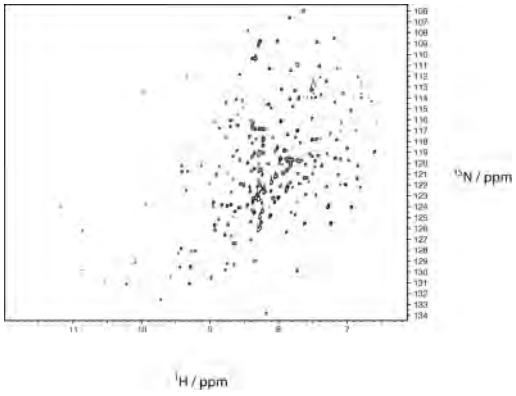
Key word: SAM, Ionic Liquid, Cyclovoltammetry

A room-temperature ionic liquid (IL) is a salt in the liquid state at a temperature below 100 ^{oC}. ILs are merely consisting of ions and short live ion pairs. ILs have recently become the focus of an always growing interest due to their remarkable properties such as negligible vapor pressure, low melting points, non-flammability, good solvents to many organic and inorganic chemicals, and high ionic conductivity. These properties make ILs candidates for numerous applications including the electrolytes of electrochemical processes. When an IL is used as electrolytes, it possesses larger electrochemical window, compare with aqueous solutions and many organic solutions. The diffusion of electroactive species and the charge-transfer at ionic liquids / electrode interface are very interest. The purpose of our work is to characterize different self-assembled monolayers of alkene thiols such as 1-dodecanthiol, 1-decanethiol and 1- tetradecanethiol in different ionic liquids. Ferrocene and other typical electroactive materials are used as probes. Cyclic voltammetry and electrochemical impedance spectroscopy results reflect the properties of the monolayers. The attenuation of Faradic current and the change of charge- transfer resistance are both observed in ILs when a compact monolayer formed on the surface of a gold electrode.

171. Towards structural characterization of the catalytic domain of bacteriophage T4 primase by NMR

Thomas H Mann, Mark D Sarcone, Lauren E Manning, William Tsai, Jayne A Kubat, Gregory A Manley, David Rovnyak., Chemistry, Bucknell University, Lewusburg, PA, United States.

Primases participate in a complicated mechanism performed by an ensemble of many proteins, collectively termed a replisome, to conduct DNA replication for all organisms. Specifically, primases are responsible for synthesizing short primers that are attached to the lagging strand of double stranded DNA. Very little structural information at the atomic scale is available for primases. A protocol has been developed to produce pure 1 mM samples of a catalytic domain of Bacteriophage T4 primase by expressing the recombinant gene through *E. coli*. Extensive optimizations of the protocol employing HSQC experiments (see Figure 1) have explored the effects of temperature, buffer, and protease inhibitors on signal-to-noise and protein stability. To date, five 3D backbone NMR experiments have been conducted. Resonance assignments have been initiated. New NMR techniques to study large, unstable proteins and their utility in this project, will be discussed. Plans for future work will be described.



172. Adsorption of Lanthanides on Cellulose Carbamate - Silica Hybrid Materials

Ivana McNeal., Chemisty, Prairie View A&M University, Priarie View, TX, United States.

Lanthanides are an important group of elements with wide range of applications such as catalysts, super conductors, and thermal neutron absorbents. Separation of lanthanides from aqueous solutions is usually carried out by solvent extraction, but this process requires large volumes of organic solvents and multiple extractions. Lanthanide separation using selective adsorbents is an alternative and attractive technique. In this report we present the preparation of a novel cellulose carbamate - silica hybrid material by sol-gel method and selective adsorption of lanthanides from aqueous solutions. The cellulose carbamate - silica hybrid was prepared in 1-butylmethylimidazolium chloride (BMIMCl) ionic liquid medium by dissolving cellulose in the ionic liquid and then reacting with 3-triethoxysilylpropylisocyanate. This hybrid material was exposed to the lanthanide ions in aqueous medium at room temperature and adsorptions were measured by determination of the free metal ion concentrations by colorimetric methods.

173. Synthesis of a Pentaphenyl Benzene Bridging Ligand

Adolfo Pertuz, Ken Yamaguchi., Department of Chemistry, New Jersey City University, Jersey City, NJ, United States.

Studies with polyaromatic molecules have received a lot of attention because of their favorable PET process and light emissive properties. The synthesis of a pentaphenyl benzene phenylacetylene bridged 8-quinolinol capable of binding metal ions will be discussed. Metal complexes formed with these ligands are thought to exhibit favorable electrochemical and luminescent properties.

174. Systematic Investigation of Phage Elution from Calcite Crystal Suraces

Stephanie Stanley, Ryan Sours., Department of Chemistry, Towson University, Towson, MD, United States.

Biomineralization is the highly evolved process by which biological organisms produce minerals, often to harden existing tissues. These minerals can form complex structures such as seashells or bones as a result of specific interactions between organic molecules and inorganic crystal surfaces. By studying these interactions, it may be possible to rationally design and synthesize new composite materials.

Phage display employs a bacteriophage with a foreign DNA sequence inserted into a protein gene, which causes a short peptide sequence to be displayed on the outer surface of the phage. Using a multitude of different DNA inserts, a "library" of phage with unique peptide sequences is created, some of which will selectively bind to a given target[1,2]. The bound phage can then be eluted, and collected for amplification. The process is repeated several times using this amplified phage in order to evolutionarily select the peptide sequence with the highest binding affinity. This method of the phage display technique has been widely used to determine peptide affinity for molecular interactions and has only recently been applied to inorganic substrates[3]. The elution step in particular has been identified as a potential point at which peptides strongly bound to the target may be missed due to the acid elution being less effective when using inorganic targets, rather than biological molecules[4,5].

We have observed that the standard, single-step elution method may be ineffective in removing all bound phage from the surface of the biomineral calcite (calcium carbonate). A systematic comparison of eluted and crystal-bound phage fractions (see Fig. 1) using peptide sequence analysis, fluorescence microscopy observations, and phage titers has indicated that modification of the elution step may be necessary to select phage with the highest binding affinities for calcite.

Optimizing the phage display technique for identification of peptide binding sequences for inorganic targets has a widespread potential use, including synthesis of nanomaterials, identification of growth modifiers for crystals, and general understanding of peptide interaction in crystal formation.

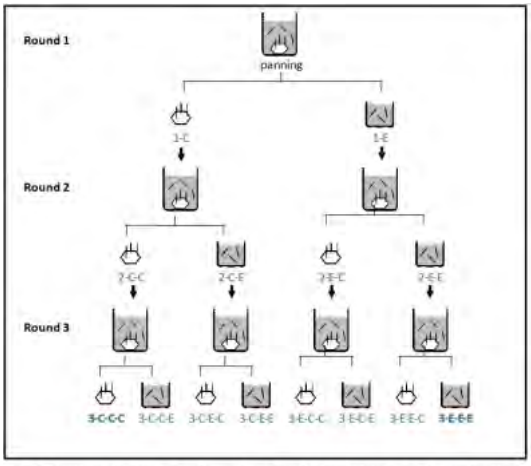


Figure 1: A comparison of titers and sequences between phage collected by elution and phage collected by crystal incubation

1. Baneyx, F; Schwartz, D, Selection and analysis of solid-binding peptides. *Curr. Opin. Biotechnol.* 2007, *18*, 312-317.

2. Merzlyak, A; Seung-Wuk, L, Phage as templates for hybrid materials and mediators for nanomaterial synthesis. *Curr. Opin. Chem. Biol*. 2006, *10*, 246-252.

3. Li, C; Botsaris, G; Kaplan, D, Selective in vitro effect of peptides on calcium carbonate crystallization. *Cryst. Growth Des.* 2002, *2*, (5), 387-393.

4. Naik, R; Jones, S, Peptide templates for nanoparticle synthesis derived from polymerase chain reaction-driven phage display. *Adv. Funct. Mater.* 2004, *14*, 25-30

5. Sarikaya, M; Tamerler, C, Molecular biomimetics: nanotechnology through biology. *Nat. Mater.* 2003, *2*, 577-585.

Frontiers in Magnetic Resonance in Liquids and Solids

Sponsors: Varian, Inc. (NMR); Bruker Corporation - Bruker BioSpin NMR; Cambridge Isotape Labs
Organizers: Donald Mencer, David Rovnyak

Session Overview: Applications of nuclear magnetic resonance spectroscopy (NMR) continue to expand into new disciplines, while new NMR technologies and methods are emerging at a rapid pace. In this session, a diverse selection of highlights of nuclear magnetic resonance spectroscopy in the liquid and solid state will be featured, including also recent pedagogical perspectives in response to the heightening challenge to best prepare future scientists.

175. Characterization of cation-exchanged NH4NaY and USY zeolites by ^{27}Al MAS NMR spectroscopy

David J. Aurentz,[1] Kevin J. Sutovich.[2], [1]Division of Science, Penn State Berks College, Reading, PA, United States; [2]Refining Technologies, Grace Davison, Columbia, MD, United States.

The effects of cations on the local electromagnetic environments of catalytic sites in Y-zeolites are studied as a function of cation type and concentration. Extensive study of cation-exchanged faujasite zeolites for the optimization of Y-zeolites as the principle source of activity in fluid catalytic cracking (FCC) catalysts is well known. Quadrupolar coupling parameters measurable using ^{27}Al magic angle spinning (MAS) NMR at multiple field strengths, provide a window to study aluminum's local electronic structure. With knowledge of the total shifts at two field strengths, a calculation based on the total chemical shift and the isotropic second-order quadrupolar shift yields the isotropic chemical shift and a "quadrupolar product." Quadrupolar parameters calculated for framework tetrahedral aluminum are related to cation concentration and Brønsted acidity for potassium-, zinc-, and lanthanum-exchanged NH_4NaY and USY zeolites. Increasing percentages (up to 4%) of Zn and La in USY systems increases the C_Q in 4- and 6-coordinate sites. Further increase in cation concentration past 4% decreases the C_Q. This yields a maximum C_Q at concentrations of about 4% in USY zeolites. These results indicate a change in proximity of the cation relative to the framework aluminum and a distortion of the lattice producing aluminum coordination with increased symmetry.

176. Solid-state NMR studies of CAP-Gly domain of mammalian dynactin and the CAP-Gly/microtubule complex

Shangjin Sun,[1] Si Yan,[1] Amanda E Siglin,[3] John C williams,[2,3] Tatyana Polenova.[1], [1]Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States; [2]Department of Molecular Medicine, Beckman Research Institute at City of Hope, Duarte, CA, United States; [3]Department of Biochemistry and Molecular Biology, Thomas Jefferson University, Philadelphia, PA, United States.

Assemblies of microtubules (MTs) and microtubule-associated proteins (MAPs) are difficult to address by conventional structural biology techniques due to their intrinsic insolubility and lack of long-range order. Lack of atomic level structural and dynamics information impeded the effort to understand this large class of biological systems, which are important for a broad range of physiological functions such as cell division, cell motility and organelle or vesicle transport. This knowledge gap hence impeded the effort of designing effective therapeutic strategies to treat many diseases that directly link to the dysfunctions of microtubule-associated proteins. We present a solid-state NMR study of the

CAP-Gly domain of mammalian dynactin and its complex with microtubule, demonstrate that magical angle spinning (MAS) solid state NMR spectroscopy as a novel yet viable technique to investigate the structure and dynamics of MT/MAPs.

177. Structures of Phospholamban Monomer and Pentamer by a Hybrid Solution and Solid-State NMR Refinement Protocol

Nathaniel Traaseth, Raffaello Verardi, Lei Shi, Martin Gustavsson, Gianluigi Veglia., Biochemistry, Molecular Biology and Biophysics, University of Minnesota, Minneapolis, MN, United States.

A single-pass membrane protein, phospholamban (PLN), regulates the sarcoplasmic reticulum (SR) Ca^{2+}-ATPase (SERCA). PLN is believed to exist in two oligomeric forms: a) a monomer that directly binds to and inhibits SERCA (1, 2) and b) a pentamer that acts as a storage form within the membrane (1, 2). To completely describe the fold space and ultimately the biological function of PLN and other membrane proteins, it is necessary to determine the specific interactions of the protein with respect to the lipid bilayer. This property is known a *structural topology* and can best be probed by oriented solid-state NMR experiments in lipid bilayers. In this work, we describe a new hybrid method to calculate the structures of the PLN monomer and pentamer using a combination of solution and solid-state NMR restraints in detergent micelles and lipid bilayers, respectively (3, 4). These high-resolution images of the PLN not only describe the structures, but also the topologies of all the protein domains with respect to the lipid bilayer.

In order to minimize the structure/topology of the PLN monomer and pentamer, we implemented our hybrid objective function into XPLOR-NIH software (5) that utilizes geometrical (E_{chem}) and solution ($E_{sol\text{-}NMR}$) and solid-state NMR (E_{ssNMR}) restraints:

$$E_{total} = E_{chem} + E_{sol\text{-}NMR} + E_{ssNMR}$$

We obtained short-range distance and angular restraints from solution NMR of PLN reconstituted into DPC detergent micelles and orientational restraints (anisotropic chemical shifts and dipolar couplings) from 2D separated local field experiments such as PISEMA (6, 7) in mechanically aligned lipid bilayers. The final stage of refinement was to incorporate explicit lipids around the protein structure and carry out minimization to reveal the interactions between the lipid and protein domains. In our structures, we find that the N-terminal amphipathic helical domain Ia (residues 1-16) rests on the surface of the lipid membrane with the hydrophobic face of domain Ia embedded in the membrane bilayer interior. The helix comprised of domain Ib (residues 23-30) and transmembrane domain II (residues 31-52) traverses the bilayer with a tilt angle of ~24° in the monomer and an angle of ~16° in the pentamer. Hybrid methods such as the one presented in this work will be necessary to tackle challenging biophysical problems such as membrane protein structure determination.

References

1. Kimura Y, Kurzydlowski K, Tada M and Maclennan DH (1997). J Biol Chem 272, 15061-4.

2. Reddy LG, Jones LR and Thomas DD (1999). Biochem 38, 3954-62.

3. Traaseth NJ, Shi L, Verardi R, Mullen DM, Barany G and Veglia G (2009) PNAS 106, 25, 10165-70.

4. Shi L, Traaseth NJ, Verardi R, Cembran A, Gao J and Veglia G (2009) J Biomolec NMR 44, 195-205.

5. Schwieters CD, Kuszewski JJ, Tjandra N and Clore GM (2003) J Magn Reson 160, 65–73

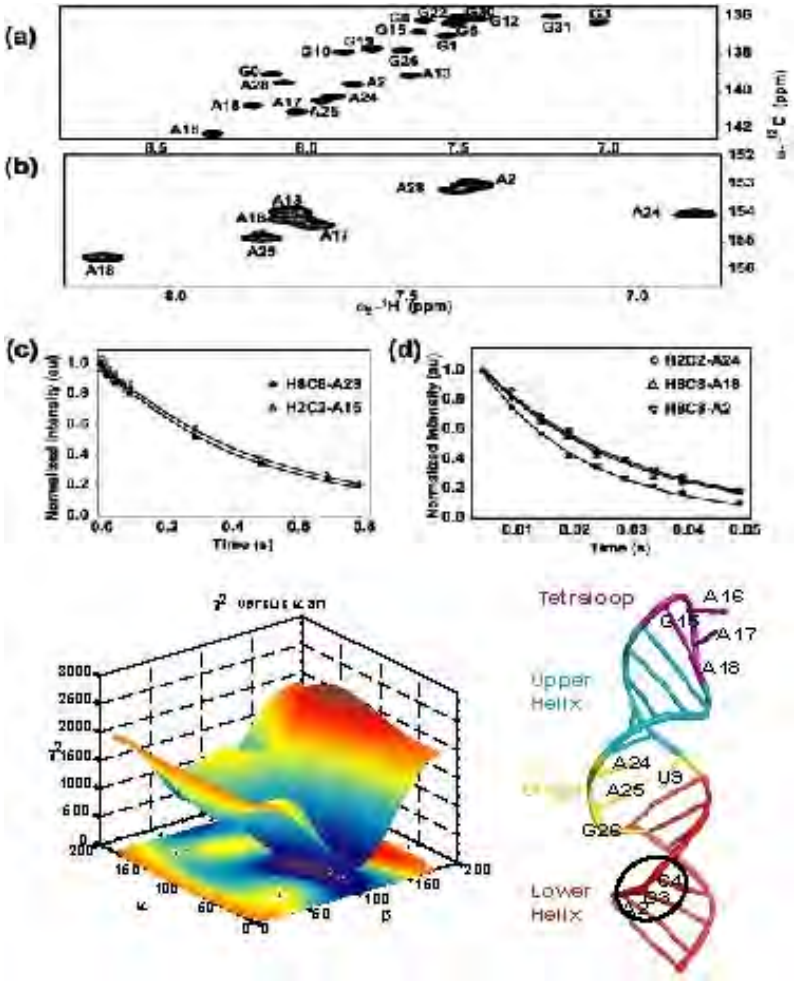
6. Wu CH, Ramamoorthy A and Opella SJ (1994) J Magn Reson 109, 270-2.

7. Gopinath T and Veglia G (2009) J Am Chem Soc 131, 5754-6.

178. Structural switch model for Group II Intron RNA catalytic function

T. Kwaku Dayie., Chemistry and Biochemistry, University of Maryland, College Park, MD, United States.

RNA molecules are expected to carry out cellular functions that rival those of proteins, yet the three-dimensional (3D) structures of RNA and their dynamics characterization lag far behind those of proteins. To address the impact of flexibility on RNA biomolecular structure and function, we reconstructed a group II intron from *Pylaiella littoralis* into a highly active form by combining an unstructured 22nt substrate, a 36nt domain 5 (D5) hairpin, and a 493 nt domains 1 through 3 (D123). This new tripartite ribozyme system functions under low salt conditions attractive for NMR structural and dynamics studies. We will show that using this divide and conquer approach, we can obtain chemical shift perturbation data on D5 binding to the large 100 kDa D123 fragment. Additionally using NMR relaxation measurements and newly developed software for RNA dynamic analysis, we will show that regions of D5 important for catalysis and binding are flexible, suggesting that motion is an important and necessary component of catalysis.



179. NMR based screening tool for quality control of botanical dietary supplements

Kimberly L. Colson,[1] Joshua M. Hicks,[1] Jan A. Glinski,[2] Stefan Gafner,[3] Jonathan Ferrier,[4] Kristina McIntyre,[4] John T. Arnason,[4] Alain Cuerrier,[5] Brian Killday.[1], [1]R&D, Bruker BioSpin, Billerica, MA, United States; [2]Planta Analytica LLC, Danbury, CT, United States; [3]Tom's of Maine, Kennebunk, Maine, United States; [4]Department of Biology, University of Ottawa, Ontario, Canada, United States; [5]Montreal Botanical Garden, Montreal, Quebec, Canada.

Assessment of quality of botanical dietary supplements is challenging due to the complex nature of the molecular components that vary with growing location, seasonal conditions, harvesting conditions and processing conditions. The ability of NMR to analyze complex mixtures as a non-targeted fingerprinting method combined with rapid sample preparation makes it an attractive analytical tool for the routine analysis of botanical extracts. In this presentation we will show our work towards developing an NMR based quality control tool for crude botanical extracts including grape seed, pine bark, skullcap, ginseng, cranberry and blueberry. This presentation includes (1) evaluation of NMR reproducibility between different instruments and different operators to establish robust screening methods, (2) statistical methods used to characterize the botanical extracts, (3) sample characterization to provide information such as the varietal, sample purity, and natural variation in samples, and (4) identification of the presence of single components within a crude extract and quantification of these components.

180. A fresh look at triosephosphate isomerase reaction mechanism

Sharon Rozovsky., Department of Chemistry & Biochemistry, University of Delaware, Newark, DE, United States.

Triosephosphate isomerase (TIM) is one of the most efficient enzymes known, and also one of the most extensively studied. Our understanding of TIM is often used to explain the mechanism by which all enzymes bring about their remarkable rate acceleration. The classical view of TIMs catalytic power holds that the geometry of the substrate is strained, and resembles that of the transition state. NMR spectroscopy enable a detailed analysis of chemical entities bound to TIM during catalysis. Remarkably, rather than straining the substrate, TIM appears to provide an optimal environment for the initial proton transfer. Analysis of the enzyme bound species suggests that the proton transfer is the reaction rate limiting step. Implications for the reaction mechanism and the classical view of this textbook enzymatic reaction are discussed.

181. Database mining applications for NMR protein structure determination

Frank Delaglio., Software Science Consultant, NMR Science, North Potomac, MD, United States.

Conventional NMR protein structures rely on identification of short-range inter-proton distances from NOE peaks, usually the most time-consuming step in structure generation. Furthermore, NOE information cannot easily be interpreted quantitatively, so large numbers of distance restraints must be included in order to generate precise structures. We present novel alternatives to NMR protein structure determination, based primarily on quantitative orientational restraints from backbone chemical shifts and residual dipolar couplings. To exploit these orientational restraints effectively, we use database mining of small fragments from known protein structures. This forms the basis of NMR structure calculation protocols that can be both quicker and more precise than traditional methods. Protein backbone chemical shifts are strongly correlated with backbone structure, but with no simple numerical relationship. In the TALOS+ approach, we search a database of residue triplets from known structures to find entries whose measured backbone shifts match those in the target protein, and use the best matches to predict backbone angles in the target. When combined with a neural-network classification scheme, this yields automated phi and psi torsion restraints for 88% of residues on average, with an error rate of 2.5%, and an RMSD for "correct" restraints of better than 15 degrees. This same approach can be "reversed" in order to predict the shifts of a proposed structure. This

method, called SPARTA, yields shift predictions with typical deviations of N 2.36, HN 0.46, HA 0.25, CA 0.88, CB 0.97 and CO 1.01 ppm. Orientational information from dipolar coupling is a powerful complement to conventional short-range NOE distance information. However, the orientational information is also ambiguous, because there are continuous ranges of orientations that would all give rise to the same measured dipolar coupling. One way to help circumvent this ambiguity is to limit consideration to physically realistic arrangements of orientations. In the case of proteins, we do this via NMR homology database mining, in an approach called Molecular Fragment Replacement (MFR).

MFR identifies short fragments in known protein structures whose simulated NMR parameters (such as shifts and dipolar couplings) are a good match for the observed NMR parameters of the target. MFR was used to determine the structure of Gamma-S crystallin (177 residues), based primarily on dipolar couplings and chemical shifts, supplemented by small numbers of easy-to-assign HN-HN and methyl-methyl distances from specially labeled samples. The final MFR-derived structure of Gamma-S agrees with its homolog (50% sequence identity) Gamma-B to 0.63 angstroms RMSD for the N-terminal domain backbone, and 1.09 angstroms for the C-terminal domain. In particular, the N-terminal agreement is among the best between any NMR structure and homolog.

MFR has also been applied in conjunction with the well-known ROSETTA program for ab-initio structure prediction. This combined approach was applied to blind structure prediction of nine small proteins with sizes from 65-129 residues, yielding predictions which matched subsequent experimentally determined folds with RMSDs of 1.14 to 2.85 angstroms, using sequence information and chemical shifts alone.

Your Company Fosters Innovation - Now how do you protect it?

Sponsor: Division of Chemistry & the Law
Organizer: Sarah Perlinger Hasford

182. Whether And How To Protect Your Innovations: Initial Considerations

Roberte Makowski., Connolly Bove Lodge & Hutz LLP, United States.

The initial evaluation process on whether and how to protect your innovations will be discussed, including trade secrets, patent protection, and patentable subject matter. This presentation will also highlight strategies for best protecting your invention from its initial discovery/development.

183. Drafting your Patent Application to Avoid Written Description, Enablement, and Obviousness Rejections

Eamonn Morrison., Connolly Bove Lodge & Hutz LLP, United States.

A claimed invention must be novel, non-obvious, and enabled, as well as be supported by an adequate written description, in order to be patentable. This presentation will provide a primer on drafting chemical and pharmaceutical patent applications in order to avoid rejections from the USPTO based on a failure to meet these requirements.

184. A Former Examiner's Guide to the Patent Office: How to Work Effectively and Efficiently with Examiners to Patent Your Innovations

Sarah Hasford, **James Balls**., Connolly Bove Lodge & Hutz, LLP, United States.

James and Sarah will give a basic primer on how patent applications are handled by Examiners at the U.S. Patent and Trademark Office. Their presentation will also include tips on how to effectively work with Examiners to optimize patent protection.

185. Potential Pitfalls to Protecting Innovation: Activities Now that Can Affect Patentability in the Future

Geoffrey Zelley., Connolly Bove Lodge & Hutz, LLP, United States.

This presentation will discuss a variety of regularly undertaken activities which could hamper future patentability of an invention. In addition, suggestions will be presented to prevent or minimize problems down the line.

186. IP Strategy: Licensing, Legal Opinions and Due Diligence

Mark Freeman., Connolly Bove Lodge & Hutz, LLP, United States.

Our discussion considers some of the IP management issues addressed by legal opinions and due diligence. Contexts for these considerations include obtaining patent protection, investigating licensing options, and encountering third party IP challenges.

ACS Undergraduate Research Symposium - III

Organizers: Narmada Gunawardena, Andrea Martin

Session Overview: Posters may be set up time around 1:15. The symposium provides an excellent opportunity for undergraduate chemistry students to present the results of their research. Presenters should be by their posters from 1:30 - 3:00.

187. Synthesis of a Ruthenium Complex of a Chiral Tetradentate Aminosulfoxide Ligand

Krista N. Taylor,[1] Tim J. Brunker,[1] Arnold L. Rheingold.[2], [1]Department of Chemistry, Towson University, Towson, MD, United States; [2]Department of Chemistry, University of California, San Diego, La Jolla, CA, United States.

A new tetradentate diamino-disulfoxide ligand was synthesized as a single enantiomer by conjugate addition of (*R*,*R*)-*N*, *N*'-dimethylcyclohexanediamine to (*R)-p*-tolyl vinyl sulfoxide. Reaction of this ligand with $RuCl_2(PPh_3)_3$ gave the corresponding $RuCl_2$ complex and a *trans*-$RuCl_2$(ligand) stereoisomer was characterized by single crystal x-ray diffraction. Both sulfoxide donors were shown to be S-bound to the Ru center. Sulfoxide ligands are of interest in coordination chemistry as they may bind through oxygen or sulfur, and may also be chiral at sulfur. Complexes of sulfoxides with redox-active metals could be useful as a redox-based chiroptical molecular switch if the binding mode of a chiral sulfoxide changes upon oxidation/reduction.

188. Cloning, expression, and purification of a putative acetylcholine binding protein from Nostoc punctiforme

Kasey M Johnson, Victoria Pisciella, Barry S Selinsky., Department of Chemistry, Villanova University, Villanova, PA, United States.

A homology search of bacterial genomes has uncovered three putative ligand gated ion channels and an acetylcholine binding protein in *Nostoc punctiforme*. We have successfully cloned the gene for the acetylcholine binding protein and inserted it into a bacterial expression vector as a small ubiquitin related modifier (SUMO) fusion protein with an added $(his)_6$ tag for visualization and purification. We were able to overexpress the SUMO fusion protein in *E. coli* BL21(DE3) cells. Fractionation experiments indicated that the fusion protein was associated with the bacterial plasma membrane. A detergent screening found that only sodium dodecyl sulfate was capable of solubilizing the expressed protein. We are currently developing methods to purify the SDS-solubilized protein using a Ni-affinity column.

189. Synthesis of new Heterocyclic Inhibitors of the Helicase of Hepatitis C Virus

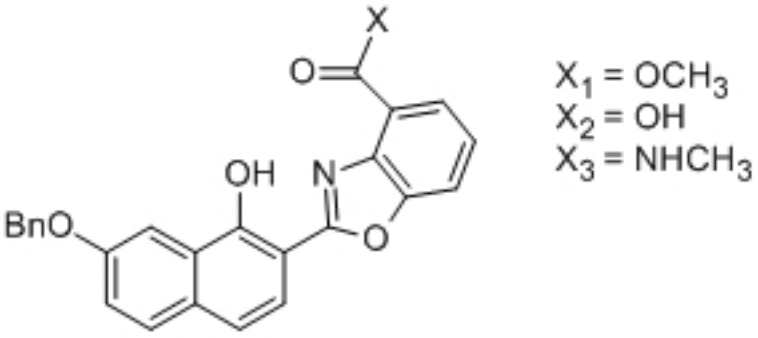
Kevin W. O'Malley, Dawn N. Ward, Paul J. Smith., Department of Chemistry and Biochemistry, University of Maryland, Baltimore County, Baltimore, Maryland, United States.

The Hepatitis C virus (HCV) is a blood borne pathogen that infects 3 percent of the world's population. In the United States, HCV is a leading cause of liver cirrhosis, liver carcinoma, and chronic hepatitis. The damage that HCV yields is exacerbated by limited treatment options. Currently the only approved therapies for HCV are combined pegylated alpha-interferon with ribavirin, and pegylated alpha-interferon alone. While the combination therapy is most effective, it only yields long-term improvement in 55 percent of patients. Considering the severity of the disease, sparse treatment options, and sub-optimal efficacy of existing HCV drugs, the development of new therapeutic compounds for HCV is highly warranted.

The natural product UK-1 is known to have significant anti-cancer activity. In our lab, new novel heterocycles (e.g. **1**) based on UK-1 were synthesized that are effective against HCV in the whole cell replicon assay and in the HCV helicase assay. Interestingly, the activity of **1** in the whole cell replicon assay was ten times higher than its activity in the helicase assay. It was hypothesized that a methyl-ester functional group on **1** may become cleaved by intracellular esterases; thus it may be the resulting carboxylic acid that is the actual active species.

To test this hypothesis, variations of the lead compounds were synthesized with carboxylic acid (**2**) or amide (**3**) functional groups in place of the methy-ester functional group. High activity of the carboxylic acid in the HCV helicase assay, compared with that of the methyl-ester (**1**) will confirm the hypothesis. The amide (**3**), which is isosteric to the methyl-ester (**1**), is not subject to hydrolysis by intracellular esterases, and will serve as a valuable control.

The synthesis of these compounds will be presented along with the results from biological assays, including both the whole cell HCV replicon assay and the in vitro HCV helicase assay. The ultimate goal of this project is to develop more potent and bioavailable analogs for the lead compound (**1**) for the creation of a new class of HCV theraputics.



190. Explorations in the synthesis of new Troger's base derivatives

Alyson DeStefano, Donald L Jameson., Department of Chemistry, Gettysburg College, Gettysburg, PA, United States.

Troger's base (TB), a chiral diamine providing a moderately rigid, roughly 90 degree angle between two aromatic rings, is intriguing as a potential element in the construction of nanometer scale molecules and assemblies. Construction of diastereomerically pure molecules or assemblies containing two or more TB fragments requires enantiomerically pure TB building blocks. We have prepared both 2,8-diiodo and 2,8-dibromo Troger's base and resolved them via diastereomeric salt formation into their entantiomers with > 95 % e.e. The method is applicable to a variety of other TB deriva-

tives, including the parent 2,8-dimethyl Troger's base. Progress on the application of this resolution method to the construction of diastereomerically pure molecules containing two TB fragments will be reported.

191. Simple and efficient green methylation of phenols, carboxylic acids and heteroaromatic nitrogen compounds using dimethyl carbonate

Marc Fialkoff, **Andrew Krasley**, Donald L Jameson, Timothy W Funk., Department of Chemistry, Gettysburg College, Gettysburg, PA, United States.

A central theme of the organic laboratory curriculum at Gettysburg College is the demonstration of "green chemistry" concepts. Towards that end, experiments are designed to minimize use of hazardous materials, utilize catalytic processes and exhibit atom economy. As part of this project, we were motivated to develop a process for the methylation of heteroatomic functional groups, which avoided the commonly used, but highly toxic reagents such as methyl iodide or dimethyl sulfate. Dimethyl carbonate has been widely explored as a "green" methylating agent, but its use has often required high temperatures and/or inconvenient reaction conditions. We report convenient experimental conditions for the methylation of phenols, carboxylic acids and heteroaromatic nitrogen compounds using dimethyl carbonate as the methylating agent. The reactions, which take advantage of the concept of organocatalysis, occur at 100 – 110 degrees C and atmospheric pressure and generally provide yields of 70-90 %. The conditions have been adapted to an organic chemistry lab experiment in which p-phenylphenol is converted to its methyl ether.

192. Electrochemical sensors based on poly[4-vinylpyridine Os(bipyridine)$_2$Cl]-co-ethylamine on glassy carbon electrode for glucose analysis

Phong Trinh, Amos Mugweru., Chemistry & Biochemistry, Rowan University, Glassboro, NJ, United States.

The Polycationic redox polymer, poly[4-vinylpyridine Os(bipyridine)$_2$Cl]-co-ethylamine (POs-EA) was synthesized and then covalently attached onto glassy carbon electrode. Glucose oxidase (GOx) was then attached to the redox polymer modified electrode through electrostatic interaction. This electrode containing the redox polymer and glucose oxidase was found to respond to glucose in solution. Another sensor arrangement that responded to glucose was prepared by trapping the redox polymer, Pos-EA and GOx in polyethylene glycol diacrylate hydrogel (PEG-DA) on glassy carbon using photopolymerization. In this work we compare the results of cyclic voltammetry and amperometry of the two types of sensors.

193. Synthesis of functionalized cyclic boronic acids via hydroxy assisted Baylis Hillman reaction of a-boronoaldehydes

Sravan K Jonnalagadda,[2] **Subash C Jonnalagadda**,[1] Michael A Corsello,[1] Chase P Gomez,[2] **Venkatram R Mereddy**.[2], [1]Department of Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States; [2]Department of Chemistry and Biochemistry, University of Minnesota Duluth, Duluth, MN, United States.

2-Boronobenzaldehyde undergoes a facile Baylis Hillman reaction with variety of electrophilic alkenes such as methyl acrylate, acrylonitrile, methyl vinylketone and acrolein in the presence of DABCO to furnish the corresponding benzoboroxoles. The reaction of 4-boronobenzaldehyde under similar conditions was observed to be very sluggish and the products could not be obtained in synthetically useful yields. All the new compounds were evaluated for their anti-bacterial and anti-fungal activity. The synthetic studies as well as the biological activity will be presented.

194. Synthesis and Quantization of Z-(9)-Pentacosene, A Honey Bee Pheromone Given Off During The Waggle Dance

Yonaton N Heit, Spyros Mavropoulos, Amber F. Charlebois., Department of Chemistry and Pharmaceutical Science, Fairleigh Dickinson University College at Florham, Madison, New Jersey, United States.

Pentacosane, tricosane, Z-(9)-pentacosene, and Z-(9)-tricosene are four chemicals or pheromones that are given off by the honey bee during the waggle dance to increase number of bees that forage and gather food. Our collaborator in this project, David Gilley of William Paterson University, is a honey bee expert and has asked us to synthesize one of these pheromones as it is not commercially available, and to subsequently quantitate the amount of these pheromones present above the dance floor during the waggle dance. We have successfully synthesized Z-(9)-pentacosene in a two step synthetic process and currently in the process of using Solid Phase Micro Extraction (SPME) fibers to collect and analyze these compounds for quantitative purposes.

195. Effects of Osmotic Stress and Macromolecular Crowding on the B-to-Z Transition in DNA

Crista Nguemeta, Richard S. Preisler, Alan J. Pribula., Department of Chemistry, Towson University, Towson, MD, United States.

Electrostatic interactions between transition metal complexes and DNA have been a continuous interest in research over several decades. The ability of the +3 complex hexamminecobalt (III) to drive the transition from righthanded B-DNA to lefthanded Z-DNA at very low complex concentrations has been attributed to the formation of both charge-charge interactions with the DNA backbone and site-specific hydrogen bonds with DNA phosphates and bases (Gessner, Quigley,Wang, van der Marel, van Boom, and Rich (1985) *Biochemistry 24*, 237-240). We have used circular dichroism spectroscopy to observe the effects of several +3 and +2 complexes on the conformation of the DNA copolymer poly[d(G-C)]. We have observed that various complexes with a charge of +3, such as hexamminecobalt (III), require much smaller concentrations (5-15 micromolar) compared to +2 complexes, such as chloropentamminecobalt (III) (200-600 micromolar). When an osmotic stress was applied to the system using sucrose, the conformational equilibrium was shifted toward Z-DNA. The osmotic effect was relatively small with a +3 complex, but much greater when a +2 complex was used. The difference in osmotic sensitivity may occur because the weaker binding of the lower charge complex to the DNA backbone allows greater competition of water molecules for hydrogen bonding sites on DNA. Currently we are investigating the effect of conformational flexibility in +3 complexes by comparing the effects of osmotic stress with monodentate ligands (greater conformational flexibility), such as the ammonias in hexamminecobalt (III) and bidentate ligands (greater conformational rigidity), as in trisethylenediaminecobalt (III). We predict that the more constrained hydrogen bonding interactions of the bidentate ligand will be correlated with a greater sensitivity to water activity. Macromolecular crowding agents, which simulate the sterically crowded environment in cells, have been shown to influence protein folding equilibria (Qin and Zhou (2009) *Biophysical Journal 97*, 12-19). We have investigated the effect of various concentrations of Ficoll-70 on the B-to-Z transition induced by hexamminecobalt (III). At higher Ficoll concentrations the equilibrium was shifted toward the formation of Z-DNA, but the results at lower Ficoll concentrations were less clear-cut. This study is funded by Undergraduate Research Committee grants to C. N. from Towson University and the Jess and Mildred Fisher College of Science and Mathematics at Towson University.

196. Computational analysis of aromatic oligoamide foldamers

Marc Luong, Jhenny Galan, Zhiwei Liu, Christian Tooley, Vojislava Popristic Popristic., West Center for Computational Chemistry and Drug Design, University of the Sciences in Philadelphia, Philadelphia, PA, United States.

Foldamers are synthetic oligomers that exhibit secondary structures found in nature and has great potential in medicinal applications, such as drug delivery. Understanding foldamers at the atomic level in various polar protic and non-polar environments is essential for the rational design of foldamers. Our group focuses on the study of arylamide which is a special class of foldamers containing repetitive units of aromatic rings and amide groups, and we are specifically concerned with the effects of the aromatic substituents on torsions around the $C_{aromatic} - C_{peptide}$ or $C_{aromatic} - N_{peptide}$bonds. My study focuses on two group of model compounds with the $C_{aromatic} - N_{peptide}$ linkage and *ortho*-flouro or *ortho*-methoxy substituents. We have'analyzed the effects of different substituents, molecular scaffold'and solvent polarity on the strength of the intra-molecular hydrogen'bonds and conformational distribution of the foldamer building'blocks by using methods such as *ab initio* calculations and'molecular dynamics simulations.

197. Biodiesel: From the Frier to the Laboratory

Joseph G Jablonski, Amber F Charlebois., Department of Chemistry, Fairleigh Dickinson University, Madison, NJ, United States.

The growing importance of alternative energy sources in our society has provided an excellent opportunity to introduce undergraduate students to the concepts of green chemistry and the use of analytical techniques while reinforcing the applicability of chemistry to their daily lives. We have optimized a process for converting used cooking oil obtained from campus dining services into biodiesel which can then ultimatly be used to power equipment used by campus facilities. Presented here is the synthesis and analysis of the biodiesel synthesized on campus. The Gas Chromatography/Mass Spectrometry (GC/MS) and the Fourier Transform Infrared (FTIR) data of the biodiesel produced confirm that biodiesel has been produced. Bomb calorimitry was also performed on the synthesized biodiesel of various concentrations, and the results were compared to that of commercial petrolium diesel.

198. Core-shell hydrogel particles incorporating Acid Black 48

Tiffany Ha,[1] Alexis Patanarut,[1] Prianka Debnath,[1] Davide Tamburro,[2] Alessandra Luchini,[2] Emanuel F. Petricoin,[2] Lance Liotta,[2] Barney Bishop.[1], [1]Department of Chemistry and Biochemistry, George Mason University, Fairfax, VA, United States; [2]Center for Applied Proteomics and Molecular Medicine, George Mason University, Fairfax, VA, United States.

Hydrogel microspheres containing Acid Black 48 constitute a new and powerful tool for protein harvesting. Acid dyes such as Acid Black 48 have been used in the quantification of protein content in milk. These studies suggested that Acid Black 48 could be a suitable affinity bait for incorporation in hydrogel particles intended for biomarker harvesting. Thermoresponsive core-shell hydrogel particles based on N-isopropylacrylamide (NIPAm) with cores that incorporate acrylic acid (AAc) were generated to provide the stationary scaffold upon which acid dye was immobilized. The core-shell pNIPAm-*co*-AAc particles were synthesized using precipitation polymerization in the absence of surfactants, and the aryl amine groups of Acid Black 48 molecules were covalently affixed to the carboxyl groups of AAc in the particle core using basic peptide coupling chemistry. Dynamic light scattering was used to determine particle size and uniformity. Preliminary sieving and harvesting performance was ascertained by incubating particles in solutions containing a known mixture of proteins and then evaluating protein uptake using SDS-PAGE. However, residual unbound dye within the particles can complicate analysis of the sequestered protein species. In light of this finding, considerable effort has gone into refining the protocols and conditions used in the washing, handling and storage and handling of particles containing Acid Black 48.

199. Characterization of Sacharolyticum degradans xylanases activity

Richard Negri, Brittany Nixon, Gbekeloluwa B. Oguntimein., Civil Engineering, Morgan State University, Baltimore, Maryland, United States.

Second generation biofuels from forest and crop residues, energy crops and municipal wastes will require development of effective hemicellases to hydrolyze hemicelluloses which account for about thirty percent of plant materials. One of the major hemicellulases is xylanases which hydrolyze xylan a major fraction of hemicelluloses. The xylanases activity of Sacharolyticum *degradans*, a bacterium *isolated* from the Chesapeake Bay with respect to temperature and pH has been studied. Three optima temperatures at 45^{o}C, 55^{o}C and 65 ^{o}C at pH 6.0 and pH optimum of 7.62 at 50^{o}C'were observed

200. Studies of the conformational rigidity of monomer units of arylamide oligomers with H-bond acceptors embedded in the aromatic ring

Chi Ngong Tang, Jhenny F Galan, Zhiwei Liu, Vojislava Pophristic., Department of Chemistry & Biochemistry/West Center for Computational Chemistry and Drug Design, University of the Sciences in Philadelphia, Philadelphia, PA, United States.

Polymers, such as arylamide foldamers, that resemble naturally occurring polypeptides have gained increasing interest because of their potential biomedical uses and their low cost synthesis. Arylamide oligomers usually contain an aromatic ring and a peptide bond. The secondary structure of foldamers, which dictates its function, is governed by noncovalent interactions such as pi-pi stacking, hydrogen bonding and electrostatics. Previous studies have shown that H-bonding substituents in various sites influence the conformational flexibility and overall shape of an oligomer. In this study, we investigate the influence of embedded H-bond acceptor in the *ortho* position of the aromatic ring on the X-$C_{aromatic}$-$C_{carbonyl}$-N torsion and the intramolecular H-bond strengths using a combination of quantum mechanics and molecular dynamics. We compare the results to our earlier studies with the H-bond acceptor attached at the *ortho* position. We also examined the effect of various solvents on the rigidity of the foldamer backbone. Based on the model compounds we have studied, we discovered that embedding the H-bond acceptor in the aromatic ring generates a more rigid structure. Our quantitative assessment of the backbone rigidity of these various foldamer building blocks will provide further insights in the design of functional foldamers.

201. Computational function annotation of structural genomics proteins in the enolase superfamily using THEMATICS

Ee Leng Terng,[1] Jaeju Ko,[1] Mary Jo Ondrechen.[2], [1]Department of Chemistry, Indiana University of Pennsylvania, Indiana, PA, United States; [2]Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA, United States.

One of the most critical tasks in genome research is to discover the function of the many gene products, particularly enzymes, whose sequences we now know for humans and other organisms. Computational approaches are expected to contribute'significantly in this task. Here we present a new computational procedure for assigning functions to proteins of unknown function. The method is based on THEMATICS, a highly selective method for identifying active-site residues from 3D structure only. The THEMATICS-predicted active site of the query protein is aligned with the THEMATICS-predicted active site of each structural homologue whose biochemical function is known. Based on the degree of matching at the predicted active sites, a tentative assignment is made. 'The proposed method is applied to several structural genomics proteins in the enolase superfamily. We make use of the 20 distinct chemical-reaction families in the enolase superfamily, according to the Structure-Function Linkage Database. It is shown that the new approach can be applied to classifying these structural genomics proteins into the chemical-reaction families.

202. Drug-lipid interaction studies via fluorescence anisotropy and molecular dynamics simulations

Harsh Amin, Nicolas Chen, Jhenny Galan, Zhiwei Liu, Preston Moore, Julian Snow., Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, Pennsylvania, United States.

The effects of lipid-drug interaction are crucial in understanding the efficiency and toxicity, and can be very useful in drug design. In this project , we employ fluorescence anisotropy studies and coarse grain molecular dynamics simulations to better understand drug-lipid interactions. Dibucaine, also know as cinochocaine, is a local anesthetic which block both initiation and conduction of nerve impulse by decreasing the neuronal membrane's permeability to sodium ions. A comprehensible explanation of the effects of dibucaine-lipid membrane interactions on membrane fluidity has yet to be elucidated. In order to better understand this phenomenon, we use 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) vesicles marked with the fluorescent tag 1,6-diphenyl-1,3,5-hexatriene (DPH) to study changes in membrane fluidity upon binding with dibucaine. The coarse grain simulations are used to study the thermodynamic effects, such as changes in enthalpy and entropy, caused by lipid-drug binding. The experimental results show an increase in anisotropy which correlates with increase in membrane fluidity. The computational simulations display an increase in entropy which correlates with increase in chain mobility of the lipid membrane.

203. Synthesis, structure and reactivity of an Azaferrocene-borane sandwich complex

Benjamin T. Roembke,[1] Tim J. Brunker,[1] James Golen,[2] Arnold L. Rheingold.[2], [1]Department of Chemistry, Towson University, Towson, MD, United States; [2]Department of Chemistry, University of California, San Diego, La Jolla, CA, United States.

Azaferrocenes are analogs of ferrocene in which an h^5-pyrrolyl ring replaces a cyclopentadienyl ring. Various azaferrocenes, particularly planar-chiral versions, have been found to be effective as nucleophilic catalysts and as ligands for metal-catalyzed reactions. Synthetic methods to new azaferrocene-derivatives are, however, limited by the nucleophilicity and basicity of the nitrogen center although this might be avoided by coordination of the nitrogen to a Lewis acidic group. To investigate this idea, the borane-protected azaferrocene $Fe(h^5\text{-}C_5(CH_3)_5)(\ h^5\text{-}C_5H_4N\text{-}BH_3)$ has been synthesized and completely characterized including a single crystal X-ray structure. Studies have also shown that the borane can be readily removed to regenerate deprotected azaferrocene. Some reactivity of the azaferrocene has been explored including electrophilic aromatic substitution reactions and the results of these studies are presented.

Sustainability, Green Chemistry, and Policy Symposium

Sponsor: American Chemical Society
Organizer: Martha Hollomon

204. Sustainability – What is it and what does it mean to me?

Frankie K Wood-Black., Trihydro Corporation, Ponca City, OK, United States.

Sustainability is a hot topic and everyone is trying to find was to achieve it. In fact if you "Google" sustainability, you will get over 30 million hits. As scientist and engineers, this topic has crept into our research, our business practices, our communities and our homes. But, what does it really mean? How as students, instructors, researchers, engineers, and applied scientist utilize the concepts involved in "sustainability" to move forward. What challenges are faced? Are there barriers? Are there unintended consequences? This presentation will provide a bit of history and outline some of the dilemmas that are faced with implementing sustainable practices.

205. Enhancements of enzymatic saccharification of hardwood biomass using oxalic acid pretreatments

David W Berke-Schlessel, Robert Wexler, Sudipto Das, Yen Wei., Department of Chemistry, Drexel University, Philadephia, PA, United States.

When untreated, enzymatic saccharifation of hardwood biomass is a slow process; in order to make the process more feasible for use in the production of cellulosic ethanol, pretreatments are necessary to increase glucose output. There are many types of pretreatments used to enhance glucose output, but many are inefficient, expensive, and can produce hazardous byproducts. When hardwood is treated with the cellulase enzyme from t. reesei, there is an output of 0.32 mg/mL/hr of glucose. After being pretreated in a 2.5% solution of oxalic acid (w/v) and 0.5M NaOH the glucose output can be augmented 275% to a glucose output of 0.88 mg/mL/hr. Other combinations of oxalic acid and NaOH concentrations were investigated, but the 2.5% solution of oxalic acid and 0.5M NaOH showed the best results.

206. Sustainability from innovative chemistries to legislative policy

Catherine T. Hunt., Technology Collaboration Development, The Dow Chemical Company, Spring House, PA, United States.

In short, sustainability is about prospering today without compromising tomorrow. This talk will quickly review the principles of green chemistry and green engineering, highlight award winning innovative sustainable chemistries, and put a spotlight on how we as chemical professionals and private citizens can come together with scientific societies around the world to advance a 'global sustainable chemical enterprise'. It will take all of us working together to create a sustainable planet for future generations; *so let's get started!'***CATHERINE T. *"Katie"* HUNT** is the Senior R&D Director for External Science & Technology at The Dow Chemical Company. She began her career as a senior scientist in analytical research at Rohm and Haas in 1984 after completing an NIH Postdoctoral Fellowship at Yale University. During her 25 years at Rohm and Haas[1], Katie held positions of increasing responsibility, from research scientist to process chemist to plant laboratory manager to Director of their worldwide Analytical and Computational Competency Network (better known as ACNET) and ultimately, Corporate Sustainability Director and Leader for Technology Partnerships.

[1] Rohm and Haas Company was acquired by The Dow Chemical Company on April 1, 2009.

207. Sustainable future: century of challenge and change for our plant

Pat N. Confalone., Crop Agriculture and Nutrition Platform, DuPont, Newark, DE, United States.

This is a century of challenge and change for our planet. Chemists and chemical engineers will play a decisive role in confronting these challenges and bringing about changes that improve people's lives and help us create a sustainable future. Doing these things will not be easy. But the ACS and its members can and will do their best to transform these visions into reality.

Pat N. Confalone, Ph.D., an executive with DuPont in Wilmington, Del., has been elected to the board of directors of the American Chemical Society (ACS), the world's largest scientific society. He will begin a three-year term Jan.1, 2009, as director from District III, which covers 11 ACS Local Sections in New Jersey, Pennsylvania, Delaware, Maryland and the District of Columbia.

Confalone, who is vice-president, Global Research & Development, Crop Protection, Agriculture and Nutrition Platform at DuPont, received his B.S. from Massachusetts Institute of Technology in 1967, his M.S. in 1968 and Ph.D. in 1970, both from Harvard University. He and his wife, Dianne, live in Wilmington. An ACS member since 1970, Confalone has been the chair of the ACS Division of Organic Chemistry, a member of the advisory board of the ACSs *Journal of Organic Chemistry*, and chair of the Committee on Chemistry & Public Affairs.

208. Sustainability and the chemical enterprise

William F. Carroll., Occidental Chemical Corporation, Dallas, TX, United States.

The power of chemistry to improve people's lives is extraordinary. That's particularly important now as we face a number of emerging global challenges. The need for innovative solutions to these challenges has never been greater, and the ACS and our members are on the forefront of those efforts. We are committed to finding solutions to these problems and creating a sustainable future for Earth and its peoples.

William (Bill) Carroll is a vice president of Occidental Chemical Corporation in Dallas, TX, with nearly 30 years of industrial experience. He holds a B.A. in chemistry and physics from DePauw University in Greencastle, IN, an M.S. from Tulane and a Ph.D. from Indiana University. The latter two degrees are in organic chemistry. He is adjunct professor of chemistry at Indiana, where he teaches polymer chemistry. In 2005, Bill was president of the American Chemical Society. Contact e-mail: William_F._Carroll@oxy.com

ACS Graduate and Post-Doc Research Symposium - Poster Session

Sponsor: American Chemical Society
Organizer: Narmada Gunawardena

209. Master of the 7 C's

Thomas Lane., Director of Global Science and Technology Outreach, Dow Corning Corporation, Midland, MI, United States.

Strengthing the bonds: chemistry,members, the world - together

210. Molecular dynamics of amphiphathic peptides embedded in a lipid bilayer

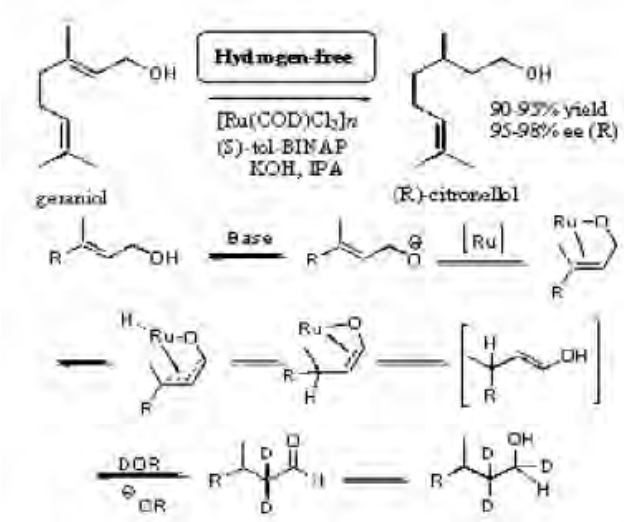
Thuy Hien T Nguyen, Zhiwei Liu, Preston B Moore., Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, United States.

Membranes and their embedded ion-channels play a crucial role in numerous cell processes such as signaling, energy conversion, and ion conductance. One common class of ion-channels is the homo-oligomeric ion-channels which are found in many membrane protein structure studies. The overall goal of this research is to quantify the structural, dynamical, and energetic properties of transmembrane amphipathic peptides which form these homo-oligomeric ion-channels. In order to achieve this goal, we performed a series of molecular dynamics (MD) simulations using a rigid tubular coarse grain (CG) model, specifically we elucidated the mechanism and energetic of four amphiphathic a-helical peptides, particularly the dimerization free energy and pathway to assembly. While the tubular CG peptide model provides us with vital information on ion-channel assembly and structure, it does not allow the model to be flexible enough to fully form an ion-channel. Therefore, we are in the process of designing a new CG model that is structurally and physically more suitable for our studies than our previous tubular CG model. We ran a series of all-atom (AA) and CG MD simulations using different oligomeric states which not only allow us to design a new CG model, but also allow us to determine if different oligomeric states are stable. In summary, our simulations can lead us to further understanding of the assembly of peptides in membranes, which is of great importance when designing antimicrobial, antiviral, and other pharmaceutical agents that will target ion-channels.

211. Asymmetric transfer hydrogenation of allylic alcohols with chiral ruthenium catalysts

Ruoqiu Wu, Marie G. Beauchamps, Joseph M. Laquidara, John R. Sowa., Department of Chemistry and Biochemistry, Seton Hall University, South Orange, NJ, United States.

Chiral alcohols are the key chiral building blocks to many single enantiomer pharmaceuticals.[1] Asymmetric reduction of the corresponding prochiral ketones to produce the chiral alcohols is one of the most common synthetic routes. Asymmetric transfer hydrogenation (ATH)[2] is a well developed method for enantioselective reduction of ketones, imines, and aldehydes that both rivals and compliments asymmetric reductions with hydrogen gas.[3] Asymmetric transfer hydrogenation (ATH) of allylic alcohols is a novel reaction, and provide a very promising method to prepare chiral alcohols. In our study, a range of substrates, including aliphatic and cyclic allylic alcohols have been screened by using ruthenium-based catalysts made *in-situ* with chiral bidentate phosphine ligands, ATH occurs in > 90 % yield and > 90 % ee. The mechanism investigated with deuterated isopropanol indicates that the reaction occurs via tandem enantioselective isomerization-transfer hydrogenation process. The reaction provides the product with the same chirality as the gaseous hydrogenation reaction and comparable yield and ee. Reaction conditions can be optimized using pure chiral ruthenium complexes.



References:

1. Zhong-Hua Yang Z.-H., Zeng R., Yang G., Wang Y., Li L.-Z., Lv Z.-S., Yao M and Lai B., *Journal of Industrial Microbiology and Biotechnology*, **2002**, *35*, 1047-1051.

2. (a) Gladiali, S.; Alberico, E. *Chem. Soc. Rev*. **2006**, *35*, 226–236; b) Samec, J. S.; Backvall, J. E.; Andersson, P. G.; Brandt, P. *Chem. Soc. Rev*. **2006**, *35*, 237-248.

3. (a) Noyori, R. *Angew. Chem. Int. Ed.,* **2002***, 41,* 2008-2022; b) Noyori, R. *Asymmetric Catalysis in Organic Synthesis;* John Wiley: New York*,* **1994**; c) Krische, M. J.; Sun, Y.-K. *Acc. Chem. Res.* **2007***, 40,* 1237 and accompanying articles.

212. Role of Dichloromethane and Phenol in Chemical Paint Strippers

Kelly E. Watson,[1] James H. Wynne,[2] James P. Yesinowski,[2] Christopher N. Young,[3] Clive R. Clayton.[3], [1]Science Applications International Corporation, Washington, DC, United States; [2]Department of Chemistry, Naval Research Laboratory, Washington, DC, United States; [3]Department of Materials Science and Engineering, Stony Brook University, Stony Brook, NY, United States.

Chemical paint strippers that include dichloromethane and phenol have long been used to remove polymer coatings from metallic substrates. These paint strippers are inexpensive and remove polymeric coatings quickly and easily from a variety of metallic substrates without damage to the substrate. However, due to environmental and health concerns there is increasing pressure to replace dichloromethane with a less hazardous alternative. Although various alternatives to these organic solvent based paint strippers have been developed, none equal their effectiveness in performance or cost. The mechanism of action of chemical strippers has not been adequately characterized. We report here changes in physical and molecular-level properties of four polymer coatings after exposure to components of the paint stripper including dichloromethane and phenol. The coatings studied are polyurethane topcoats and epoxy primers and are similar to coatings in current military use. In particular we characterize the coatings using DSC, TGA, solid-state proton NMR and FTIR-ATR.

213. Progress towards a light activated self-decontaminating coating

Jeffrey G Lundin,[1,2] Robert F Cozzens,[2] Kelly E Watson,[3] James H Wynne.[1], [1]Chemistry Division, Naval Research Laboratory, Washington, DC, United States; [2]Department of Chemistry, George Mason University, Fairfax, VA, United States; [3]Science Applications International Corporation, Washington, DC, United States.

C_{60} fullerene molecules exhibit intriguing photochemical properties which hold exciting potential for novel self-decontaminating coating applications. Of these properties, the production of chemically reactive singlet oxygen by the fullerenes from the immediate environment due to UV/visible light exposure presents particular interest. The assimilation of this property into a coating could create a surface which, when exposed to sunlight, would automatically oxidize and decompose harmful or undesired chemical species contaminating the surface. Catalytic self-decontamination by a coating eliminates the need for corrosive washing solutions and greatly reduces the risk of human exposure. Herein, the effects of fullerene molecules as additives into a commercial polyurethane coating system and their degradation of pesticides on the surface in various UV/visible light environments are reported. Results demonstrate that exposure to intense light increases degradation of surface contaminates upon coatings containing C_{60} fullerene. A proposed mechanism of action and also the degradation by-products detected utilizing GC/MS are presented.

214. Characterization of a novel, putative trypanosome transcription factor

Allison Sing, Kellie Whitecavage, Jennifer Palenchar., Chemistry, Villanova University, Villanova, Pennsylvania, United States.

African sleeping sickness, caused by the parasite *Trypanosoma brucei*, is endemic in regions of Sub-Saharan Africa. Unusually, these parasites trans-splice a 39-nucleotide capped Spliced Leader RNA (SL RNA) onto the 5' end of their messenger RNA (mRNA). RNA cannot be translated without the addition of SL RNA. SL RNA is transcribed by RNA Polymerase II. The SL RNA gene contains the only RNA Polymerase II promoter element identified to date in trypanosomes. The complement of proteins involved in transcription, and their roles, are not well understood in these parasites. Recent studies of a known trypanosome transcription factor, TFIIB, revealed an association with a protein essential for parasite survival, *Tb*TAF49 (*Trypanosoma brucei* TFIIB-Associated Factor, 49kDa). *Tb*TAF49 contains transcription-related motifs, yet appears unique to trypanosomes. Promoter pulldown assays reveal *Tb*TAF49 interacts with DNA and we are currently studying the nature of that interaction, including the interaction with the SL RNA gene promoter. Studies are also underway to determine the oligomeric state of *Tb*TAF49 in the presence and absence of DNA.

215. Atmospheric oxidation mechanisms of trichloroethylene and tetrachloroethylene: ab initio studies

Carrie J Christiansen, Joseph S Francisco., Department of Chemistry, Purdue University, West Lafayette, Indiana, United States.

A number of experimental studies have investigated the atmospheric oxidation of trichloroethylene and tetrachloroethylene. However, confusion has arisen over the role chlorine atom initiated reactions may play in the oxidation of these compounds, including the influence on resulting products. In order to gain a more thorough understanding of the atmospheric oxidation mechanism of these compounds, this study presents a comprehensive computational investigation of the energetic of the hydroxyl radical initiated and chlorine atom initiated atmospheric oxidation mechanisms of both trichloroethylene and tetrachloroethylene. Analysis of the *ab initio* computed energetics of these systems suggests that the chlorine atom initiated oxidation is likely to play a significant role in the atmospheric oxidation of both compounds. Products from this mechanism will include phosgene from both compounds, dichloroacetyl chloride from trichloroethylene and trichloroacetyl chloride from tetrachloroethylene, as well as other minor products.

216. OxyR dependent stress response

Salvador Gomez, Matthew Harter, Peter M Palenchar., Department of Chemistry, Rutgers, The State University of New Jersey - Camden, Camden, New Jersey, United States.

OxyR is a redox-sensitive transcriptional regulator which activates the expression of defense genes responsible for an oxidative stress response in *Escherichia coli*. The transcription factor is activated by the modification of thiols. There are six cysteine residues in the amino acid sequence of OxyR; two are evolutionarily conserved at positions 199 and 208. It has been shown that C199 is essential for protein activity and C208 is critical for protein activity. An oxyR knock out line, TA4112, was complemented with plasmids containing OxyR with altered cysteines. Cysteine to serine point mutations allows us to further study the role of cysteins in OxyR. The cell lines researched encoded for OxyR with C208S, C143S, and C25S. TA4112 producing C199S OxyR had a phenotype that prevented us from further research. The resulting bacteria were grown on LB agar plates containing different chemical stressors. Using Carestream Molecular Imaging camera/software system, the total colony number and the mean of the area of the colonies were recorded. Our results have shown TA4112 containing plasmids producing C208S, C25S, and C143S OxyR all have independent effects. Cell lines producing C25S OxyR have a similar phenotype to C208S compared to C143S. The bacterium with mutation C208S OxyR causes differences in the area and distribution of colonies in both the background and when treated with H_2O_2 when adjusted. However, our studies of diamide show an OxyR cysteine independent response.

217. Theoretical study on protonated water clusters: enumeration of structures and classification of OH bonds

Maihemutijiang Jieli, Misako Aida., Center for Quant Life Science & Chemistry Deapartment of Graduate School of Science, Hiroshima University, Hiroshima University, Higashi-Hiroshima, Hiroshima, Japan.

1. Introduction

In this work graph representation is introduced and used in order to represent HB pattern in PW cluster $H_3O(H_2O)_{n-1}$(n=2-8). A rooted digraph is regarded as PW cluster and an HB matrix represented by a rooted digraph. **[figure1]** We numerated all possible topology-distinct patterns corresponding to PW clusters. From close investigation of the structural patterns obtained, several restrictions which should be satisfied in the stable structures of PW clusters were found. The generated HB matrices of

the restrictive rooted digraph were used as the theoretical framework to obtain all the local minima of those PW clusters using ab initio MO and DFT methods. We classified all the O–H bonds in PW clusters up to heptamer accompanied with a specific range of stretching frequencies.

2. Computational Methods and Results

The H-B matrix is used to enumerate all the possible structures, in which the hydrogen bonding patterns are different. We found several restrictions which should be satisfied in the stable structures of PW clusters given belove (we call a vertex which corresponds to a protonated water molecule P vertex, and a vertex which corresponds to a water molecule W-vertex):

(1) There is no arrow directed toward the P-vertex. (2) The number of the arrows directed from the P-vertex is 2 or 3. (3) When two arrows are directed from the P-vertex, a W-vertex which accepts an arrow from the P-vertex cannot accept any arrow from other vertex. (4) When three arrows are directed from the P-vertex, all of the three W-vertices, each of which accepts an arrow from the P-vertex, cannot accept other arrow from other vertex.

The OH stretching modes are divided into nine types by analyzing the characteristic IR frequencies of local minimum structures of PW clusters $H_3O^+(H_2O)_{n-1}$ (n=2~7).

3. Conclusion

We showed here the systematical method to find all possible structures of PW clusters. Combination of graph theoretical enumerations with ab initio MO calculations allows us to find all topology-distinct stable structures for PW clusters. We found some new PW pentamer and hexamer structures.

Stretching modes of different OH bonds in local minima of PW clusters are generated systematically at the MP2/aug-cc-pVDZ level of theory. The vibrational frequencies distribution and their changing order of different types of OH in PW clusters are classified systematically. Vibrational frequencies of different OH types agree reasonably well with the recent experimental and theoretical results.

4. References

(1) Jieli M.; Miyake, T.; Aida, M. Bull. Chem. Soc. Jpn. 2007, 80, 2131–2136

(2) Jieli M.; Aida M., The Journal of Physical Chemistry A 2009 113 (8), 1586-1594

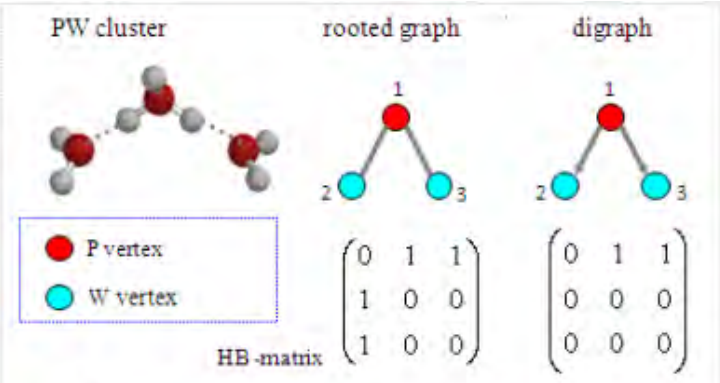


Fig. 1. A structure of a PW cluster (n=3) with the equivalent rooted graph, rooted digraph and the corresponding hydrogen bond matrix.

218. Mechanism of anesthetic binding to lipid bilayer

Nicolas Chen., Chemistry & Biochemistry, University of Science in Philadelphia, Philadelphia, PA, United States.

The study of drug interactions with lipid bilayers is essentially for drug design, efficacy, and toxicology. Computational molecular dynamic simulation of physical parameter determination was carried out in this research. The drug Dibucaine and the lipid bilayer POPC (1-palmitoyl-2-oleoyl-glycero-3-phosphatidylcholine) were chosen to use for the study because the research interest will be focused on studying the binding of anesthetics to lipid bilayers. The long term goal of these studies is to gain insight into anesthetics binding to lipid bilayer mechanism, especially the thermodynamics of the system. We hypothesize that the increased entropy upon binding of drugs comes mainly from the tails of the lipid, while the enthalpy term is dominated by the headgroup-drug interaction. The analysis of the output from the computational trajectories could provide evidence for this hypothesis. Furthermore, these computational results could lead us to a generalized principal for a certain drug class such as anesthetics binding to membrane.

219. Engineering magnetic hydrogel microspheres for the capture and concentration of dilute proteins and peptides: Application as biomarker harvesting platforms

Alexis Patanarut,[1] Tiffany Ha,[1] Elissa H. Williams,[1] Emanuel F. Petricoin,[2] Lance A. Liotta,[2] Barney Bishop.[1], [1]Department of Chemistry and Biochemistry, George Mason University, Fairfax, VA, United States; [2]Center for Applied Proteomics and Molecular Medicine, George Mason University, Fairfax, VA, United States.

Biomarker harvesting represents a novel application for functionalized magnetic hydrogel microspheres. Introduction of magnetic elements into the polymeric network enhances their overall utility by simplifying particle recovery following harvesting. Engineering magnetic hydrogel particles toward biomarker harvesting applications requires magnetic particles of suitable size and the appropriate affinity baits. The magnetic core component of magnetic hydrogel particles is typically coated with an inert compound in order to prevent undesirable events such as agglomeration and oxidation. The described work focuses on magnetic microspheres functionalized with reactive dye, Cibacron Blue F3G-A, and their sequestration performance. The hydrogel particle microspheres were synthesized via precipitation polymerization, and the magnetic component in the form of iron oxide was subsequently incorporated within the hydrogel matrix. The reactive dye was then immobilized onto the polymeric scaffold to facilitate the harvest of target proteins and to prevent their escape from the particle. The ability of these particles capture and sequester low molecular weight and low abundance species from complex solutions portends their potential utility in applications other than biomarker harvesting.

220. Carbon nanotube-based electrochemical sensors for single-cell NO detection

R. Venkat Kalyana Sundaram,[1] Fei Li,[3] Roozbeh Ghavami,[3] Riju Singhal,[2] Zulfiya Orynbayeva,[2] Eric Borguet,[3] Yury Gogotsi,[2] Elisabeth S Papazoglou,[1] **Michael G Schrlau**.[2], [1]School of Biomedical Engineering, Drexel University, Philadelphia, Pennsylvania, United States; [2]Department of Materials Science and Engineering, Drexel University, Philadelphia, Pennyslvania, United States; [3]Department of Chemistry, Temple University, Philadelphia, Pennsylvania, United States.

We have developed an electrochemical sensor using non-catalytic chemical vapor deposition (CVD) of carbon on pulled quartz glass capillaries. Deposition of carbon happens mostly on the inner surface of the glass capillary and using buffered hydrofluoric acid, the glass is etched and the exposed carbon used as an electrode. Based on pulling parameters and etching times, we can control the conicity and dimensions of the electrode as low as 10 nm tip diameter and a few hundred nanometers in length. For the purpose of our experiments, we created an electrode with a tip diameter of 200 nm and length

of 210 μm. Existing, commercially available electrodes for single cell detection require exposing a threaded metal wire through a glass capillary or coating a wire with insulating material to provide a conducting surface to study redox reactions. Such methods are time consuming and require a great amount of skill to produce electroactive surfaces that are not reproducible from one electrode to the next. Our manufacturing protocol provides an automated method to produce a controlled surface that is reproducible batch-after batch. Using this tool, we were able to detect Potassium Ferricyanide concentrations down to 1 nM in static solutions with cyclic voltammetry. We were also able to detect Nitric Oxide (NO) in a solution of phosphate buffered saline down to 1 μM. Using cyclic voltammetry, we determined an appropriate potential of 1 V vs. Ag/AgCl reference electrode for NO detection in chronoamperometric studies. Finally, we detected up to a 20 pico-ampere increase due to extracellular NO from Human Osteosarcoma (HOS) cells using chronoamperometry when stimulated by the addition of L-arginine and Bradykynin. The use of glass capillaries and the automated nature of production make this a possible venture for commercialization. While we have probed cells in the past, we are well positioned to start intracellular electrochemical measurements with ~100 nm diameter tips. These measurements can be amplified by functionalizing the carbon surface with the addition of metals such as platinum or gold for specific detection properties or proteins via linkers to detect the presence of biological species. Further work will involve measuring extracellular NO from endothelial cells using a wider variety of stimulants for NO detection and moving to intracellular electrochemical measurements. These developments are leading to the first intracellular electrochemical detectors of oxidative species.

221. Synthesis of imidazole and pyrrolidine containing ionic liquids and study of their biodegradation properties

Samanta Boursiquot,[1] Firmause Payen,[1] Sharon I. Lall-Ramnarine,[1] Marie Thomas,[2] James F. Wishart,[2] Cleveland J. Dodge,[2] A. J. Francis.[2], [1]Department of Chemistry, Queensborough Community College, CUNY, Bayside, NY, United States; [2]Department of Chemistry, Brookhaven National Laboratory, Upton, NY, United States.

Ionic liquids (ILs) compounds with melting points below 100 °C, are currently being used as alternative solvents in industrial and academic laboratories. Therefore, it is important to study their polluting effects on people and the environment. The goal of this project is to synthesize ILs that are commonly being used such as those containing imidazole and pyrrolidine and to study their biodegradation properties. We have successfully synthesized seven halide ILs: 1-(3-hydroxypropyl)-3-methylimidazolium chloride, *N*-(3-hydroxypropyl)-*N*-methylpyrrolidinium chloride, 1-(6-hydroxyhexyl)-3-methylimidazolium chloride, *N*-(6-hydroxyhexyl)-*N*-methylpyrrolidinium chloride, *N*-ethyl-*N*-methylpyrrolidinium diethyl phosphate, *N*-methoxyethyl-*N*-methylpyrrolidinium bromide and 1-methoxyethyl-3-methylimidazolium bromide. These liquids were synthesized by reacting the amine (1-methylimidazole, *N*-methylpyrrolidine) with the alkyl halide 3-chloro-1-propanol, 6-chloro-1-hexanol, and 2-bromoethyl methyl ether under reflux conditions at 60 °C in acetonitrile. *N*-ethyl-*N*-methyl pyrrolidinium diethyl phosphate was prepared under microwave conditions. The structures of these ILs have been confirmed using H-1, P-31 and C-13 nuclear magnetic resonance spectroscopy. Future work will focus on synthesizing similar ionic liquids bearing different side chains and anions and determining their biodegradation properties. This work was supported in part at BNL by the U. S. DOE Office of Basic Office of Basic Energy Sciences under contract # DE-AC02-98CH10886.

222. Immobilization of horseradish peroxidase on modified chitosan beads

Mohammed Monier,[1] Yen Wei,[1] A Sarhan.[2], [1]department of chemistry, Drexel University, United States; [2]Mansoura University, Egypt.

A method has been developed to immobilize horseradish peroxidase (HRP) on modified chitosan beads by means of graft copolymerization of polyethylacrylate in presence of potassium persulphate and Mohr's salt redox initiator. The activity of free and immobilized HRP was studied. FTIR spectroscopy and scanning electron microscopy were used to characterize HRP immobilization. The efficiency

of the immobilization was investigated by examining the relative enzymatic activity of free enzyme before and after the HRP immobilization. The obtained values were found to reach 98.4%. The results show that the optimum temperature of immobilized HRP was 45 ^{0}C, which was identical to that of free enzyme, and the immobilized HRP exhibited a higher relative activity than that of free HRP over 45 ^{0}C. The optimal pH for immobilized HRP was 10, which was higher than that of the free HRP (pH 9.0), and the immobilization resulted in stabilization of enzyme over a broader pH range. The apparent kinetic constant value (K_m) of immobilized HRP was 3.784mmol ml^{-1}, which was higher than that of free HRP. On the other hand, the activity of immobilized HRP decreased slowly against time when compared to that of the free HRP, and could retain 65.8% residual activity after 6 consecutive cycles.

223. Hydration effects on ion polarizability: Insights from iterative Hirshfeld partitioning

Brad A. Bauer, Timothy R. Lucas, Sandeep Patel., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

Recent studies of alkyl-halide ions at aqueous liquid-vapor interfaces have suggested the importance of polarizability for the density enhancement of larger anions at the surface. The nature of ion polarizability variation upon hydration may offer insight to the fundamental driving force for such processes as well as provide the basis for development of sophisticated new force fields. The Iterative-Hirshfeld method is implemented to study the effects of hydration on ion polarizability in ion-water clusters of various sizes. Such an approach allows for the partitioning of ab initio estimates of cluster polarizability into atomic contributions. The variation of polarizability as a function of cluster size using several levels of theory and basis sets is considered for fluoride, chloride, bromide, and sodium ions. Furthermore, effects of ions on the polarizability of neighboring water molecules are examined. Results suggest decreased ion and water polarizability in condensed environment, in agreement with recent studies and theoretical arguments based on Pauli's Exclusion Principle.

224. Solvation Properties of N-acetyl-beta-hexosaminides: A Molecular Dynamics Study Incorporating Electrostatic Polarization

Yang Zhong, Sandeep Patel., Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States.

N-acetyl-D-glucosamines (NAG) are common in nature and are found in molecules such as chitin, glycosaminoglycans and as an essential component of the carbohydrate structure of glycoproteins and glycolipids. They are also implicated in molecular recognition processes, acting as ligands for a variety of ribonucleases. We present the development of a polarizable force field for the carbohydrate functionality with NAG as the paradigmatic model compound. These studies will present the first application of polarizable force fields to carbohydrates. We discuss condensed phase properties of the NAG monomer as well as polymeric NAG species that are relevant as ligands to naturally occurring receptors (HEWL). The hydration energies of NAG oligmers are computed via Thermodynamic integration (TI) and the Bennett acceptance ratio (MBAR).

225. Molecular dynamics simulation of hydrated DPPC monolayers using charge equilibration force fields

Timothy R Lucas, Sandeep Patel., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

Membranes and membrane-bound proteins are vital components of biological systems. Indeed, membrane-bound proteins are involved in a number of physiological functions including passive and active transport, signaling processes, and interfacial enzymatic processes. Membrane-bound proteins have been found to make up 20-30% of the human genome, a fact that further emphasizes their significance. Of equal importance is the lipid environment within which these proteins function.

Even current state-of-the-art experimental measurements are not always able to provide the type of detailed atomic level resolution that would provide meaningful insight into the mechanisms of membrane systems. To this end, computational methods such as molecular dynamics simulations have been employed to study the properties and processes in such systems at the atomic level.

We explore several properties of the monolayer-water interface of dipalmitoylphosphatidylcholine (DPPC) based on molecular dynamics simulations using a recent charge equilibration (CHEQ) force field for DPPC (and saturated PC lipids in general) and the TIP4P-FQ polarizable force field for water. We present our results which include density profiles, deuterium order parameters, dielectric constant profiles, surface tension and surface pressure calculations, and relative interfacial dipole potentials. We compare several aspects of the monolayer properties with experimental values as well as with predictions made using the CHEQ force field on DPPC bilayers.

226. Effect of ions on hydrophobic assembly and properties at the water/hydrophobe interface

Shuching Ou, Brad A. Bauer, Sandeep Patel., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

The study of aqueous electrolyte interfaces is important for understanding a multitude of physicochemical processes ranging from the depletion of atmospheric ozone to the transport of ions across cellular membranes. Aqueous salt solutions also play a significant part in "salting-out" and "salting-in" effects for proteins as described by the Hofmeister series and the ions' ability to amplify or suppress hydrophobic interactions. We investigate the role of ions in hydrophobic interactions using molecular dynamics simulations. For our study, two large-scale (d=2 nm) hydrophobic plates are solvated in aqueous salt solutions comprised of polarizable TIP4P-FQ water and nonpolarizable NaCl/NaI salts. The potential of mean force for plate dimerization, interfacial profiles (density, dipole moment), and the wetting/dewetting transition for each salt solution and pure water are examined. We also discuss effects of concentration and ion-hydrophobe interaction strength on these properties. Emphasis is placed on the similarities and differences of the ions' behavior at the water/hydrophobe and water/air interfaces. Results highlight and further characterize the role of solvent polarizability in hydrophobic effects.

227. Investigating intramolecular hydrogen bonding in aromatic oligoamide foldamers

Jessica Amber Geer, Zhiwei Liu, Vojislava Pophristic, Jhenny Galan., Chemistry & Biochemistry, Univeristy of the Sciences in Philadlephia, Philadlephia, PA, United States.

We investigate aromatic oligoamide foldamers, which can be designed to have medical functions. As the shape of a foldamer strongly influences its function, an atom-level understanding of interactions that govern the foldamer shapes and stabilities is necessary for rational design. Hydrogen-bonding (H-bonding) plays a critical role in the conformation of an oligomer along with its related function. The formation of a stable, intramolecularly H-bonded system is associated with solvent effects and intricate arrangements of the proton donor/acceptor units, which can be oriented to enhance stability.

A comprehensive ab initio study followed by molecular dynamic calculations has been performed on diarylamide model compounds containing various intramolecular H-bond patterns, with an aim of studying the influence that the presence of one H-bond has on the strength of another, shared one. Our results demonstrate to what extent the cooperativity between shared H-bonds exists in this type of foldamer monomer unit.

228. Development of a coarse-grain intramolecular forcefield for proteins

Kenny Nguyen,[1] Jhenny Galan,[1] Zhiwei Liu,[1] Russell DeVane,[2] Preston Moore.[1], [1]Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, Pennsylvania, United States; [2]Department of Chemistry, Temple University, Philadelphia, Pennsylvania, United States.

We introduce a method to create a coarse-grain intramolecular forcefield for proteins. This project is two-fold where (1) coarse-grain molecular dynamics will be used to simulate proteins and (2) where intramolecular parameters will be developed to simulate them. Our coarse-grain potential is a reduced model method, which allows spatial and temporal scales to exceed all-atom molecular dynamics by three orders of magnitude. An intermolecular forcefield was already developed by DeVane and co-workers for amino acids, and will be used for our study (DeVane *et al*., *J. Chem. Theory Comput.* **2009**, *5*, 2115). Intramolecular parameters, which are bond lengths, bond angles, and dihedral angles, will be used to create our forcefield from its all-atom simulations. We employ different techniques to best determine which parameters will be used, such as using the Ca or the center-of-mass to define the protein backbone, or using the entire secondary structure information of the protein itself. The goal is to determine which set of parameters to accurately simulate proteins beyond conventional all-atom techniques. We have used our forcefield on the following proteins: rhodopsin, aquaporin, potassium ion channel, photosynthetic reaction center, myoglobin, and barnase-barstar.

229. Novel method to control pressure in molecular dynamics simulations

D Vladimir Pérez,[1] Preston B Moore,[1] Steve O Nielsen.[2], [1]Department of Chemistry & Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, United States; [2]Department of Chemistry, University of Texas at Dallas, Richardson, TX, United States.

Pressure is a fundamental thermodynamic quantity and most precesses occurs at constant pressure. Many Molecular Dynamics (MD) simulations algorithms use the NPT ensemble (Constant Number of particles, Pressure, and temperature) for this reason. The usual computational way to control pressure in MD simulations is to use the viral expressions which involve modifications of the distances between all the particles in the simulation cell in order to emulate the volume fluctuation of real systems. For many systems this method is satisfactory, but in certain systems this method may be inadequate, e.g. the simulation of adsorption energy on a crystal surface where the lattice parameters must be kept constant. We present a new way to control the pressure by the use of a wall or piston that would compress or dilate the system (depending on the desired pressure) and keep the lattice spacing constant. We present results for confined Lennard-Jones systems and compare and contrast the current barostat methods.

230. Targeting the human Andorgen Receptor with steroidal CYP17 inhibitors: A Molecular Docking approach

Eleonora Gianti,[1] Randy J. Zauhar,[1] Puranik Purushottamachar,[2] Vincent C. O. Njar.[2], [1]Departments of Chemistry & Biochemistry, Bioinformatics & Computer Science, University of The Sciences in Philadelphia, Philadelphia, PA, United States; [2]Department of Pharmaceutical Sciences, Jefferson School of Pharmacy, Thomas Jefferson University, Philadelphia, PA, United States.

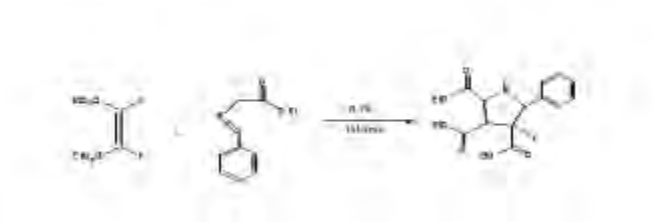
Prostate cancer (PCA) is the most frequently diagnosed malignancy and cause of cancer death worldwide. Androgen dependent and androgen-independent prostate cancers both rely on the Androgen Receptor (AR) for growth and proliferation. The last step in the biosynthesis of the natural AR agonist Testosterone (T) is catalyzed by the CYP17 enzyme. A novel class of potent CYP17 inhibitors (steroidal C-17 benzoazole and pyrazine derivatives) has been identified. Interestingly, these compounds have been found to also posses AR modulating properties, including AR antagonism and AR down-regulation (ablation) and they have been shown to be potent antagonists of both wild type and mutant androgen receptors. No CYP17 three-dimensional structures have been resolved so far, making difficult any Structure Based Drug Design (SBDD) effort to study these compounds. In contrast

the Protein Data Bank includes more than 70 AR Crystallographic Structures, either in the apo-form or bound with several small molecule inhibitors. The impressive multiple in vitro biological activities exhibited by the steroidal C-17 benzoazole and pyrazine derivatives (i.e. inhibition of CYP17, strong anti-proliferative prostate cancer cell and anti-androgenic activities) justify the need to elucidate, at a fine level, the molecular mechanism for their AR modulating activities. The present study was essentially focused on two main purposes. First, put in place a SBDD approach to generate a putative binding hypothesis for the steroidal CYP17 inhibitors to the human Androgen Receptor. To do so, and in order to deal with the flexibility of several residues buried in the AR binding pocket (which is known to accommodate a variety of ligand structures), we implemented a flexible receptor docking protocol using the Glide Induced-Fit methodology (www.schrodinger.com). Second, we aim to use the molecular docking results generated for the most active compounds (like the first in class, VN124/1), as a starting point to guide the rational design and synthesis of novel VN124/1 analogs with improved AR modulating properties.

231. Synthesis and cycloaddition reactions of diethyl (E)-2-fuoromaleate

Mehrdad Shadmehr, Timothy B Patrick., Department of Chemistry, Southern Illinois University, Edwardsville, IL, United States.

The importance of organofluorine compounds are is because of their application to pharmaceuticals. Fluorine increases metabolic stability, binding interaction, and selective activities of different kinds of medicines.



The objective of our research is to synthesis bioactive heterocyclic systems in which fluorine improves lipophilicity, and improves thermal and oxidative stability. These properties play an important role when making molecules that are designed to be active in vivo.

We have investigated the synthesis of diethyl (E)-2-fluoro-2-butendioate and studied its reactions with different kind of imines and nitrones, whic have potential biological activities.

References:

[1] William K. Hagmann,. J. Med. Chem., 15 (**2008**) 4359.

[2] James M. Longmire, Bin Wang, and Xumu Zhang,. J. Am. Chem. Soc. 124 (**2002**) 13400.

[3] John A. Wilkinson. Chem. Rev., 92 (**1992**) 505.

ACS Career Management Workshop

Sponsor: American Chemical Society

232. Today's Job Searching Strategies

James D. Burke., Career Consultant, American Chemical Society, Washington, DC, United States.

Dr. James D. Burke worked nearly 35 years in chemical industry: 8 in R & D as a research chemist, 3 in management of information security, and 24 in design and management of programs for technical recruiting (scientists and engineers) and university relations. He has published about 20 papers and articles - principally on the topics of technical recruiting, employment interviews, and professional development of technical employees. Principal co-author of original version of ACS tutorial Managing a Successful Job Search. He has presented more than 300 seminars and tutorials at universities and conferences of professional societies on the topics of managing ones job search, career self-management, employment interviews, professional development, minority recruiting, strategic planning, and related topics.

Member of ACS Board of Directors since 2000. Councilor for Philadelphia Section ACS, 1990-1998. Philadelphia Section Chair, 1989. Philadelphia Organic Chemists Club Chair, 1972. ACS Career Consultant since 1990.

Dr. Burke is Past Board member of National Association of Colleges and Employers, Midwest Association of Colleges and Employers, GEM, and Big Brother/Big Sister Association of Philadelphia. Current member of University of Pennsylvania Chemistry Department's M.S. Chemistry Education Advisory Board.

233. Preparing your résumé or CV

James D. Burke., Career Consultant, American Chemical Society, Washington, DC, United States.

Your résumé or CV is a personal introduction and leaves an impression. In this one hour workshop you will learn which personal data format is right for your "marketing plan," and construct a winning résumé.

234. Effective Interviewing

James T. Burke., Department of Career Management and Development, American Chemical Society, Washington, DC, United States.

Many job seekers think their work ends once an interview is secured. Think again! This one hour workshop will examine the entire interview process, types of interviews, frequently asked questions, and how to evaluate an offer.

235. Resume reviews and career assistance

James D. Burke., Department of Career Management and Development, American Chemical Society, Washington, DC, United States.

ACS Career Consultants will be available to provide resume reviews and career assistance. Individual 30 minute resume reviews will be offered. You must bring a copy of your resume. Sign-up will be available at meeting registration.

Analytical Chemistry II

Organizer: Narmada Gunawardena

236. Analysis and determination of the chemical constituents of turmeric and its anti-microbial activity

Bibi Javeria, Aheda Saber., Department of Chemistry, Governors State University, University Park, IL, United States.

Turmeric (*Curcuma longa*) is a rhizome of a perennial plant of the ginger family Zingiberaceae. It is native to tropical south Asia. Turmeric is extensively used in Indian cuisines as a spice and coloring agent. It is also used traditionally for medicinal purposes. Curcumin, a polyphenolic compound is the principal constituent of turmeric. Polyphenol is known for its anticancer activities which include, among others, anti-oxidative, pro-apoptotic, DNA damaging, anti-angiogenic, and immunostimulatory effects. The aim of this study is to establish a reliable analytical procedure to extract and characterize the curcumin extracted from powdered turmeric using Gas Chromatography, Gas Chromatography-Mass Spectroscopy, and Liquid Chromatography-Mass Spectroscopy. The extraction is done by using both soxhlation and shaker methods with a polar solvent, ethanol. The extracts are further investigated for its antimicrobial activity by examining them against a range of microorganisms using the Kirby Bauer method and broth cultures. Based on the results of this study, it is likely that Curcumin may be used as antimicrobial agents in alternative medicines, and in natural therapies.

237. Antibacterial activity determination and extraction quantification of cuminaldehyde in cuminum cyminum seeds

Divya Varadarajan, Aheda Saber., Department of Chemistry, Governors State University, Univeristy Park, IL, United States.

Cuminum cyminum seeds are from an aromatic plant family Umbelliferae commonly used as a flavoring and seasoning agent in foods. Cuminaldehyde , the major constituent of these seeds is known to participate in the plants defense against diseases; however, the mechanism of its antimicrobial action against fungi or bacteria is still unclear. The aim of this study is to establish a reliable analytical procedure to extract and characterize the cuminaldehyde extracted from Cumin seeds using Gas Chromatography and Gas chromatography-Mass Spectrometry. The extraction is done using two different solvents by soxhalation. Both polar extraction and non-polar extraction is done using a methanol/chloroform mixture and hexane respectively. These Extracts are then analyzed using analytical procedures involving Gas Chromatography and Gas chromatography-Mass spectrometry. The extracts are further investigated for its antimicrobial activity by examining them against a range of microorganisms using the Kirby Bauer method and broth cultures. The results obtained from these procedures are then compared along with data obtained using standard cuminaldehyde. Based on the results of this study, it is likely that cuminaldehyde may be used as antimicrobial agents in alternative medicines, and in natural therapies.

238. Analysis of mineral contents in seed coat in relation to canning quality of selected cultivars of dark red kidney beans (Phaseolus Vulgaris L .)

Alfred Anderson., Department of Family Sciences, Kuwait University, Safat, Kuwait.

This study investigated the influence of the mineral content of the seed coat of kidney bean on the canning quality among different cultivars of the bean. Three dark red kidney bean *(Phaseolus vulgaris L.)* cultivars (cvs. 85, 453, and Nickols) were studied. In the canned product, highly significant differences (p £0.01) in percentage of split seed coats were observed among the three cultivars studied. Canned cultivar 85 significantly showed fewer seed coat splits than the other two cultivars. Significant negative correlations were observed between the percentage of seed coat splits and so-

dium (r = - 0.89, p £ 0.01), calcium (r = - 0.74, p £ 0.01) and iron (r = - 0.79, p £ 0.05) contents in the seed coat. This study suggested that the mineral content of the seed coat of kidney beans may play important roles in the integrity of the seed coat during thermal processing.

239. Analysis of polyhexamethylene biguanide in multipurpose contact lens solutions

Anne D Lucas, Edward A Gordon., Center for Devices and Radiological Health, US Food and Drug Administration, Silver Spring, MD, United States.

The objective of this study was to establish a reasonably simple and reliable method to measure very low concentrations of polyhexamethylene biguanide (PHMB) in multipurpose contact lens solutions (MPS). By using a weak cation exchange solid phase extraction cartridge to extract the PHMB from MPS, followed by HPLC analysis using an evaporative light scattering detector, low levels (0.1 ppm) of PHMB were detected. Application of this method to a series of off-the-shelf MPS with PHMB as the active ingredient demonstrated these solutions contain 1 ppm. The contact lens solution with hydrogen peroxide as the active ingredient gave no peak where the PHMB peak eluted. The Polyquad ® contact lens solution generated a peak close to the retention time of PHMB. Recovery of PHMB from fortified hydrogen peroxide contact lens solution was good at 0.25 ppm and above; 105% with a RSD of 17% or less. The repeatability of the HPLC system ranged from 4 to 11% RSD; the reproducibility of the entire method was less than 17.5% RSD. Storage and stability studies indicated that storage of MPS with PHMB for chemical analysis are not temperature dependent, but are affected by the composition of the container in which the contact lens solution is stored.

240. Evaluation of the oxidative metabolites of w-6 and w-3 fatty acids by LC-ESI-MS and their implication in the progression of rheumatoid arthritis

Deepti R Varma, Susan Jansen Varnum., Chemistry, Temple University, Philadelphia, PA, United States.

Inflammation is implicated in diseases such as from hypertension, atherosclerosis and rheumatoid arthritis (RA). A mechanistic understanding of the inflammation process as it relates to the disease state and injury needs to be developed. Specifically, the role and modulation of inflammation needs to be assessed as well as the mechanism which produces oxidation of arachidonic acid. Gender and age also affect the level and nature of the inflammatory process. Eicosanoids are specific biomarkers for inflammation. Their biosynthesis from arachidonic acid, and related fatty acid molecules can be catalyzed by either lipoxygenases (LOX), COX-2 or P450 enzymes. Depending on the mechanism/ pathway or parent molecule, different distributions of eicosanoids are found. The oxidation of arachidonic acid gives hydroxy eicosatetraenoic acids (HETEs), dihydroxy eicosatetraenoic acids (DiHETEs), epoxy eicosatetraenoic acids (EETs), and prostaglandins (PGs) and thromboxane (TX). The metabolites of eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA) (the w-3 fatty acids) along with the metabolites of AA regulate inflammation.

We have developed and validated an LC-ESI-MS method to quantify 35 of these lipid biomarkers. The separation was performed on a C18 column using gradient elution of 0.1% formic acid and acetonitrile. This method provides an assessment of thequantitative reliability of the extraction and chromatographic procedure necessary for valid comparison between the various inflammatory biomarkers to study the mechanism involved in rheumatoid arthritis.

241. Tuning of nanohole array surface plasmon resonance wavelength by varying nanohole diameter and array periodicity

Laurel L Kegel, Karl S. Booksh., Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

The surface plasmon resonance (SPR) wavelength, l_{SPR}, of gold nanohole array structures with 220-1500nm periodicity has been tuned for optimal coupling with the localized surface plasmon resonance (LSPR) of nanoparticles as well as for increased surface sensitivity over planar gold to change in refractive index. SPR biosensors offer universal detection based on refractive index change of analyte binding to the recognition element employed on the surface. Nanohole array structures are of interest for SPR sensors as a more sensitive platform than planar gold or as a substrate for coupling with an LSPR sensor. The LSPR of a nanoparticle has a shorter penetration depth than that of the propagating SPR and thus increased sensitivity to surface binding. This may be exploited and increased by achieving gap mode SPR by coupling the nanohole and nanoparticle SP. Nanohole arrays were prepared by nanosphere lithography in which a monolayer of polystyrene spheres are deposited onto a glass cover slip, plasma etched, coated with gold, and removed by sonication in chloroform. The hole width and periodicity is controlled by etch time, sphere size, and gold deposition. Nanohole arrays with hole widths of 160-700 nm and periodicity of 220-1500nm have been fabricated by this procedure with order over a region of 5-50 mm^2. The arrays were physically characterized by atomic force microscopy and scanning electron microscopy; **[figure1]** The l_{SPR} was determined in total internal reflection (TIR) and transmission configurations; **[figure2]** The setup was comprised of a white light source, collimating lens, polarizer, dove prism (TIR), spectrometer, and CCD detector. The sensitivity of l_{SPR} of short range, near propagating surface plasmons has been shown to be more sensitive to change in refractive index than the propagating surface plasmon of planar gold. The sensitivity of the nanohole structures was determined by calibration with a series of sucrose solutions of known refractive index in TIR. The l_{SPR} for various nanohole size and periodicity was determined and may be matched to that of a given nanoparticle probe. The l_{SPR} is tuned by changing the periodicity and width of gold nanoholes. A series of nanohole arrays have been fabricated and optimized for maximum sensitivity and tunability for potential sensor applications.

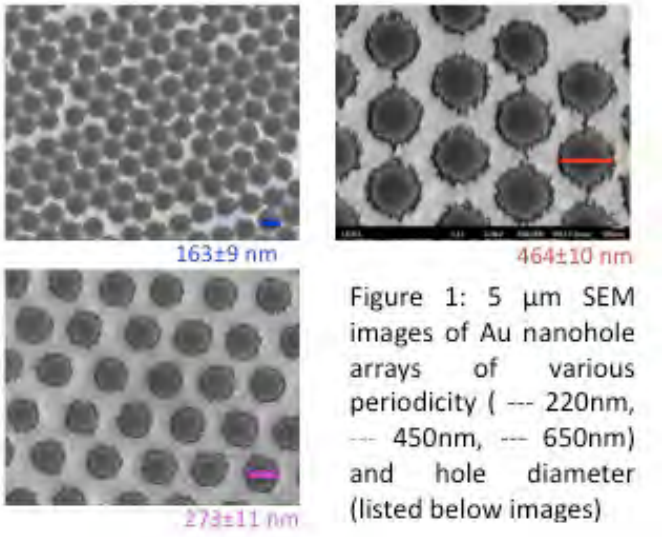


Figure 1: 5 µm SEM images of Au nanohole arrays of various periodicity (--- 220nm, --- 450nm, --- 650nm) and hole diameter (listed below images)

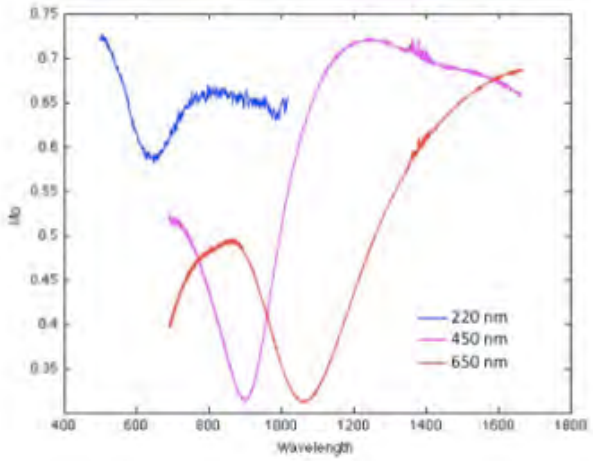


Figure 2: Transmission Spectra of Au nanohole arrays of various periodicity (--- 220nm, — 450nm, — 650nm)

242. Implementation of liquid chromatography and UV-Vis spectrometry for the quantification of a low level colored impurity formed during the process optimization of Trityl Losartan

Stephen M Marcinko, Robert Hartman, Tony Hudgens., Analytical Development and Commercialization, Merck Manufacturing Division, Merck and Company, Rahway, NJ, United States.

Several synthetic routes have been reported for the synthesis of Losartan Potassium, the active pharmaceutical ingredient (API) in COZAAR®, along with an assessment of the resultant quality of the API. The comparability of the quality of the API is typically assessed by assay and or impurities by HPLC to ensure each synthetic route produces equivalent material. However, HPLC alone may not produce a complete picture when it comes to colored impurities which can impact the subsequent elegance of the formulated drug product. In the recent development of a more cost effective route we encountered low level colored impurities that were not readily detecable by HPLC alone. The impurity found to be the major contributor to the color was identified as the aldehyde of the unreduced Trityl Losartan intermediate. This impurity could have the potential of being carried forward as the unreduced Losartan causing a similar change in color of the final drug substance. A correlation between the level of the impurity quantified and the degree of yellow color present in the drug substance was investigated. The data shows that a linear relationship exists between the level of the unreduced Losartan impurity measured by HPLC and the intensity of the color as measured by UV-Vis spectrometry.

What a Chemist Needs to Know About Patent Law

Sponsor: Division of Chemistry & the Law
Organizers: Justin Hasford, Sarah Perlinger Hasford

243. Requirements for Patentability: Utility, Novelty, Nonobvious, Enablement, and Written Description

Christine Hlavka., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

Every patent covers an invention, but not every invention may be patented. This presentation will provide a brief overview of the basic requirements necessary to successfully obtain a patent on an invention in the United States, including utility, novelty, nonobviousness, enablement, and written description.

244. What Constitutes an Invention: Conception, Reduction to Practice, and Inventorship

Krista Bianco., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

An invention requires more than just an idea. The making of an invention involves three stages: (1) conception, (2) activities leading toward a reduction to practice, and (3) reduction to practice (either actual or constructive). This presentation will explain the three stages for chemical inventions and what contributions one must make to be named as an inventor. In addition, it will discuss what records should be kept to establish the actual date of invention and for use in the patent drafting process.

245. Best Practices in Drafting and Prosecuting a Patent Application

Maureen Queler., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

Navigating an invention from the idea stage to the grant of a patent takes the combined effort of inventors and patent attorneys alike. This presentation will focus on some best practices for inventors and patent attorneys during the different stages of patent prosecution, with a particular focus on the do's and don'ts of drafting a patent application.

246. A Patent Litigation Primer

Krista Bianco., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

A patent is infringed when another party makes, uses, offers to sell, or sells any patented invention, within the United States, or imports into the United States any patented invention during the term of the patent. This presentation will discuss patent infringement and the steps and procedure involved in enforcing a patent through litigation. Specifically, it will focus on initiating a suit, defenses to patent infringement, fact discovery, expert discovery, trial, and appeal.

247. Overview of ANDA Pharmaceutical Patent Litigation in the United States

Justin Hasford., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

Pharmaceutical patent litigation arises under the Hatch-Waxman Act when a generic pharmaceutical company submits an Abbreviated New Drug Application (ANDA) seeking approval from the U.S. Food and Drug Administration (FDA) to market a generic copy of an innovator drug before the expiration of a patent covering that drug. Upon filing an ANDA with the FDA including a so-called Paragraph IV certification, which is an act of patent infringement, the generic company must send to the patent owner and New Drug Application owner a detailed statement of the factual and legal bases for the generic company's challenge that the claims of the patent are invalid and/or not infringed, and/or

that the patent is unenforceable because of alleged inequitable conduct before the U.S. Patent and Trademark Office. The patent owner then has 45 days to file suit against the generic company for infringement, at which time a statutory stay of FDA approval of the generic company's ANDA will commence so that the patent infringement suit may be adjudicated. This presentation will discuss the basic substantive and procedural law underlying pharmaceutical patent infringement litigations that arise from ANDA submissions.

Chemical Engineering/AIChE Symposium

248. Evaluating Miscibility Tests for Planning Gas Injection Projects for Four Major Kuwaiti Oil Reservoirs

Adel Elsharkawy,[1] Osamah Al-Omair,[1] Moudi Al-Ajmi.[1], [1]Petroleum Engineering, Kuwait University, Safat, Kuwait, Kuwait; [2]Kuwait University, Kuwait; [3]Kuwait Oil Company, Kuwait.

The escalating oil demand and maturity of most of the giant oil fields in the world, especially in the Middle East, the techniques for improving oil recovery have became more feasible and essential. Kuwait long term strategy is to increase oil production to meet marked demand. Currently, miscible gas injection is considered for enhancing oil production from Kuwaiti oil reservoirs. A key parameter for assessing the applicability of gas injection for a given reservoir is the minimum miscibility pressure (MMP). In this paper various miscibility experiments for planning gas injection projects in major producing fields in Kuwait are discussed. These experiments include swelling tests, slim-tube tests, and core flooding studies. These tests are useful tool for screening of the potential reservoirs for improving their future oil production and for developing suitable EOS for planning gas injection projects of the chosen fields.

249. Colloidosomes: Controlling transport from alginate hydrogels

Rachel Rosenberg, Nily Dan., Department of Chemical and Biological Engineering, Drexel University, Philadelphia, PA, United States.

Colloidosome-based microgels consist of an aqueous polymer gel core with a shell of colloidal particles adsorbed to the surface by electrostatic interactions. Their applications span several areas including drug delivery, cell encapsulation, cosmetics, and household cleaners. The packing and distribution of the colloidal shells determine the pore size; however, the rate of transport of molecules encapsulated inside is independent of the particle size. In the presence of the coating, the rate of release of small hydrophilic molecules is suppressed by nearly 33% and the time to reach 100% release is doubled. In this study, we use sodium alginate as an aqueous gel scaffold, synthesized into microgels via microfluidics. Internal gelation of the alginate core is achieved by crosslinking with calcium ions while flowing in the microfluidic device. The shells consist of packed polystyrene nanoparticles which are functionalized to yield the appropriate charge.

250. Cross-dimerization of isoamylene and a-methylstyrene in a microreactor using Filtrol-24 catalyst

Obiefuna C. Okafor,[1] Sunitha Tadepalli,[2] Geatesh Tampy,[2] Adeniyi Lawal.[1], [1]Department of Chemical Engineering and Material Sciences, Stevens Institute of Technology, Hoboken, New Jersey, United States; [2]R&D Center, International Fragrances and Flavors, Union Beach, New Jersey, United States.

The cycloaddition reaction between isoamylene and a-methylstyrene yields indane compounds 1,1,2,3,3,-pentamethylindane and 3-ethyl-1,1,3-trimethylindane, which are intermediate cyclic products used in the synthesis of musk fragrances. This exothermic reaction is conventionally carried out industrially in large semi-batch reactors, which have high heat and mass transfer resistances, are difficult to optimize, and scale-up. Aqueous sulfuric acid is conventionally used as the catalyst for the

cycloaddition reaction, but solid catalysts offer many advantages over the corrosive aqueous sulfuric acid catalyst including the elimination of expensive separation and purification steps, and the need to use corrosion resistant materials of construction. A microreactor, which has enhanced heat and mass transfer characteristics, high surface to volume ratio, and improved fluid mixing, was used for the reaction using an acidic solid catalyst, Filtrol-24. A parametric study to obtain the dependence of product yield, reactant conversion and space-time yield on process variables such as catalyst particle size, residence time, velocity, temperature, pressure and the molar ratio of the reactants in the feed, was conducted.

Through this study the optimum reaction conditions were obtained. The cycloaddition reaction was also performed in the semi-batch reactor using Filtrol-24 catalyst in order to compare its performance to that of the microreactor.

Higher product yields were obtained in the microreactor compared to the semi-batch reactor, and the space-time yield in the microreactor was 4.4 times larger than that obtained in the semi-batch reactor at optimum reaction conditions in both reactors.

251. Vascularized scalable networks: Electrohydrodynamic viscous fingering and electrical treeing

Kristopher D. Behler, Eric D. Wetzel., Composite and Hybrid Materials Branch, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, United States.

Vascular networks provide a method to distribute fluid throughout a system. An uninterrupted and controllable supply of liquid is optimal for many applications such as continual self-healing, drug delivery and thermal management. Two such approaches to induce vascular networks are electrohydrodynamic viscous fingering (EHVF) and electrical treeing (ET).

[figure1]Viscous fingering occurs in an immiscible liquid system when one liquid of lower viscosity is forced through a higher viscosity liquid causing the flowing liquid to branch, or form fingers due to capillary and viscous forces. EHVF is a modification on viscous fingering in which a DC voltage is applied to the low viscosity conductive fluid (Fig. 1a) and forced through a dielectric matrix material. The application of a large electrical potential, 10-60 kV, induces fingers with a reduction in size and an increased branching behavior. The ensuing patterns mimic those found in biology and geology (lung tissue and plants as well as river beds). Using a silicone oil system as the matrix material, the surfactant concentration was optimized, through a reduction in the interfacial tension, thereby producing a branched pattern of small diameter fingers while still maintaining continuity when dyed water is pushed through the system. Various loadings of glass beads where subsequently used to represent a more 3D system. Typically, in a two fluid system, the fingers relax as soon as the applied voltage is removed. Addition of glass beads, up to 60 v/v%, aids in a retardation of finger relaxation while producing fine channels throughout the porous system. Delayed relaxation allows for greater control of the curing process in UV-curable systems, such as polydimethylsiloxane (PDMS). Fabrics were also investigated as another material inserted into the liquid matrix to provide a different porosity structure.

Electrical treeing (ET) is the result of partial discharges in a dielectric material. In the vicinity of a sharp electrode, the local electric field is greater than the global dielectric strength, causing localized breakdown to occur. Inducing this breakdown by using small diameter electrodes, complex branched structures can be formed from various electrode geometries (Fig. 1b). ET is a viable method to produce networks in 2D systems and in more robust 3D systems on a smaller, micron, scale than EHVF. AC driven electrical current, harnessing a sine wave at 100 Hz, grows a bush-like structure with many branches and therefore volume within the epoxy samples. The use of multi-walled carbon nanotube (MWCNTs) coated electrodes have aided in reducing the time required for tree growth. Liquid filling is observed through the hollow channels produced by ET resulting in vascularized networks capable of fluid flow.

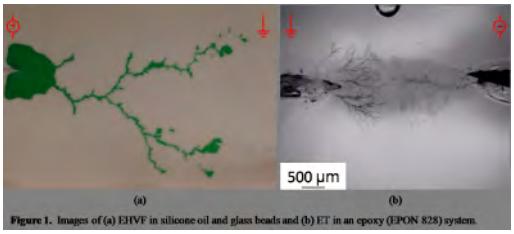


Figure 1. Images of (a) EHVF in silicone oil and glass beads and (b) ET in an epoxy (EPON 828) system.

Medicinal Chemistry I

Sponsor: Division of Medicinal Chemistry

252. Using computer-aided drug design to identify new antimicrobial lead compounds

Malela Werner,[1] Mohammed Bamajboor,[2] Randy Zauhar.[1,2], [1]Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, United States; [2]Department of Bioinformatics and Computer Science, University of the Sciences in Philadelphia, Philadelphia, PA, United States.

We are applying Computer-Aided Drug Design (CADD) tools to identify new lead compounds expected to inhibit ATP hydrolysis at the ATP-binding sites of gyrase (GyrB) and topoisomerase IV (ParE), and in separate studies to stabilize the DNA double-stranded break at the DNA binding sites of gyrase (GyrA) and topoisomerase IV (ParC). Gyrase and topoisomerase IV are attractive enzyme targets for antimicrobials, as they are required for bacterial replication but not found in the host. We have used Shape Signatures, a novel computational method developed in our laboratory, to scan the ZINC database (a large chemical library of readily-available compounds) for molecules similar in shape and electrostatic properties to known inhibitors. Top hits from this initial scan are further validated by molecular docking using the simulation tools GOLD and GLIDE. These are widely-used methods for predicting and scoring binding modes of small-molecule ligands against protein targets. Receptor models of GyrB and ParC of *Staphylococus aureus* were constructed by homology modeling using the Molecular Operating Environment (MOE), taking experimental structures for GyrB of *Thermus thermophilus* and ParC of *Streptococcus pneumonia* as templates. Our research plan is to acquire the most promising candidate compounds identified through the docking experiments for antimicrobial assay. The validated best leads will be further optimized by substituent scans, coupled with free-energy simulations to predict consequent variations in binding affinity.

253. Benzylthiocarbamate inhibitors of endothelial lipase: A drug target for atherosclerosis

D. J. Hlasta, A. Darrow, M. Hawkins, Z. Huang, J. Kranz, G. Leo, M. Olson, E. Powell, C. Smith, W. Sun, H. Xin, M. Connelly, M. Greco., Johnson & Johnson Pharmaceutical Research & Development, Spring House, Pennsylvania, United States.

Endothelial lipase (EL) is a serine phospholipase that functions in the metabolism of lipoproteins. Lipases hydrolyze the ester bonds of water-insoluble lipids to release fatty acids. EL is synthesized by endothelial cells and functions at the plasma membrane. The phospholipase activity of EL is associated with higher rates of HDL phospholipid hydrolysis and a reduction in HDL-cholesterol (HDL-C) and apo A-I levels. In EL knockout mice, HDL particle levels are reported to increase, while animals that over express EL show a reduction in HDL-C levels. Clinical study data indicate that increasing plasma HDL levels will decrease the risk of coronary artery disease. Therefore, an EL inhibitor is expected to be effective in the treatment of coronary artery disease.

By screening directed libraries from other in-house serine hydrolase programs using a cell surface form of EL, a phenyl carbamate analog was discovered. While the screening hit was a potent inhibitor (IC_{50} = 140 nM), the compound was unstable. As the structure-activity relationship study progressed, inhibitor potency was maintained in analogs that were stable in plasma. A tool compound raised HDL-C levels in mice in a dose-related fashion, and a correlation was found between plasma HLD-C and compound levels. The structure-activity relationship study and in vivo data will be presented.

254. Design and structure-activity relationships of a dipeptidyl peptidase-1 inhibitor series

D. J. Hlasta, R. Alexander, S. Ghosh, Y. Huang, D. Johnson, A. Jordan, J. Kervinen, J. Kirkpatrick, L. Kuo, E. Lawson, R. Malaviya, M. Parker, I. Petrounia, A. Reitz, C. Schubert, R. Steele, E. Strobel, B. Tounge, K. White, M. Winters., Johnson & Johnson Pharmaceutical Research & Development, Spring House, Pennsylvania, United States.

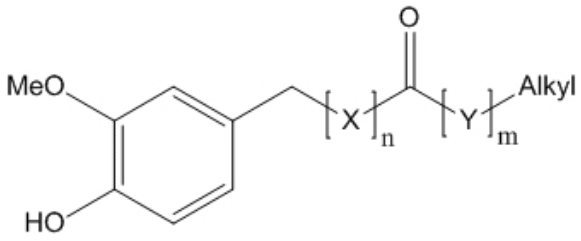
Dipeptidyl-peptidase 1 (DPP-1 or cathepsin C) is a member of the lysosomal cysteine protease family that includes cathepsins B, C, F, H, K, L, and S. Most cathepsins are comparatively small monomeric proteins, whereas DPP-1 is a dimer of disulfide-linked heavy and light chains with a third exclusion domain, that drives exopeptidase activity. DPP-1 cleaves the inactive pro-enzyme forms into the active forms of granule associated serine proteases: cathepsin G, elastase, and proteinase 3 in neutrophils, granzyme A in T-cells, and chymase and tryptase in mast cells. Targeting this single enzyme should have a multitarget effect on these inflammatory mediators and a DPP-1 inhibitor should thus prove useful in the treatment of COPD, asthma and rheumatoid arthritis.

After a high-throughput screening campaign did not identify progressible screening hits, we pursued a fragment-based design approach to generate high content data of fragment location and orientation in the active site of DPP-1. A fragment library was screened by x-ray crystallography which identified sets of fragments that were detected in the S1' and S1/S2 sites. Using this information, analogs were designed and prepared that linked these fragment hits and a 430 nM inhibitor was discovered. The discovery of the lead compound and the structure-activity relationship study will be presented.

255. Synthesis and anti-inflammatory acitivity in a lipophilic vanilloid amide platform

Abhilash N Pillai,[1] Carl J Lacey,[1] Cynthia A Fianu Velgus,[1] Sherri C Young,[1] Karine M Fabio,[1] Christophe D Guillon,[1] Ned D Heindel,[1] Jeffrey Laskin,[2] Diane Heck,[3] Irene Wohlman,[2] Mou-Tuan Huang,[2] Anna Vetrano.[4], [1]Chemistry, Lehigh University, Bethlehem, PA, United States; [2]UMDNJ / EOHSI, Rutgers University, Piscataway, NJ, United States; [3]Environmental Health Science, New York Medical College, Valhalla, NY, United States; [4]of Pediatrics, Rutgers University, School of Pharmacy, Piscataway, NJ, United States.

In vivo screening of candidate anti-inflammatory drugs is traditionally conducted by studying the dose-dependent suppression of inflammation induced by s.c., topical, or i.p. administration of carrageheen, phorbol ester, chloroethyl ethyl sulfide or gelatin. Other methods are also employed but all are difficult to carry out and fraught with large experimental errors. A simple *in vivo* method is required and the inhibition of fatty acid amide hydrolase (FAAH) represents a possibility. We wish to report the design and synthesis of a broad class of FAAH inhibitors containing a vanilloid moiety and an amide-like carbonyl. IC_{50}'s against FAAH and percent suppression of inflammation *in vivo* models will be compared.



n and m = 0 or 1; X and Y = NH, O, NR or CH_2

256. Novel tricyclic inhibitors of IKK2: Synthesis, SAR, PK/PD and activity in a preclinical model of rheumatoid arthritis

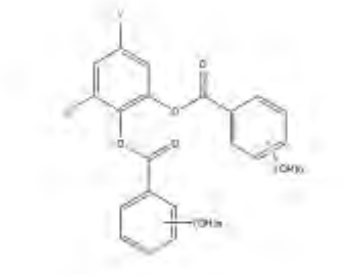
Alaric J. Dyckman, Charles M. Langevine, Claude Quesnelle, James Kempson, Junqing Guo, Patrice Gill, Steven H. Spergel, Scott H. Watterson, Tianle Li, David Nirschl, James R. Burke, Kathleen Gillooly, Mark A. Pattoli, Kim W. McIntyre, Laishun Chen, Punit H. Marathe, Zheng Yang, David Wang-Iverson, Murray McKinnon, John H. Dodd, Joel C. Barrish, William J. Pitts., Research and Development, Bristol-Myers Squibb, Princeton, NJ, United States.

The NF-kB family of nuclear transcription factors regulates the expression of a variety of genes relating to immune and inflammatory disorders, among others. NF-kB is held in an inactive state by inhibitor proteins known as IkBs, with activation requiring phosphorylation by IkB-kinases (IKK), in particular IKK2. Modulating NF-kB activity through small molecule inhibition of IKK2 represents an attractive approach towards beneficially impacting a number of disease states. The synthesis, structure activity relationships and biological evaluation of inhibitors of IKK2 based on imidazo[4,5-d] oxazolo[5,4-b]pyridine and imidazo[4,5-d]thiazolo[5,4-b]pyridine scaffolds are described. The pharmacokinetic properties, activity in a pharmacodynamic model and efficacy in a murine model of rheumatoid arthritis will be presented.

257. Novel inhibitors of basal glucose transport as potential anticancer agents

Weihe Zhang,[1] Yi Liu,[2] Xiaozhuo Chen,[2,3,4] Stephen C Bergmeier.[1], [1]Department of Chemistry and Biochemistry, Ohio University, Athens, OH, United States; [2]Department of Biological Science, Ohio University, Athens, OH, United States; [3]Department of Biomedical Science, Ohio University, Athens, OH, United States; [4]Edison Biotechnology Institute, Ohio University, Athens, OH, United States.

Cancer cells commonly show increased levels of glucose uptake and dependence. We envisioned that inhibit the basal glucose transport maybe a potential strategy to treat cancers. Recently, we successfully built a small library of polyphenolic esters, which can inhibit basal glucose transport in H1299 lung and other cancer, and can also inhibit cancer cell growth in H1299 cells. [figure1] Lead compound was selected from this library after SAR staudy. In a further animal studies, it showed the polyphenolic esters are not very stable. Thus, based on the structure of WZB-115, we will design and synthesize more stable analogus.



Advances in Infra-red (IR) and Terahertz (THz) Spectrometry Symposium

Organizer/Presider: Anis Rahman

258. Applications of terahertz spectrometry in biopharmaceutical reagent quantification and characterization

Trevor L. Broadt,[1] Anis Rahman.[2], [1]Biopharmaceutical Development Program, SAIC-Frederick, Frederick, MD, United States; [2]Applied Research and Photonics, Inc., Harrisburg, PA, United States.

The interaction of terahertz radiation with a given molecular system is greatly influenced by the characteristic parameters of the molecule such as its molecular weight and vibrational properties. As such terahertz transmission (or equivalently terahertz reflection) is a function of the concentration of each species. This hypothesis has been successfully tested on macromolecular systems [1]. In the present work, terahertz spectrometry was used to measure the sensitivity of detection and spectral features of two non-ionic detergents from aqueous solution. It was found that a wide range of detection sensitivity can be achieved. Concentrations ranging from ~1 parts per billion (ppb) to ~17 parts per million (ppm) exhibit a lower slope region (Region 1) where the data can be fitted well by a single exponent power law, while for the range above 17 ppm the slope is much steeper (Region 2) but the data still can be fitted with another single exponent power law. Initial attempt of terahertz spectral characterization shows that the spectra of the two detergents are significantly different. It is expected that a well controlled experiment will allow us to discern between the two detergents by their terahertz spectral characteristics. Details of the findings will be presented with exemplary data.

[1] Anis Rahman, Bruce Stanley and Aunik K. Rahman, "Ultrasensitive label-free detection and quantitation of DNA hybridization via terahertz spectrometry," Paper Number: 7568-8, SPIE conference on Imaging, Manipulation, and Analysis of Biomolecules, Cells, and Tissues VIII, January 23-28, 2010, SPIE Photonics West, San Francisco, CA.

259. Terahertz spectral analysis of FCGR3A genotypes

Gulshan Ara,[1] Aunik K Rahman,[1] Bruce A Stanley,[2] Anis Rahman.[1], [1]Applied Research Photonics, Inc., Harrisburg,, PA, United States; [2]Penn State College of Medicine, Hershey, PA, United States.

Monoclonal antibodies (mAb) can kill tumor cells by blocking ligand-receptor mediated signaling, through antibody-dependent cell-mediated cytotoxicity (ADCC) and complement-mediated cytotoxicity. ADCC are triggered when mAb of the IgG1 subtype bind FCGR3A receptors on effector cells, encoded by FCGR3A gene, resulting in cross linking of effector cells to target cells such as CD20-positive B and non-Hodgkin's Lymphoma (NHL) cells. Rituximab, a chimeric anti-CD20 IgG1 mAb, has been shown to be effective in the treatment of NHLs (1). However, 30–50% of patients with low-grade NHLs exhibit no clinical response. Both binding affinity and target cell lysis by Rituximab are influenced by the single nuclear polymorphisms (SNPs) of FCGR3A. After treatment with Rituximab NHL patients having FCGR3A 4985 G/G genotype show high probability of response and patients having FCGR3A 4985 G/T and T/T genotypes show average probability of †response. Hence, detection of FCGR3A SNPs in patient's blood is of crucial importance for identifying better responding population to Rituximab treatment. To identify patient's FCGR3A genotypes SNP detection service is currently available from genomic DNA extracted from patient's blood (PGxPredict:Rituximab from PGxHealth). The assay is time consuming, requiring DNA amplification by PCR and dye-terminating chemistry. A label-free SNP detection by terahertz (THz) spectroscopy has been used to analyze DNA-DNA interactions with minimal sample preparation and with biologically available quantity specimens (~ few femto moles) [2]. We now propose to carry out THz spectral analysis for detection of FCGR3A genotypes.

Preliminary data on THz spectra of ssDNA & hybridized dsDNA of known sequence have shown that three different peaks can be identified for both ssDNA and dsDNA and the peaks are significantly shifted compared to each other thus allowing an easy comparison. We will carry out spectral analysis of FCGR3A ssDNA having various genotypes and with hybridized dsDNA and generate a pattern of

DNA concentration dependent temporal pulse. We will then use DNA from unknown samples and carry out spectral analysis for FCGR3A SNPs using THz spectroscopy and compare the data with known reference e.g., that of PGxPredict:Rituximab test. First, the spectral signature of pure FCGR3A will be acquired. Then, a methodology will be developed to identify the signature of FCGR3A and its polymorphs in the presence of solvents such as DI water. A library of known signatures will be developed that will be used for subsequent detection of the known SNPs. Finally, the work will be extended to detect SNPs of FCGR3A in clinical samples such as commercially available blood. In this talk, we shall report on some details of the concept with exemplary results.

1. Cartron G, Dacheux L, Salles G, Solal-Celigny P, Bardos P, Colombat P and Watier H. Therapeutic activity of humanized anti-CD20 monoclonal antibody and polymorphism in IgG Fc receptor FcgRIIIa gene. Blood, 99: 754-758, 2002.

2. Anis Rahman, Bruce Stanley, Anuk K. Rahman, "Ultrasensitive label-free detection and quantitation of DNA hybridization via terahertz spectrometry,"Paper Number: 7568-8, SPIE conference on Imaging, Manipulation, and Analysis of Biomolecules Cells, and Tissues VIII, January 23-28 2010, SPIE Photonics West, San Francisco, CA

260. Terahertz study of transdermal drug delivery

Aunik K Rahman,[1] Anis Rahman,[1] Diksha Kaushik,[2] Bozena Michniak-Kohn.[2], [1]470 Friendship Road, Ste 10, Applied Research & Photonics, Harrisburg, PA, United States; [2]Department of Pharmaceutics/ Pharmacy, Rutgers-The State University of New Jersey, Piscataway, NJ, United States.

Terahertz spectrometry is an emerging novel technique that has great potential in diagnosis of certain disease conditions as well as in the analysis of actives in certain biological tissues. Broadband terahertz technology utilizes frequencies from ~100 GHz to over 10 THz that can be used to obtain spectrographic information on the tissue surface and its interior, as well as interaction of the actives with tissue. The interaction of terahertz radiation with a given molecular system is greatly influenced by the characteristic parameters of the molecule such as its vibrational properties. This hypothesis has been successfully tested on macromolecular systems [1].

The present study investigates the feasibility of using terahertz spectrometry in the field of transdermals/topicals and cosmetic formulations. Transdermals and topicals often involve use of compounds that either enhance or retard the permeation of the active ingredient across the skin. The agents that either enhance or retard the permeation of the actives across the skin are termed as permeation modifiers. Permeation enhancers play a great role in increasing the bioavailability and efficacy of therapeutic agents by compromising the barrier properties of the skin and lead to enhancement in the delivery of the active across the skin. On the other hand, the retardants help in limiting the skin absorption of agents such as agrochemicals (pesticides), chemical warfare agents, mosquito repellants, sunscreens and household chemicals that have the attributes of easily permeating through the barrier of the skin.

We report the detection and quantification of the penetration modifiers (enhancer and retardants) across the stratum corneum. The terahertz absorption spectra showed that the control exhibited higher absorption without significant absorption peaks. The N-0915 (3-dodecanoyloxazolidin-2-one) treated specimen showed distinct absorption peaks that can be assigned to the N-0915 in the formulation. Some details will be discussed with exemplary data.

[1] Anis Rahman, Bruce Stanley and Aunik K. Rahman, "Ultrasensitive label-free detection and quantitation of DNA hybridization via terahertz spectrometry," Paper Number: 7568-8, SPIE conference on Imaging, Manipulation, and Analysis of Biomolecules, Cells, and Tissues VIII, January 23-28, 2010, SPIE Photonics West, San Francisco, CA.

261. Mid-IR reflectance spectroscopy for surface analysis: in-situ applications of grazing-angle methods

Mary Thomson., Remspec Corporation, Sturbridge, MA, United States.

Reflectance spectroscopy in the mid-IR is a well-established technique for materials identification and it can be calibrated for quantification of oil layers etc. on metal surfaces down to a thickness of about 1 micrometer*. Contamination below that level cannot be quantitatively measured by conventional reflectance. The technique of grazing-angle reflectance, however, is sensitive enough to measure organic films that are tens of Ångstroms thick (equivalent to sub-microgram amounts per square centimeter). The grazing-angle mid-IR method has been adapted for in-situ use both on flat surfaces and inside small hollow items, making it suitable for cleaning verification and validation in situations where high levels of surface cleanliness are critical, e.g., reactive gas handling and pharmaceutical reactors**. This talk will describe several applications of reflectance spectroscopy in the area of surface cleanliness and will explore the potential for using mid-IR reflectance as a real-time, in-situ technique for surface analysis.

* Bley H, Behrning S**,** Fischer N, *JOT, J. fuer Oberflaechentechnik* (2004), **44(8)**, 48-50.

** see, for example, Hamilton M L, Perston B B, Harland P W, Williamson BE, Thomson M A, Melling P J**,** *Organic Process Research & Development* (2005), 9(3), 337-343.

Chromatography Forum of Delaware Valley Student Award Symposium

Organizer/Presider: Marshall Fishman

262. Synthesis and characterization of isoquinoline urea derivatives of A-425619 as TRPV1 antagonists

Neha A Gujarati,[1] Bradley J Undem,[2] Vijaya L Korlipara.[1], [1]College of Pharmacy & AHP, St. John's University, Queens, NY, United States; [2]John's Hopkins Asthma and Allergy Center, Baltimore, MD, United States.

Transient receptor potential vanilloid receptor 1 (TRPV1), expressed widely in various tissues including skin, gut, airways and conjunctiva, acts as a key signaling complex in the pain pathway. TRPV1 is activated by a number of stimuli and modulation of this receptor through sensitization/desensitization or through antagonism is an area of active research for treatment of various types of pain. The isoquinoline urea derivative A-425619, a potent TRPV1 antagonist, was used as a lead (starting) compound in an effort to design a series of thirteen TRPV1 receptor antagonists. The phenyl ring of A-425619 was modified to obtain compounds with a potential to understand the binding site characteristics of the TRPV1 receptors. Synthesis of target compounds involved a common intermediate 2,2,2,-trichlor-N-isoquinolin-5-yl-acetamide which was obtained by reacting the commercially available 5-aminoisoquinoline with trichloroacetylchloride in presence of triethylamine. The *m*- and *p*- nitro, *p*-trifluoromethyl, *p*-chloro, *p*-bromo and *o*-amino analogues were obtained by reacting the substituted benzylamines with 2,2,2,-trichlor-N-isoquinolin-5-yl-acetamide under reflux conditions in presence of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU). The *m*- and *p*-nitro analogues were reduced to their corresponding amino derivatives, which were then reacted with various reagents to obtain the target acetamides and isothiocyanates. Purification of the target compounds by flash column chromatography presented some challenge due to the poor solubility characteristics of these compounds in various polar and nonpolar solvents. The target compounds were evaluated for their biological activity as TRPV1 antagonists in the guinea pig trachea assay.

263. Effects of temperature on the neutral lipid content of Biomphalaria glabrata as determined by modern, instrumental high-performance thin-layer chromatography with densitometry

Jeff Bolstridge,[1] Joseph Sherma,[1] Bernard Fried.[2], [1]Department of Chemistry, Lafayette College, Easton, PA, United States; [2]Department of Biology, Lafayette College, Easton, PA, United States.

High-performance thin-layer chromatography (HPTLC) with visible mode densitometry was used to examine the effects of extreme temperatures (14, 28, and 32ºC) on the neutral lipid content of the medically important snail *Biomphalaria glabrata*. Lipid samples were extracted from snail whole body samples using the Folch method with chloroform-methanol (2:1). Aliquots of extracts were spotted on Analtech channeled HPTLC silica gel plates with a preadsorbent zone, and the plates were developed with the Mangold mobile phase, petroleum ether-diethyl ether-glacial acetic acid (80:20:1). After drying the mobile phase, plates were sprayed with 5% ethanolic phosphomolybdic acid and then heated for 10 min at 110ºC to detect lipids as blue zones on a yellow background. Free sterols, free fatty acids, and triacylglycerols were qualitatively identified by comparing the R_f values of their zones in sample chomatograms to the corresponding R_f values of the lipid zones in standard chromatograms. Densitometric quantification of the three identified lipids was performed using a CAMAG TLC Scanner II with the tungsten light source set at 610 nm. Lipids were quantified at 2 and 4 weeks after the initiation of the experiment. At week 2, there were significant differences in the triacylglycerol fraction (Student's *t*-test) between all three temperatures, suggesting that snails were building reserves of depot fat at the higher temperatures. Global climate changes have led to concerns about the spread of infectious disease, including snail-born infections such as schistosomiasis. Some of these concerns relate to the ability of vector snails to adapt to climate change, making studies on lipid use of vector snails at temperature extremes crucial to a better understanding of the potential spread of snail-borne disease.

Jeff Bolstridge was supported by a Camille & Henry Dreyfus Foundation Senior Scientist Mentor Program award to Professor Joseph Sherma.

264. QuEChERS as a Sample Preparation Technique for Samples Analyzed by GC/MS

Kelsey M Smith, Mackenzie L Lauro, Karyn M Usher., Department of Chemistry, West Chester University, West Chester, PA, United States.

The QuEChERS technique, which stands for **Qu**ick, **E**asy, **Ch**eap, **E**ffective, **R**ugged and **S**afe was developed in 2003 by scientists at the USDA to clean up and prepare food samples for multi-class, multi-residue pesticide analysis. This technique has been widely used as a sample clean-up technique for fruits and vegetables. In this study, this sample preparation technique was used prior to analysis by GC/MS. In order to achieve the best sensitivity for the analytes of interest, single ion monitoring (SIM) mode was used. By selecting specific ions to be monitored during different segments of the experiment, sensitivity for the pesticides was greatly increased. In this study, Agilent QuEChERS extraction kits were used to analyze for pesticides in apple samples and in samples of green coffee and roasted coffee. Methods that offered high recovery of the pesticides in these very different matrices are presented.

265. High-throughput single-cell toxicity screening of biocidal compounds in a microfluidic device

Michael F Santillo,[1] Michael L Heien,[1] Andrew G Ewing.[1,2], [1]Department of Chemistry, The Pennsylvania State University, University Park, PA, United States; [2]Department of Chemistry, University of Gothenburg, Göteborg, Sweden.

Microfluidic and lab-on-a-chip systems are useful tools for biological assays. These devices require small volumes of reagents and sample sizes, and allow multiple steps of an analysis including derivitization, separation, and detection to be integrated into a single system. In addition, measurements on microfluidic chips can be multiplexed and automated allowing simultaneous analyses to be performed in a high-throughput fashion. Here, a microfluidic device was fabricated and characterized for studying cell lysis of *Arcella vulgaris*, a nonpathogenic amoeba, over time. The device contains a series of chambers that capture cells allowing them to be subsequently perfused with constant, hydrodynamic flow of biocidal compounds. With this microfluidic system, individual cells are observed as they undergo lysis. This allows high-throughput measurements of individual lysis events, which are not possible with conventional techniques. Differences in lysis and decay times for *Arcella* were seen at different flow rates and concentrations of benzalkonium chloride, a biocidal detergent. The efficacy of benzalkonium chloride, chlorhexidine digluconate, phenol, sodium dodecyl sulfate, and Triton X-100 were compared, revealing information on their mechanisms of action on cell membrane disruption. Observations at the single cell level give insight into the mechanistic details of the lysis of individual *Arcella* cells *vs.* the population; lysis times for individual *Arcella* cells were much shorter when compared to a population of 15 cells. In the future, this system could integrate electrophoretic-based separations, allowing intracellular contents to be derivitized and subsequently analyzed with electrochemical or fluorescence-based detection.

266. Evaluation of the precision of dual-opposite injection capillary zone electrophoresis and comparison with conventional capillary zone electrophoresis

Donna M Blackney, Joe P Foley., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

Dual-opposite injection capillary zone electrophoresis (DOI-CZE) is a method of dual sample introduction and separation in capillary electrophoresis that has no bias in resolution and analysis time and is used for the simultaneous separation of anions and cations [1]. In this study, the precision of DOI-CZE separations is evaluated and compared with the precision of conventional CE separations in terms of the precision of migration times, resolution, and peak areas.

[1] Brian S. Weekley and Joe P. Foley. *Electrophoresis*,

2007, *28*, 697-711.

267. Enantiomeric separation of phenylalinine by micellar electrokinetic chromatography using a chiral surfactant, N-dodecoxycarbonylvaline

Joseph A Vena, Donna Blackney, Joe P Foley., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

Electrokinetic chromatography (EKC) has been used to separate charged and neutral chemical species with high efficiencies and good resolution. EKC differs from capillary zone electrophoresis (CZE) because the former employes pseudostationary phases such as a micelles, microemulsions, or vesicles that may be used to achieve the desired separation. This study investigates ways to separate the enantiomers of selected amino acids and/or their chiral phenylthiohydantoin derivatives using 2-(Cyclohexylamino)ethane sulfonic acid (CHES) buffer with varied concentrations of a chiral surfactant, N-dodecoxycarbonvaline(DDCV), or if time permits a different buffer with DDCV or one or more types of cyclodextrins.

268. Investigating the mechanism responsible for MEKC separations of chiral compounds by bile salt micelles using CE and NMR

Jenna B. Yehl, Greg A Manley, Kyle W. Eckenroad, Christine M. Hebling, Laura E. Thompson, Timothy G. Strein, David Rovnyak., Department of Chemistry, Bucknell University, Lewisburg, PA, United States.

Micellar electrokinetic chromatography (MEKC) was initially developed to separate neutral analytes, but this technique is also capable of chiral separations when the pseudostationary phase has chiral selectivity. Bile salt micelles facilitate chiral separations in MEKC, but the structural and mechanistic details of how they accomplish such separations remain unclear. We have employed nuclear magnetic resonance (NMR) spectroscopy to study the molecular-level micellar structure, the nature of inter- and intra-molecular communication between atoms, and, ultimately, the interactions which govern chiral separations by MEKC. NMR chemical shift data have been studied for R,S-1-1'–binapthyl-2-2'-diylhydrogenphosphate(R,S-BNDHP) in the presence of aggregates of cholate and deoxycholate, two bile salts that form chiral micelles. We have found that BNDHP chemical shifts are sensitive reporters on the primary critical micelle concentrations (CMC) of bile salts, indicating which micellar aggregates are needed to perform successful chiral separations by MEKC. Both NMR chemical shifts and 2D-NOE data demonstrate that OH-12 (on the hydrophilic edge of cholate and deoxycholate) participates in chirally selective interactions between BNDHP and the cholate or deoxycholate micelles. Significantly, MEKC and NMR studies with chenodeoxycholate (lacking OH-12) show that OH-12 is in fact necessary for chiral selection of R,S-BNDHP by cholate and deoxycholate micelles. In addition, gradient field NMR techniques have recently allowed the investigation of the changes in diffusion coefficient of the micelle/micelle analyte complex as a function of bile salt concentration. Overall, these NMR data, have allowed us to develop a structural model to explain chiral recognition of R,S-BNDHP, as well as to determine the size of the micelle-analyte complex.

269. Investigation of the effects of buffering and mixing conditions for the in-line jaffe reaction with capillary electrophoresis

Sarah Schubert, Sarah Findeis, William Napoli, Timothy Strein., Department of Chemistry, Bucknell University, Lewisburg, Pennsylvania, United States.

Renal function is generally determined by blood serum creatinine levels. Clinical determination of creatinine is often based on the Jaffe reaction, in which creatinine in the serum reacts with sodium picrate, resulting in a spectrophotometrically quantifiable product. Previous work from our lab has introduced an electrophoretically mediated initiation of this reaction, in which nanoliter plugs of individual reagent solutions can be added to the capillary and then mixed and reacted. Following electrophoretic separation of the product from excess reactant(s), the product can be directly determined on column.

This work aims to gain a detailed understanding of the in-capillary reagent mixing dynamics, in-line reaction yield, and product degradation during electrophoresis, with an overall goal of augmenting assay sensitivity. Initial experiments have focused on maximizing product formation through manipulation of various conditions such as pH, voltage applied, and timing of the applied voltage, while recent work has focused on controlling the post-reaction product degradation. In that vein, we have systematically explored the importance of the identity, concentration, and pH of the background electrolyte on the overlap dynamics and post-reaction degradation rate of the product. While no single set of optimal conditions for both maximal reactant overlap and minimal product degradation was determined, a deeper understanding of the complexity of this in-line reaction system and the significance of product stability on assay sensitivity was gained. Some general trends that were observed include: increasing background electrolyte concentration increases peak efficiency, higher pH favors product formation, and product degradation occurs more rapidly in background electrolytes with higher pH and higher ionic strength.

270. Chemical reactions within CE capillaries: transferring an antioxidant power assay to the nanoliter level Shelly A. McCormack, Adam D. Catherman, Timothy G. Strein PhD

Shelly A McCormack,[1] Timothy G Strein,[1] Adam D Catherman.[2], [1]Department of Chemistry, Bucknell University, Lewisburg, Pennsylvania, United States; [2]Department of Chemistry, Northwestern University, Chicago, Illinois, United States.

Electrophoretically mediated microanalysis (EMMA) is a technique by which chemical reagents can be mixed within a capillary electrophoresis tube. EMMA has been widely applied to enzymatic reactions, but can also be performed with small molecules. The purpose of this research is to rapidly carry out a common assay for antioxidant capacity known as the FRAP reaction using EMMA. The Ferric Reducing Antioxidant Power (FRAP) assay is one of the more popular methods for determining the Total Antioxidant Capacity (TAC) in everyday foods such as teas, red wine, citric fruits, etc. The FRAP method employs ferric 2,4,6-tripyridyltraizine (Fe^{III}-TPTZ) complex, buffered at pH = 3.6 (with acetate), to directly react with antioxidant molecules to form the blue ferrous form of the complex. The traditional assay requires a milliliter of sample and the absorbance at 593nm, the absorbance maximum for the reduced ferrous form of the complex, is measured over a period of ten minutes. With our EMMA work, a few nanoliters of an antioxidant-containing beverage sample is injected between plugs containing Fe^{III}-TPTZ. The antioxidant sample and the Fe^{III}-TPTZ plugs are then mixed by applying a voltage field, allowing a redox reaction to proceed. A high voltage separation potential then separates the product from the reactants and moves all zones past a single on-line detector. The product absorbs strongly at 593nm. Linear calibration data on both "long" and "short" end of the capillary have been obtained, and the short end method has been used to successfully determine the TAC of several over the counter beverages.

Medicinal Chemistry II

271. X-ray imaging contrast agent based on nanoparticles of bismuth compounds

Oded Rabin.[1,2], [1]Department of Materials Science and Engineering, University of Maryland, College Park, MD, United States; [2]IREAP, University of Maryland, College Park, MD, United States.

Bismuth compounds have been suggested as excellent contrast producing agents for x-ray imaging due to the large attenuation coefficient of the element. However, bismuth compounds are generally very poorly soluble in water and in serum. The utilization of nanoparticles allows us to circumvent this difficulty and generate bismuth suspensions with a high concentration of the attenuator in water. The negligible biological availability of the bismuth ion in these suspensions in the extra-cellular environment greatly reduces the toxicity of these suspensions compared to that of the ions. Thus, bismuth sulfide nanoparticles were demonstrated to be suitable as blood-pool contrast agents by x-ray CT of laboratory mice. However, all inorganic nanoparticle formulations are limited by the rate in which the nanoparticles are excreted from the body. These rates were shown to be highly size-dependent. Naturally, there is a disconnect between the sizes of nanoparticle that show long circulation times and those that show efficient renal clearance. As a result, effective contrast agents have the tendency to accumulate in the reticuloendothelial system (primarily, the spleen).

The author discusses strategies by which the nanoparticle suspensions can be made as an effective contrast agent while reducing the load on the RES. One strategy is molecular imaging, where the nanoparticles are targeted to bond a receptor on the surface of the cells of the organ to be highlighted. The other is dynamic size evolution, where the nanoparticles possess an internal hierarchical nanostructure that gradually fragments in physiological conditions. Opportunities and challenges will be discussed.

272. Antitrypanosomal activities of some novel imido- substituted 1,4-naphthoquinone derivatives

Mozna H Khraiwesh,[2] Clarence M Lee,[2] Yakini Brandy,[1] Emmanuel S Akinboye,[1] Solomon Berhe,[1] Genelle Gittens,[1] **Oladapo Bakare**.[1], [1]Department of Chemistry, Howard University, Washington, DC, United States; [2]Department of Biology, Howard University, Washington, DC, United States.

American trypanosomiasis, also known as Chagas disease, is a parasitic disease, caused by the protozoan *Trypanosoma cruzi* and transmitted by triatomine bugs. It affects millions of people in Central and South America. Chagas disease commonly occurs in poor and rural areas of Central and South America. However, occurrence of the disease appears to be on the rise as more people immigrate to the United States. Currently used drugs have been reported to have undesirable side effects including gastrointestinal, neurological and mutagenic effects. In addition, problems such as bone marrow depletion, skin rashes, weight loss and dizziness have been reported for these drugs. Consequently, there is a search for safer drugs with more selective mode of action. Compounds containing the quinone moiety are known to possess a number of useful biological activities including antiviral, antifungal, antineoplastic, anti-hypoxic, anti-ischemic, anti-platelet, anti-inflammatory and anti-allergic activities. We have previously developed some imido-substituted 1,4-naphthoquinones as a unique class of MEK1 inhibitors with some of them showing anticancer activities. In our ongoing studies on the synthesis and biological activities of quionone-containing compounds, we have developed some quinonoid compounds with selective antitrypanosomal activities. We herein report the antitrypanosomal activities of some imido-substituted naphthoquinone derivatives. Subsequent cytotoxic activities on Balb/C 3T3 mouse fibroblasts cell lines revealed that some of these compounds possess excellent selectivity index and trypanosomal activity when compared to one of the commercial drugs.

273. Investigations of heterocyclic sulfones as medicinal compounds

Kristen N Barrett, James McKee, Murray Zanger., Department of Chemistry & Biochemistry, University of the Sciences in Philadelphia, Philadelphia, Pennsylvania, United States.

Heterocyclic sulfones have been shown to have a high level of activity against human immunodeficiency virus type 1. In addition they have been shown to have a variety of other medicinal properties including activity against tuberculosis, pneumocystis carinii pneumonia, which is the leading cause of death in AIDS patients, and as tranquilizers. Due to this wide spectrum of medicinal properties, currently in this project sulfones are being investigated for activity using computational methods. First, a ligand-ligand comparison using the computational program Shape Signatures was used to find ligands similar in shape to sulfones. Second, the shape similar ligands were investigated for activity using Similarity Ensemble Approach (SEA). Lastly, to ascertain any activity the sulfone candidates were docked into molecular targets discovered from SEA using GOLD_Suite docking program. From these studies two new molecular targets for heterocyclic sulfones have been established: aldose reductase and phosphodiesterase 4b. Inhibitors of aldose reductase have been suggested for the treatment of a variety of diseases including diabetes and heart disease. Phosphodiesterase 4b inhibitors are used in the treatment for COPD and other asthma related diseases. Further screening is being accomplished using GOLD_Suite to find sulfones with increased binding affinity to the above targets. Sulfones determined to have the most affinity for the target(s) will be synthesized and assayed in the future as part of this project. This poster elaborates on the computational determination of these targets and the chemistry of the corresponding heterocyclic sulfones.

274. Free radical scavenging assay for comprehensive analysis of individual and multi-component anti-oxidants

Michael M Koganov, Artyom Duev., Integrated Botanical Technologies, Ossining, NY, United States.

Free radical scavenging activity of anti-oxidants is often analyzed *in vitro* with "conventional" DPPH assay as described by Brand-Williams *et al*, 1995. This assay takes into consideration predominately stationary level of absorbance, and dynamic of scavenging process is assessed only in general

as "fast", "moderate" or "slow". Quantitative kinetic analysis of free radical scavenging process is required to calculate reaction characteristic time and stoichiometry. These parameters determine whether the scavenging is realized by individual or multi-component anti-oxidants. To achieve above objectives, "conventional" DPPH assay was modified for use with high-speed computer-controlled microtiter plate reader, focusing on ability of equipment to take rapid absorbance measurements of all wells of a 96-well plate. Absorbance curves were analyzed as superposition of complex-valued exponents to determine the number (A) of "elementary" first-order irreversible reactions, their amplitudes (B) which represent the amount of consumed DPPH and characteristic times (C). Individual anti-oxidant (A=1) is characterized by two parameters: stationary free radical scavenging capacity (B) and speed of scavenging reaction reflected by characteristic time (C). This modified assay was successfully used for evaluation of plant-derived phenols , their mixtures and selected natural products which are developed for personal care products capable of countering skin oxidative damage.

275. SAR of tertiary carbinamine derived BACE1 inhibitors: role of aspartate ligand amine pK_a in enzyme inhibition

Hemaka A. Rajapake,[1] Philippe G. Nanternet,[1] Harold G. Selnick,[1] James C. Barrow,[1] Georgia B. McGaughey,[2] Sanjeev Munshi,[3] Stacey R. Lindsley,[1] Mary Beth Young,[1] Phung L. Ngo,[1] M. Katherine Holloway,[2] Ming-Tain Lai,[4] Amy S. Espeseth,[4] Xiao-Ping Shi,[4] Dennis Colussi,[4] Beth Pietrak,[4] Ming-Chih Crouthamel,[4] Katherine Tugusheva,[4] Qian Huang,[4] Min Xu,[4] Adam J. Simon,[4] Lawrence Kuo,[3] Daria J. Hazuda,[4] Samuel Graham,[1] Joseph P. Vacca.[1], [1]Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA, United States; [2]Department of Structural Biology, Merck Research Laboratories, West Point, PA, United States; [3]Department of Molecular Systems, Merck Research Laboratories, West Point, PA, United States; [4]Department of Alzheimer's Research, Merck Research Laboratories, West Point, PA, United States.

The optimization of tertiary carbinamine derived inhibitors of BACE1 from its discovery as an unstable lead to low nanomolar cell active compounds is described. In the course of this study, five membered heterocycles were discovered to be stable and potency enhancing linkers. We have also discovered a clear trend where the activity of inhibitors at a given assay pH is dependent on pK_a of the amino group that interacts directly with the catalytic aspartates. The potency of compounds as inhibitors of Ab production in a cell culture assay correlated much better with BACE1 enzyme potency measured at pH 7.5 than at pH 4.5.

Nano Science, Technology, & Material Science II

276. Neurite Outgrowth on Gradients of Extracellular Matrix Proteins

William Theilacker,[1] Dianna Willis,[2] Lisa Capriotti,[1] Holt Bui,[1] Glen O'Neil,[1] Ying Len,[1] Jeffery Twiss.[2], [1]Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States; [2]Alfred I. DuPont Hospital for Children, Nemours Biomedical Research, Wilmington, DE, United States.

After sustaining a spinal cord injury, the central nervous system has a limited ability for regeneration and a promising approach is to implant biomaterial-based bridges at the injury site that will provide growth-promoting signals for nerve cells. This work details a novel method for creating millimeter scale 2-D surface gradients with the extracellular matrix proteins fibronectin and laminin. The surface coverages of the covalently attached proteins were quantified by surface analytical techniques including X-ray Photoelectron Spectroscopy (XPS) and Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS). Axonal outgrowth of dorsal root ganglia neurons was determined to increase steadily with surface coverage on both fibronectin and laminin gradients at low coverages. The rate of axonal outgrowth plateaued at intermediate coverages for fibronectin whereas on laminin, the rate of axo-

nal outgrowth continued to increase to higher coverages. An understanding of the effects of neuron outgrowth on patterned 2-D substrates with varying protein coverages and patterns is necessary for the design of future biomaterial-based bridges.

277. Surfactant mediated electrochemical polymerization of polythiophene fibers

Ian de Albuquerque,[2] Eduard Nasybulin,[1] Kalle Levon.[1], [1]Department of Chemical and Biological Sciences, Polytechnic Institute of NYU, United States; [2]Department of Chemical and Biological Engineering, Polytechnic Institute of NYU, United States.

Poly(3,4-ethylenedioxythiophene)(PEDOT) nanofibers were electrochemically polymerized in the presence of tetradecyltrimethylammonium bromide(TTAB) and cetyltrimethylammonium bromide (CTAB) surfactants and sodium nitrate electrolyte in aqueous solution. The ratios of TTAB and CTAB to EDOT monomer were shown to influence PEDOT morphology. Surfactant to monomer ratios between 1 and 2 resulted in the formation of particle-like structures while higher ratios enabled to obtain fibrous structures. Electrochemical parameters such as current and time of polymerization were shown to affect the structure of the deposited layer. Thicker deposited samples formed porous structures with ~500 nm thick fibers. Conditions were optimized to create fibrous structures and fibers of ~50 nm. SEM and AFM were used to study PEDOT morphology. UV-Vis and NMR spectra were recorded for additional characterization of the samples. The obtained materials are promising for application in organic photovoltaics due to their high porosity and small thickness of fibers.

278. Carbon Nanotube-Bioglass nanocomposite for Bone Tissue Engineering Applications

Leah E Mitchell, Aderemi Oki., Department of Chemistry, Prairie View A&M University, Prairie View, Texas, United States.

Since its discovery in the late sixties, bioactive glass has been a focal point in bone cell regeneration, and has indeed been utilized as bone fillers. Most widely used bio-glass is the 45S5® bioglass (a melt derived l with 45% silica). The Sol gel processing of bioglass has allowed expansion in bioglass composition. A major limitation of bioglass in wide range application in bone repair especially in load bearing condition is the Poor mechanical properties. Our hypothesis is that chemical integration of functionalized carbonnanotube into bioglass composition using sol-gel processing ,will yield 3-D-macroporous hybrid composite materials with tunable mechanical properties while retaining bone bonding ability**.** CNTs have been extensively investigated because of their unique one-dimensional structure with adjustable electrical conductivity and robust mechanical properties. The tensile strength and modulus of CNT are estimated to be in the range of 37-100 GPa and 640GPa to 1-2TPa respectively although they are $1/6^{th}$ as dense as steel. The approach utilized involves functionalization of carbon nanotube with methyl-methacrylate which is then process with alkoxysilane using sol-gel technique. The Functionalized-CNT-Bioglass hybrids were characterized using FTIR and TGA and bone bonding ability were tested by immersion in simulated body fluid for 5 days and surface morphology examined using SEM, TEM and x-ray powder diffraction.

The grafted CNT was characterized using FTIR confirmed the presence of the various functional groups the C=O stretching between 1600-1700cm-1, the amide linkage, and the siloxane –Si-O-Si linkage around 1080 cm-1) and weight loss from Thermogravimetric Analysis (TGA) confirmed degree of functionalization based on selective weight loss and residual mass. The ability to bond with bone was tested by dipping in simulated body fluid for 5 days. SEM picture and EDS, XRD and FTIR analysis before and after confirmed bioactivity of the nanocomposite material. Suitable Synthetic materials for bone repairs must show bone-bonding ability through the formation of apatite layer on its surface when immersed in simulated body fluid. The Xerogels formed by sol-gel processing of Arginine-MMA functionalized carbon nanotube with alkoxysilane showed bone bonding ability and hopefully with improved mechanical properties. Studies are underway testing the mechanical properties.

279. New inorganic-organic hybrid materials based on III-VI semiconductors

Ruibo Zhang, Derek Le, Thomas J. Emge, Jing Li., Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, New Jersey, United States.

It is a great global effort to seek clean, efficient and affordable energy to replace fossil fuels for the sake of reducing the greenhouse gas emission. To this end, sunlight has been chosen as a widely acceptable renewable energy source, and photovoltaics, considered as the most important technology that converts sunlight directly into electricity, has witnessed a tremendous growth during recent years. III-VI chalcogenide compounds (such as Ga_2Te_3 In_2S_3, In_2Se_3, In_2Te_3, etc.) are of great interest because of their excellent semiconductor properties and potential for photovoltaic (PV) applications such as solar cells and solar-powered LEDs. Our current research focuses on the design, synthesis and characterization of new inorganic-organic hybrid materials based on III-VI semiconductors. These materials are made of both inorganic and organic components, and can be considered as derivatives of III-VI semiconductors, with their band gaps falling in a range specifically suitable for use in PV devices.

280. Genetically encodable methods for controlling the orientation of the proteins ubiquitin, eGFP and protein G on gold nanoparticles

Alison M. Williams-Reed, Steven J. Metallo., Department of Chemistry, Georgetown University, Washington, DC, United States.

Proteins which are oriented randomly on a surface often have decreased enzymatic activity or recognition ability due to occlusion or modification of important residues. Controlling the orientation of active proteins on metal surfaces is therefore crucial to preserve the functions of native proteins. Current methods utilize covalent adsorption (chemisorption) or non-covalent adsorption (physisorption) to attach proteins to metal surfaces. We have developed a direct and stable genetically encodable method for the oriented attachment of proteins to gold nanoparticles through the tetracysteine motif (C-C-P-G-C-C). Agarose gel electrophoresis and fluorescence studies have confirmed that mutants of the proteins ubiquitin, and enhanced green fluorescent protein bind to gold surfaces in a robust, oriented manner. Gel electrophoresis experiments have also confirmed that protein G mutants bind stably to gold nanoparticles of various sizes. The ability to genetically control the orientation of proteins on surfaces is of particular interest in the development of bio-sensors.

Recent Updates in Patent Law

Sponsor: Division of Chemistry & the Law
Organizers: Justin Hasford, Sarah Perlinger Hasford

281. Bilski and Patent Eligibility of Processes in the Chemical and Biological Arts

Charles Collins-Chase., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

The landmark Court of Appeals case *Bilski v. Kappos* established a new test of patent eligibility for process inventions, including those in the chemical and biological arts. The "Machine-or-Transformation" test set out in *Bilski* could have a significant impact on what kinds of inventions are patentable in fields ranging from medical methods to genetics and biotechnology. While subsequent cases have begun to demonstrate the effects of this test, a great deal of uncertainty remains. The *Bilski* case was argued before the United States Supreme Court in November 2009, and the Court's decision may again completely alter the framework of patent eligibility for process inventions. This talk examines *Bilski*'s impact on chemical process patents, key cases decided since *Bilski*, and possible future developments.

282. Omission Without Intent is Not Inequitable Conduct: AstraZeneca Pharmaceuticals LP v. Teva Pharmaceuticals USA, Inc. (Fed. Cir. 2009)

Casey Dwyer., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

Patent owners have faced more and more accusations of inequitable conduct over the past several years, spurred on by liberal pleading standards and Federal Circuit case law seeming to lower the standard needed to prove deceptive intent. In many inequitable conduct allegations, the accused behavior is the failure to submit information that is material to patentability to the Patent Office during prosecution. In *AstraZeneca Pharmaceuticals LP v. Teva Pharmaceuticals USA, Inc.* (Fed. Cir. 2009), however, the Federal Circuit made clear that intent to withhold material information does not by itself prove the intent to deceive necessary for inequitable conduct. This presentation will take an in-depth look at the Federal Circuit's decision in *AstraZeneca Pharmaceuticals*, examine the landscape of inequitable conduct cases that led up to this decision, and look into what the future may hold for inequitable conduct allegations.

283. In re '318 Patent Litigation : The Enablement and Utility Requirements

Shana Mattson., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

On September 25, 2009, the Court of Appeals for the Federal Circuit affirmed the invalidation of a patent claiming the use of galantamine to treat Alzheimer's disease. The Court reasoned that the patent merely presented an unproven hypothesis, and that "mere ideas" are not patentable. Although the Court's decision hinged on the enablement requirement of patent law, much of the opinion focused on the separate requirement of utility. This presentation will examine the Court's decision, its impact on the enablement and utility requirements of patent law, and what this means for scientists seeking to patent their inventions.

284. Implications of Wyeth v. Kappos

Sheetal Patel., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

This presentation discusses the implications of the recent case,*Wyeth v. Kappos,* No. 09-1120 (Fed. Cir. Jan. 7, 2010), where the Federal Circuit held that the USPTO has been miscalculating the PTA. The Court also provided a new PTA framework, which primarily affects patents derived from applications that were pending at the USPTO for more than three years. Under the Court's decision in *Wyeth*, some patent applicants may qualify for a longer term adjustment. The resulting extended patent term is extremely valuable for patent holders especially those in the pharmaceutical, biotechnology and medical device industries.

285. Product-by-Process: What You Say Is What You Get

Mary Chlebowski., Finnegan Henderson Farabow Garrett & Dunner, LLP, United States.

In certain circumstances, new compounds may be difficult or impossible to accurately characterize. While such problems of characterization may no longer be the norm, polymorphs represent an important area where accurate characterization methods are still underdeveloped. Traditionally, inventors were able to patent a new product, even without complete characterization, by reciting the process by which the product was obtained in a "product-by-process" claim. With such a claim, an inventor was able to preclude others from using the product, whether or not the person used the same preparation method. This presentation will discuss *Abbott v. Sandoz*, which reversed that practice. In other words, an inventor today can only preclude others from using a product if the product was prepared by the exact process recited. The implications of this case in patenting the indescribable will be discussed.

286. Preventing premature patent retirement: Is your invention working and earning up to its full potential?

Patricia A. Carson, **Christopher T. Jagoe**, **Graham M. Pechenik**., Kaye Scholer LLP, New York, NY, United States.

Patents in the chemical field can be worth millions of dollars per month of patent life. Yet until this year, the U.S. Patent Office was calculating patent term in a way that effectively short-changed many applicants. That was altered by a recent court decision from the Federal Circuit, *Wyeth v. Kappos*. This presentation will review the historical background of patent term, analyze the basis for the *Wyeth* decision and the impact thereof, discuss the mechanics of calculating the proper length of patent term, and address the procedures for seeking a correction, for patentees who may be entitled to an adjustment.

Polymer and Nanomaterials based Photonics, Electro-optics and Tetrahertz Spectrometry

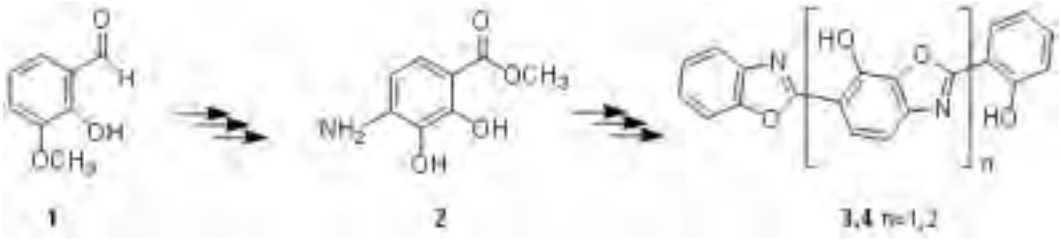
Organizer: Anis Rahman

287. Polymers for long range photoinduced proton transfer

Richard P Brown, Paul J Smith., Department of Chemistry and Biochemistry, University of Maryland Baltimore County, Baltimore, Maryland, United States.

Photonics and the development of molecular electronic devices are two exciting fields at the interface of modern chemistry and material science. Our objective is the creation of a polymer that, upon absorption of light, will propagate proton transfer over long distances. The resulting photo-induced proton transfer would ultimately be used to transfer protons across membranes, thereby establishing a proton gradient and an electrochemical potential. We envision that incorporation of large numbers of the aforementioned polymers would facilitate photochemical creation of membrane potentials. The energy associated with such potentials would be used to do physical work in energy applications. Such polarized membranes could also serve in more complex molecular electronic devices.

The specific aim of this work is to synthesize the monomer **2** (methyl 4-amino-2,3-dihydroxybenzoate), to use this to synthesize oligomeric benzoxazoles **3** and **4**, and to examine their proton transfer properties indirectly by evaluating their photochemical behavior. In particular, we hope to find that elongation of the oligomeric chain will cause nonlinear variation of absorbance or fluorescence, indicating that the individual chromophores/proton transfer units are acting in a coordinated fashion. The next step would be to implant these oligomers into a membrane and examine proton transfer behavior. Synthesis of **3** and **4**, starting with commercially available **1**, will be described.



288. Fabrication of Polycyclic aromatic hydrocarbons nanostructures from 1D to 3D by gas phase self-Assembly

Hong Wang, Karen Xu, Haifeng Ji., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

Synthesis of nanomaterials with small organic molecules has attracted increased interest.[1-3] Nanomaterials formed by polycyclic aromatic hydrocarbons (PAHs), such as pentacene and rubrene etc., are of great interest as promising candidates for supramolecular electronics and other applications in future.[4] Organic materials have natural tunable electronic and optical properties as well as greater variety and flexibility via molecular design. Besides, morphologies play important role in determining the properties of organic nanomaterials,[5-7] which enrich the applications in optical and electronic devices. However, the process on the synthesis of organic nanomateirals is slow. The low solubility in almost all solvents limits the study on the synthesis of nanostructures. Here, we report the formation of PAHs 1D to 3D nanostructures by using gas phase self-assembly (GPS) method. This is a novel and facile approach to self-assemble PAH nanostructures, which succeeds in avoiding the solubility issues and being used in fabricating organic nanomaterials from 1D to 3D. The method may find wide applications in the electronic and energy fields.

References

1. Green, J. E.; Choi, J. W.; Boukai, A.; Bunimovich, Y.; Johnston-Halperin, E.; Delonno, E.; Luo, Y.; Sheriff, B. A.; Xu, K.; Shin, Y. S.; Tseng, H. R.; Stoddart, J. F.; Health, J. R., *Nature* **2007,** 445, 414.

2. Xiao, K.; Tao, J.; Pan, Z.; Puretzky, A. A.; Ivanov, I. N.; Pennycook, S. J.; Geohegan, D. B., *Angew. Chem. Int. Ed* **2007,** 46, 2650.

3. Zhao, Y. S.; Peng, A.; Fu, H.; Ma, Y.; Yao, J., *Adv. Mater* **2008,** 20, 1661.

4. Schenning, A. P. H. J.; Meijer, E. W., *Chem. Commun* **2005**, 3245.

5. Zhang, X. J.; Zhang, X. H.; Zou, K.; Lee, C. S.; Lee, S. T., *J. Am. Chem. Soc* **2007,** 129, 3527.

6. Briseno, A. L.; Mannsfeld, S. C. B.; Ling, M. M.; Liu, S. H.; Tseng, R. J.; Reese, C.; Roberts, M. E.; Yang, Y.; Wudl, F.; Bao, Z. N., *Nature* **2006,** 444, 913.

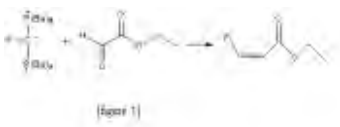
7. Oh, J. H.; Lee, H. W.; Mannsfeld, S.; Stoltenberg, R. M.; Jung, E.; Jin, Y. W.; Kim, J. M.; Yoo, J. B.; Bao, Z. N., *Proc. Nati. Acad. Sci.* **2009,** 106, 6065.

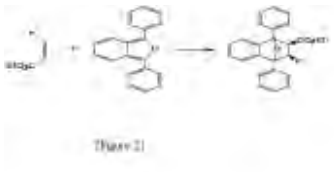
Fluorine Chemistry

Sponsor: Division of Fluorine Chemistry

289. Synthesis of ethyl cis-2-fluoroproenoate and its use in the Diels-Alder reaction

Joshua Neumann, Timothy Patrick., chemistry, southern illinois university edwardsville, edwardsville, illinois, United States.





Alkenes are an integral part of organic chemistry and are useful in nearly all branches of chemistry. With the expansion of fluorine into biochemistry, pharmaceuticals, textiles and industry, the needfor small fluorinated building blocks is in high demand. Fluoroalkenes are the perfect building blocks for placement of fluorine in a desired position. We have successfully synthesized ethyl cis-2-fluoroproenoate in high yields in a one step reaction. To compare reactivity, the ethyl trans-2-fluoropropenoate was synthesized via the Michaels reactions. Deals Alder reactions where conducted to study the effects of fluorine on the reaction.

Inorganic Chemistry II

Sponsor: Division of Inorganic Chemistry

290. Imine chelates of copper, nickel, and zinc

Molly A. O'Connor, Anthony W. Addison., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

Several Schiff base ligands with N, O, and/or S donor atoms were synthesized then complexed with an assortment of metals including nickel, copper, and zinc. The ligands and complexes were analyzed using a variety of spectroscopic, magnetic, and crystallographic methods. Chiral Schiff base ligands and complexes were also prepared. Several methods including ESR spectroscopy were used to study any changes that ligand chirality caused in the metal complexes.

291. A New Microporous Metal Organic Framework (MMOF) Material for Small Gas Separation

Jingming Zhang, Haohan Wu, Thomas Emge, Jing Li., Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, NJ, United States.

A new MMOF and member of the RPM (Rutgers Recyclable Porous Materials) family, [Zn2(bpdc)2bpe]·2DMF (DMF = N,N-dimethylformamide) or RPM4-Zn, has been synthesized and structurally characterized. Having a highly flexible three-dimensional framework containing one-dimensional channels RPM4-Zn exhibits a high adsorption selectivity towards CO_2 over other small gases such as CH_4, N_2, CO and O_2 under low pressure and room temperature. At 273K and 1 atm, it absorbs up to 8 wt% of CO_2, and features a three-step adsorption-desorption isotherm curve with very little hysteresis. The separation ratios based on the single-component isotherms at room temperature and 0.2 atm are 115:1 (v/v) and 50:1 (v/v) for CO_2/N_2 and CO_2/CH_4, respectively.

292. Comparison of the coordination chemistry of tripod ligands possessing three pyridine donors and three imidazole donors

Julie Vrana,[1] **Kathleen McGuinn**,[1] Donald L Jameson,[1] Christopher J Ziegler,[2] James Engle.[2], [1]Department of Chemistry, Gettysburg College, Gettysburg, PA, United States; [2]Department of Chemistry, University of Akron, Akron, OH, United States.

As part of a project to develop biocompatible organometallic complexes for potential medical applications, we have made a series of modifications to the "tail" of two tripod N_3 ligands: tris(2-pyridyl) methane and tris(N-methyl-2-imidazolyl)methane. These ligands bind the organometallic fragment of interest, $Re(CO)^{3+}$, with different binding modes depending on the tail modification and reaction conditions. This variability in binding has prompted us to explore the coordination chemistry of the tripod ligands with other metal ions and organometallic fragments. Reaction of $\{Ru(h^6\text{-}C_6H_6)Cl(u\text{-}Cl)\}_2$ with tris(2-pyridyl)methoxymethane (TPMOMe) results in $Ru(h^6\text{-}C_6H_6)(N,N',O\text{-}TPMOMe)^{2+}$ where x-ray crystallography revealed the tripod ligand is unexpectedly coordinated using two nitrogen atoms and the ether oxygen. Structural analysis of the analogous ruthenium complex of tris(N-methyl-2-imidazolyl)methoxymethane (timmOMe) reveals the tripod ligand is coordinated in the expected N_3 mode. We will report further synthetic results aimed at understanding the underlying reasons for the difference in reactivity between the ligand systems.

293. Nearly-Zero Anisotropic Thermal Expansion in II-VI Based Inorganic-Organic Hybrid Semiconductor Materials

Xiao Zhang,[1] Yang Ren,[2] Mojgan Roushan,[1] Jing Li.[1], [1]Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, NJ, United States; [2]Advanced Photon Source, Argonne National Laboratory, Argonne, IL, United States.

Zero thermal expansion (ZTE) is a desired but rare material property. Herein we report a unique family of inorganic-organic hybrid semiconductors with general formula $ZnSe(L)_{0.5}$ (L = organic diamine) that exhibit nearly-zero anisotropic thermal expansion behavior in temperature range between 5K and 300K. The unit cell parameters and crystal structures of $ZnSe(en)_{0.5}$, $ZnSe(pda)_{0.5,}$ $ZnSe(bda)_{0.5}$ and $ZnSe(ptda)_{0.5}$ (where *en* = ethylenediamine, *pda* = propanediamine, *bda* = butanediamine, and *ptda* = pentanediamine) were refined by Rietveld method and their thermal expansion properties were analyzed and rationalized based on their crystal structures and symmetry.

294. Tolerance of Biomphalaria glabrata to Triorganotins

James Ferguson,[1] Xueqing Song,[1] Andargachew Negash,[1] Carolyn Cousin,[2] Stephanie Graves,[2] George Eng.[1], [1]Department of Chemistry & Physics, University of the District of Columbia, Washington, DC, United States; [2]Department of Biological & Environmental Sciences, University of the District of Columbia, Washington, DC, United States.

Triorganotin (R_3SnX) compounds have been shown to have species-specific toxicity depending on the organic group attached to the tin atom. One of the biocidal activities associated with triorganotins is their toxicity to mollusks. A series of triorganotins were screened against *Biomphalaria glabrata*, a freshwater snail which hosts *Schistosoma mansoni*, the flatworm that causes *schistosomiasis*. Management of the snail population is one way to control the flatworm population, and thus, *schistosomiasia*. The effectiveness of the triorganotins was determined by their LC_{50} values. Preliminary results indicated that the most effective triorganotins were those containing the butyl moiety. Average LC_{50} values for trimethyltins, tributyltins, tricyclohexyltins, triphenyltins, and tripropyltins were 3.01 ppm, 0.11 ppm, 0.50 ppm, 0.58 ppm and 0.73 ppm, respectively. The most effective compound was tributyltin acetate, with an LC_{50} value of 0.03 ppm.

295. Luminescent MOFs for Detection of Explosives and Other Aromatic Compounds

Sanhita Pramanik,[1] Anjian lan,[2] Jing Li.[1], [1]Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, New Jersey, United States; [2]Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian, China.

The synthesis of metal organic frameworks (MOFs) has been an area of tremendous interest due to their tunable structural chemistry and potential for applications in various fields, such as gas sorption, separation, catalysis and sensing. Recently, we have focused our research on the development of a group of microporous metal organic frameworks (MMOFs) that exhibit interesting luminescent properties. The combination of luminescence and accessible porosity makes them promising candidates for sensing applications, in particular detection of nitrated explosives. While fluorescence quenching based sensing is a well known method for the detection of explosives and other molecules, our research has shown both the fluorescence quenching and enhancement phenomenon may be used for the detection of different types of aromatic compounds.

296. Toxicity of Triorganotins against Escherichia coli

Hirut Yimer,[2] Russell Knighton,[1] Joni Robinson,[2] Xueqing Song,[1] George Eng.[1], [1]Chemistry & Physics, University of the District of Columbia, Washington, DC, United States; [2]Biological & Environmental Sciences, University of the District of Columbia, Washington, DC, United States.

Studies have shown that triorganotins have a wide range of biocidal activities. The toxicity of triorganotins depends on the organic group attached to the tin atom. For example, insects have been found to be most susceptible to trimethyltin derivatives, while mammals are most vulnerable to triethyltin compounds. Triphenyltins have been reported to show activity towards fungi. *Escherichia coli (E.coli)*, a gram negative bacterium, was used as a test model for triorganotin toxicity. Thus, *Escherichia coli* were screened against three series of triorganotin carboxylates. The three series were triorganotin derivatives of modified components/fragments of pyrethroids. The data indicated that there were no significant differences between the three series, however, the methyl derivative in each series was the least effective.

297. Studies on asymmetric bis(imino)pyridines and their synthetic precursors

Rachel Hardie, Margaret D. Kennedy, Jonathan C. Axtell, Janelle E. Steves, William S. Kassel, William G. Dougherty, Timothy J. Dudley, Deanna L. Zubris., Department of Chemistry, Villanova University, Villanova, PA, United States.

The tridentate bis(imino)pyridine ligand has been studied extensively as a component of highly active iron catalysts for ethylene polymerization. Our laboratory is currently interested in bis(imino)pyridine ligands that are bulky and asymmetric at the imino carbon atoms.

We have prepared bromo mono(imines) of the form 2-Br,6-{(2,6-Me_2-C_6H_3)NC(R)}$_2$$C_5H_3BrN$, where R = *t*-Bu or Ph, and have tested them as synthetic precursors to our desired bis(imino)pyridine ligand.

Concurrently, we are using computations to evaluate the relative energies of four chemically relevant conformers for asymmetric bis(imino)pyridine ligands with a range of substitution patterns.

298. Synthesis and Study of $[Ru(bpy)_2(bpy(OH)_2)][PF_6]_2$

Samantha Klein, Jared J. Paul., Department of Chemistry, Villanova University, Villanova, Pennsylvania, United States. (Data courtesy of William G. Dougherty & W. Scott Kassel)

The complex $[Ru(bpy)_2(bpy(OH)_2)][PF_6]_2$ (bpy= 2,2′-bipyridine and bpyOH= 4,4′-dihydroxy-2,2′-bipyridine) was synthesized in order to investigate the nature of charge transfer within the complex. Synthesis was performed from a modified procedure previously reported by Z. Ji *et al.* and was

carried out under argon. Ruthenium trichloride trihydrate was converted to $Ru(bpy)_2Cl_2$ followed by addition of bpyOH which had been prepared from a 4,4'-dimethoxy-2,2'-bipyridine precursor. Characterization was performed using X-Ray crystallography, NMR, IR, UV-Visable and luminescence spectroscopies. Studies were performed with hydrogen-bonding bases such as 1-methylimidazole to understand the effects of protonation on the electronic properties of the complex. Transitions were analyzed using UV-Visable and luminescence spectroscopies. Addition of base resulted in changes in the peaks and new absorbance maxima. Similar studies were performed on the control complexes $Ru(bpy)_3$ and $Ru(bpy)_2$(bpyOMe) (bpyOMe= 4,4'-dimethoxy-2,2'-bipyrdine) to further elucidate the effects of the proton-containing bpyOH ligand on the complex.

299. Synthesis, characterization and electronic properties of $[Ru(tpy)(tpyOH)]^{2+}$

Alessa B. Wood, Kent A. Maghacut, Walter J. Boyko, **Jared J. Paul**., Department of Chemistry, Villanova University, Villanova, PA, United States.

The coupling of electron transfer with proton transfer is an intense area of interest in chemistry and biology termed Proton Coupled Electron Transfer (PCET). Ruthenium polypyridyl complexes have long been studied due to their potential for light-driven catalysis of many PCET reactions of interest, such as the oxidation of water by four electrons and four protons to molecular oxygen. The ligand structures of ruthenium complexes have been varied in many diverse ways leading to tunability of the Metal to Ligand Charge Transfer (MLCT) character of these complexes. One such way to control the electronic properties of ruthenium complexes is with ligands that can have varied protonation states. We report here, the synthesis and characterization of the mixed-ligand complex $[Ru(tpy)(tpyOH)]^{2+}$ (tpy = 2,2':6',2"-terpyridine, tpyOH = 2,6-bis(2-pyridyl)-4-hydroxy-pyridine). The tpyOH ligand contains a proton-donating phenol, which can significantly alter the electronic properties of the complex depending upon the protonation state. The complex was synthesized by refluxing $Ru(tpy)Cl_3$ with 2,6-Bis(2-pyridyl)-4(1H)-pyridone with the addition of a small amount of hydrochloric acid to ensure protonation of the tpyOH ligand once attached to the complex. The complex was characterized utilizing, 1D and 2D COSY ^{1}H-NMR spectroscopy. 2D COSY ^{1}H-NMR spectroscopy gave the couplings of each proton within the two different terpyridine ligands, most notably the differences associated with the hydroxy-substituent in the tpyOH ligand. FT-IR spectra gave a characteristic peak at ~3500 cm^{-1} associated with the hydroxyl stretch. The electronic properties of the complex, $[Ru(tpy)(tpyOH)]^{2+}$, were directly compared to the complex, $[Ru(tpy)_2]^{2+}$, which was synthesized and studied as a control complex. UV/Visible absorbance spectroscopy was utilized to study the MLCT bands of the complexes in acidic and basic acetonitrile/water solutions. In the presence of excess hydrochloric acid, a characteristic l_{max} at 479 nm was observed. When deprotonated using excess sodium hydroxide, the MLCT bands shifted significantly, yielding two significant overlapping peaks at l_{max} = 472 nm and l_{max} = 508 nm. In the control complex, $[Ru(tpy)_2]^{2+}$, no difference was observed in excess acid or base solutions, indicating that the change in electronic properties of the complex are indeed coupled to the protonation state of the tpyOH ligand. Electrochemical studies were performed on $[Ru(tpy)(tpyOH)]^{2+}$ in acetonitrile with tetrabutylammonium hexafluorophosphate as the supporting electrolyte. The complex has a reversible redox wave corresponding to the $Ru^{II/III}$ oxidation state at 1.19 V vs. SCE. This reduction potential is lower than the corresponding potential of 1.29 V vs. SCE for $[Ru(tpy)_2]^{2+}$. The lower potential is due to the electron donating properties of the tpyOH ligand, which are able to stabilize the oxidized Ru^{III} center relative to the tpy ligand.

300. Long Fluorinated alkyl chains protects Iron(III) porphyrins from self-oxidative degradation during the catalytic process

Amit Aggarwal,[1] Charles M Drain.[1,2], [1]Department of Chemistry and Biochemistry, Hunter College, New York, NY, United States; [2]The Rockefeller University, New York, NY, United States.

For the selective oxidation of olefins or other hydrocarbons, organic nanoparticles (ONPs) of matalloporphyrins can be robust catalysts. Halogenation on the periphery of macrocycle ring increases their catalytic activity but the stability towards their self-oxidative degradation is always a point of concern.

A study has been conducted on the synthesis and catalytic activity of hydrophobic porphyrin nanoparticles such as 5,10,15,20-tetrakis-[4-(1'H,1'H,2'H,2'H-heptadecafluorodecane-1-thiol)-2,3,5,6-tetrafluorophenyl] porphyrinato iron(III), [Fe(III)TPPF$_{84}$]. GC-MS analysis of the reaction mixture shows the major products formed are ene-1-ol and ene-1-one for cyclohexene oxidation and the turn over number depends upon the size of the ONPs and the nature of the oxygen source used peroxide vs. dioxygen. Initial findings show that 12 nm ONPs of Fe(III)TPPF$_{84}$ are catalytically less active than our previously reported results on Fe(III)TPPF$_{20}$, but in contrast are found to be more stable towards their self oxidative degradation. The smaller catalytic activity may be because of the formation of their μ-oxo and/or μ-dioxo dimers which are reported to be catalytically inactive. Our hypothesis is that the long fluorinated alkyl chains present on the para position of the phenyl groups may block the access to the central iron, where the oxygen is activated and protects the metalloporphyrin from their oxidative degradation.

References:

1. G. Smeureanu, A. Aggarwal, C.E. Soll, J. Arijeloye, E. Malave, and C.M. Drain, Chem. Eur. J. 15 (2009) 12133-12140.

2. A. Varotto, L. Todaro, M. Vinodu, K. J., G.-y. Liu, and C.M. Drain, Chem. Commun. (2008) 4921-4923.

3. X. Gong, T. Milic, C. Xu, J.D. Batteas, and C.M. Drain, J. Am. Chem. Soc. 124 (2002) 14290-14291.

301. Ground and excited-state coordination chemistry of Ru(bpy)$_2$(ppz)$^{2+}$ (ppz-4'7'-phenanthrolino-5'6':5,6-pyrazine)

Anthony Perri, Harry D Gafney, John Kalambogias., Department of Chemistry and Biochemistry, Queens College-City University of New York, Flushing, NY, United States.

Ru(bpy)$_2$(ppz)$^{2+}$(ppz-4'7'-phenanthrolino-5'6':5,6-pyrazine) is one of a group of compounds that exhibit enhanced Bronsted basicity upon excitation with visible light. Current research focuses on the ground and excited-state metal coordination chemistry of the complex with Zn (II) and Cd (II). UV-Vis and emission titration data along with excited-state lifetime data will be presented for both metal coordination titrations. Reactions of Zn (II) and Cd (II) with Ru(bpy)$_2$(ppz)$^{2+}$show a tenfold increase in ground state equilibrium constants, in comparison with Ru(bpy)$_2$(dpp)$^{2+}$. Reaction with Zn (II) shows sustained new emission at 785 nm with a lifetime of 60 ns at high Zn (II) concentration, which is attributed to the formation of an exciplex in which the Zn^{2+} coordinates to the peripheral ppz nitrogens of Ru(bpy)$_{2(}$ppz)$^{2+}$. Comparisons of the results with different Ru (II) diimines indicate the importance of structural factors in both ground and excited-state coordination

302. Computational study of the electronic structure and function of a novel class of cyclic Phosphazenes

Whelton A. Miller, Vincent S. Pagnotti, Edward R. Birnbaum, Preston B. Moore., Department of Chemistry and Biochemistry, University of the Sciences in Philadelphia, Philadelphia, PA, United States.

Because of their unique properties, Polyphosphazenes have generated many opportunities to explore a variety of applications. These applications include several areas of biomedical research, i.e. drug delivery systems, as well as uses in material science, i.e. fire-resistant polymers. These potential drug delivery systems and polymers can take advantage of substitution patterns, which potentially have more variations than typical carbon analog substitution patterns, such as benzene, and also allow for exploration of reactivity. Here we present a computational study of the chemical modifications to a group of cyclic phosphazenes. This study attempts to understand the electronic structure of the compounds, general reactivity, and potential applications using quantum mechanical analysis. We hope to understand this new niche of reactivity and substitution, which could allow for better design of future technology based on phosphazene chemistry.

303. On the road to controlled phosphazene dendrimers: Steps along the way. Part III

Vincent S. Pagnotti, Edward R. Birnbaum., Department of Chemistry & Biochemistry, The University of the Sciences in Philadelphia, philadelphia, Pa, United States.

In part I and II of this research we presented the rationale for synthesizing novel phosphazene dendrimers in a controlled fashion, along with the associated pitfalls. In part III of the series we take a step back to focus on synthesizing an array of monomers, many of which have not previously been described in the literature that will provide greater flexibility in achieving our end goal. In synthesizing the monomers, particular attention was paid to chain length and the number of dangling groups on the phosphazene core. By utilizing this variety of monomers, we anticipate being able to ultimately synthesize a novel series of dendrimers of varying size and properties.

304. Construction of metal-organic frameworks with enhanced properties

Yonggang Zhao, Thomas J Emge, Jing Li., Department of chemistry and chemical biology, Rutgers University, Piscataway, NJ, United States.

Metal-organic frameworks (MOFs) are a relatively new class of nano-porous material and are attracting tremendous interest during the past decades, due to their promising applications in gas storage, separation science, catalysis and sensing.

By a modular construction principle, MOFs can be rationally designed and realized with fascinating chemical and physical properties. Recently, we have been focusing on the development of metal-organic frameworks with diverse structures and multifunctionality. Our research has demonstrated that the structures of frameworks (e.g., dimensionality, framework connectivity, and topology) and pore properties (e.g., pore size, pore volume and the chemical functionality of the pore walls) of these materials can be systematically tailored by controlling and tuning experimental parameters, including metal source and functional organic linkers, solvents, pH value, reaction time and temperature. Several examples of MOFs with significantly enhanced properties and performances in gas adsorption (H2 and CO2) and light hydrocarbon separation will be discussed.

305. Use of underutilized bulky Ttz ligands for the formation of zinc based biomimetic structures

Mukesh Kumar,[1] Elizabeth T. Papish,[1] Matthias Zeller.[2], [1]Chemistry, Drexel University, Philadelphia, PA, United States; [2]Chemistry, Youngstown State University, Youngstown, OH, United States.

Ttz ligands [Ttz = tris(1,2,4-triazolyl)borate] are analogous to well known Tp ligands in terms of the sterics and the ability to structurally approximate the coordination sphere of many zinc based enzymes. In addition, these ligands provide the possibility of H-bonding and extra coordination through the use of the fourth position nitrogen. We have been interested in the biomimetic chemistry of zinc based enzymes. For this purpose, new alkyl zinc complexes, ($Ttz^{R,Me}$)ZnR' (R = *t*Bu, Ph; R' = Me, Et) were prepared. These alkyl zinc complexes react with a number of protic reagents such as fluorinated alcohols, phenols, thiophenol, acetylacetone, acetic acid, HCl and triflic acid to afford zinc complexes of the conjugate base (CB), ($Ttz^{R,Me}$)ZnCB. The X-ray structural studies on ($Ttz^{R,Me}$)ZnCB complexes showed the variation in the coordination motifs depending upon the nature of sterics around the metal and the coordination capability of the conjugate base. The Ttz ligand appears to be reasonably acid and water stable since most protic reagents used in this study do not lead to B-N bond cleavage products.

306. Departmental Hirsch Index values scale linearly with Chemistry department size

A. W. Addison, Thuong H. Tran., Department of Chemistry, Drexel University, Philadelphia, PA, United States.

In 2005, Physicist Jorge Hirsch introduced* a new citation-based index for quantifying what he referred to as individual's research output, so that many academic Physicists now cite their Hirsch Index (*h*) in their *curriculum vitæ*. A high *h* is associated with having published a large number of highly-cited research papers. Automatic computation of the *h*-index has been effected in the Thomson-ISI Web of Science citation database, and has been extended to determination of the *h*-index for entities other than individuals, such as departments. However, the inevitable dependence of *h* on the number of papers published leads to large research departments having an index advantage over smaller ones. The question thus arises, as to the nature of the dependence of departmental *h*-index on department size. Using the Web of Science as a source of Chemistry Department *h*-indices, and the ACS Directory of Graduate Research as a source of department faculty size (*N*) data, we found that for *ca*. 300 U.S. & Canadian universities, departmental *h*-index is indeed quite dependent on department size. Moreover, to a good approximation, departmental *h*-index scales in a simple linear fashion with department size, enabling one to rank the Chemistry departments according to their research accomplishment or impact on a size-normalized basis.

* J. E. Hirsch, *Proc Natl Acad Sci U S A*. (2005) 102(46): 16569–16572. doi: 10.1073/pnas.0507655102

List of Authors with Paper Numbers

Saturday, 10 April 2010 "Tear and Take" Events held at the Hotel du Pont

EVENT	TIME	ROOM*	NOTES
On-Site Registration Open	7:30 AM - 7:30 PM	Reception Area	
Welcome Reception Continental Breakfast	7:30 - 9:00 AM	Dining/ Lounge Area	
POGIL Workshop for High School Teachers	9:00 AM - 12:00 PM	King/Sullivan	
Biological Chemistry I - Oral	9:00 AM - 12:00 PM	King Sejong	
Organic Chemistry I - Posters	9:00 AM - 12:00 PM	Knowles	
Inorganic Chemistry I - Oral	9:00 AM - 12:00 PM	Montessori	
Physical Chemistry	9:00 AM - 12:00 PM	Collins	
Women Chemist Committee Luncheon	12:00 - 01:30 PM	Christiana	
Chemical Educators (K - 12) Luncheon	12:00 - 01:30 PM	Quintanilla	

*Rooms are subject to change

Saturday, 10 April 2010 "Tear and Take" Events held at the Hotel du Pont

EVENT	TIME	ROOM*	NOTES
Laboratory Waste Management	1:00 - 5:00 PM	Marshall	
Chemical Education	1:30 - 4:00 PM	Quintanilla	
Biological Chemistry II - Posters	1:30 - 4:00 PM	Knowles	
Organic Chemistry II - Oral	1:30 - 4:00 PM	King Sejong	
Regional Chemagination Competition	1:30 - 4:00 PM	Blake	
High School Research Poster Session	1:30 - 4:00 PM	Piaget	
Project SEED Poster Session	1:30 - 4:00 PM	Collins	
Plenary - Chemical Demonstrations	4:00 - 5:00 PM	King/Sullivan	
Spring Meeting RSC - USA	6:00 -10:00 PM	Delaware Suite	

*Rooms are subject to change

Sunday, 11 April 2010 "Tear and Take" Events held at the Hotel du Pont

EVENT	TIME	ROOM*	NOTES
On-Site Registration Open	7:30 AM - 7:30 PM	Reception Area	
Chemical Health & Safety (CHAS) How to Be a More Effective Chemical Hygiene Officer	8:30 AM - 4:00 PM	Marshall	
Exhibition	9:00 AM - 8:00 PM	Dining/Lounge Area	
Computers in Chemistry -Oral	9:00 AM - 2:00 PM	King Sejong	
ACS Undergraduate Research Symposium I Poster Session	8:30 - 10:00 AM	King/Sullivan	
ACS Undergraduate Research Symposium II Poster Session	10:00 - 11:30 AM	King/Sullivan	
Polymer, Colloid & Emulsion Chemistry - Oral	9:00 - 11:30 AM	Collins	
Nano Science, Technology & Material Science - Oral	9:00 - 11:30 AM	Piaget	
Analytical Chemistry I - Oral	8:00 - 11:30 AM	Newark	

*Rooms are subject to change

Sunday, 11 April 2010 "Tear and Take" Events held at the Hotel du Pont

EVENT	TIME	ROOM*	NOTES
ACS Undergraduate Student Luncheon	12:00 - 1:30 PM	du Barry Ballroom	
Chemistry and Law (CHAL) Your Company Fosters Innovation:	1:00 - 4:30 PM	Greenville	
Frontiers in Magnetic Resonance in Liquid & Solids - Oral	1:00 - 3:20 PM	Quintanilla	
ACS Leadership Development Course Fostering Innovation	1:00 - 5:00 PM	Montessori	
ACS Undergraduate Research Symposium III Poster Session	1:30 - 3:00 PM	King/Sullivan	
Plenary Symposium - Sustainability, Green Chemistry, & Policy	3:15 - 4:30 PM	King/Sullivan	
Reception Mixer	4:30 - 6:30 PM	Dining/Lounge Areas	
ACS Graduate & Post-Doc Research Symposium Poster Session	6:30 - 8:00 PM	King/Sullivan	

*Rooms are subject to change

Monday, 12 April 2010 "Tear and Take" Events held at the Hotel du Pont

EVENT	TIME	ROOM*	NOTES
On-Site Registration Open	7:30 AM - 7:30 PM	Reception Area	
Directors' Continental Breakfast	7:30 - 8:30 AM	du Barry Ballroom	
UD - Department of Chemistry & Biochemistry Alumni Breakfast	8:30 - 9:30 AM	Christina Room	
ACS Careers Management Workshop Planning Your Job Search	8:00 - 9:30 AM	Quintanilla	
Exhibition	9:00 AM - 8:00 PM	Dining/Lounge Area	
Chemistry & Law (CHAL): What a Chemist Needs to Know About Patent Law	9:00 AM - 1:00 PM	Greenville Suite	
Medicinal Chemistry I - Oral	9:30 - 11:00 AM	King Sejong	
Chemical Engineering II	9:30 - 11:00 AM	Knowles	
Delaware Academy of Chemical Sciences - DuPont's Textile Fiber Dept.	10:00 AM - 12:00 PM	Piaget	
ChemVets / Senior Chemist	10:00 AM - 12:00 PM	Collins	
ACS Careers Management Workshop Preparing a Resume	9:30 - 11:00 AM	Quintanilla	
ACS Careers Management Workshop Effective Interviewing	11:00 AM - 12:30 PM	Quintanilla	

*Rooms are subject to change

Monday, 12 April 2010 "Tear and Take" Events held at the Hotel du Pont

EVENT	TIME	ROOM*	NOTES
Delaware Section 50- and 60- member Luncheon	12:00 - 1:30 PM	du Barry Ballroom	
ACS Careers Management Workshop ACS Career Consultants	1:00 - 5:00 PM	Quintanilla	
Chemistry & Law (CHAL) Recent Updates in Patent Law	1:00 - 5:00 PM	Greenville Suite	
Chromatography Forum of the Delaware Valley - Student Award Symposium	1:00 - 4:30 PM	Sullivan	
IR & THz Spectrometry (oral)	1:00 - 3:00 PM	Blake	
Polymer & Nanomaterials (oral)	3:00 - 4:30 PM	Blake	
Analytical Chemistry II - Poster Session	1:00 -3:00 PM	King	
Medicinal Chemistry II - Poster Session	1:00 -3:00 PM	King	
Delaware Academy of Chemical Sciences - DuPont's Textile Fiber Dept.	2:00 - 4:00 PM	Piaget	
Happy Hour –Connolly Bove Lodge & Hutz, LLP Law Firm	5:00 – 8:00 PM	1007 N. Orange St.	Across the street from the Hotel du Pont
MARM 2010 Awards Banquet Carothers Award Lecture	5:30 - 9:30 PM	du Barry Ballroom	

*Rooms are subject to change

Tuesday, 13 April 2010 "Tear and Take" Events held at the Hotel du Pont

EVENT	TIME	ROOM*	NOTES
Environmental Chemistry	9:00 AM - 11:00 AM	Quintanilla	
Fluorine Chemistry	9:00 AM - 11:00 AM	Piaget	
Cope Scholars Symposium	9:00 AM - 12:00 PM	Knowles	
MARM Board Meeting	12:00 - 2:00 PM	Kent/New Castle	

*Rooms subject to change