Sunday, 22 May 2005

Science Education and Careers Day

Sunday, 22 May 2005, 10:00 AM - 5:00 PM

Biology

Room 202 (Science & Engineering Resource Center)

10:00  1  100 Years of Genetics William Sofer, Rutgers University
11:00  2  Streptomycin - Antibiotics from the Ground Up Douglas Eveleigh, Rutgers University
12:00  Break
1:00   3  Biology Teachers (BTANJ) Program Bunny Jaskot, Biology Teachers Association of New Jersey

Sunday, 22 May 2005, 10:00 AM - 2:30 PM

Chemistry III: Computers in Education

Room 308 (Allison Road Classroom Building)

Workshop Leader: Bettyann Howson, Chatham HS

10:00  4  Using Simulation to Teach Chemistry John Gelder, Oklahoma State University
11:30  Break
1:00   5  Powerful Powerpoint Workshop Patricia Duncan, High Point HS

Sunday, 22 May 2005, 10:00 AM - 5:00 PM

High School Student Posters & Displays

Poster Areas (Busch Campus Center)

6 Effect of Weather and Ozone Concentrations on the Occurrence of Stroke Death Akruti Bhalja, John F Kennedy Memorial High School
7 Catch Me If You Can Lina Zamamiri and Daria Bialik, Woodbridge High School
8 Energetic Light: a Chemiluminescence Reaction Robert Ngenzi, Monroe Township High School
9 Formation and Combustion of Acetylene Scott M Kaufman, Monroe Township High School
10 The Chemistry of the Oscillating Clock Reaction Simranjeet S Sran, Monroe Twp High School
11 The Spirit of Chemistry - The Catalytic Decomposition of Hydrogen Peroxide Yushen Qian, Monroe Township High School

Sunday, 22 May 2005, 10:00 AM - 5:00 PM

Math and Science Learning Center

Room 302 (Allison Road Classroom Building)

Workshop Leader: Kathy Scott, Rutgers University
10:00 12 Math and Science Learning Center Kathy Scott, Rutgers University

Sunday, 22 May 2005, 10:00 AM - 5:00 PM
Pre-College Research Posters

Poster Areas (Busch Campus Center)
13 The Effect of Different Bacterial Strains on the Lifespan of Wild-type and Mutant Nematodes Laura Toth, John F Kennedy Memorial High School
14 The Effects of Various Genres of Music on the Maze-Solving Abilities of Mus Musculus Vicky Du, John F Kennedy Memorial High School
15 The Effect of Grape Juice on the Adherence of Streptococcus mutans on Tooth Surfaces Manalika Ringshia, John F Kennedy Memorial High School
16 The Effects of the Magnetic Field on Primary Carrot Roots Kruti Sanghavi, John F Kennedy Memorial High School
17 The Effects of Ginkgo and Caffeine on Learning and Memory Nina Lee, Millburn High School
18 Altering Biomineralization Ilya Sabnani, Joanna Aizenberg and Bernice Feuer, (1)Kent Place School, (2)Bell Labs/Lucent Technologies
19 Effect of pH on Mycorrhizal Plant Growth in Two P Concentrations Mahak Jain and Joanna Kong, JFK Memorial High School
20 Link Between the Nematodes Divya Gupta, John F Kennedy Memorial High School
21 The Allelopathic Effect of Kava on Plants Waqar Tariq, John F Kennedy Memorial High School
22 The Antibacterial Effect of Mimosa tenuiflora Andrea Hodgson, John F Kennedy Memorial High School
23 Various sound effects on Wisconsin Fast Plants Charmi Shah, John F Kennedy Memorial High School
24 A Numerical Design Simulation of a Novel Notched Airfoil Jayanth Krishnamurthi, John F Kennedy Memorial High School
25 Traumatic Recall and Retention in Adolescents Barry P Shifrin, John F Kennedy Memorial High School
26 Can Cruciferous Vegetables Repair Damaged Cell Cycle Checkpoints? William J Zupko, Woodbridge High School
27 A Possible Role of Bilirubin In Inhibiting PKC Induced Vasoconstriction Sarah Arshad, John F Kennedy Memorial High School
28 Nutritional Basis of School Lunches and their Composistion Based on Present Requirements Sarah Heitmeyer Jr, John F Kennedy Memorial High School
29 A Scientific Way to Determine the Most Effective Suntan Lotion Krysten Thomas and Megan Mcdonald, Woodbridge High School
30 The Effect of Emissions of Volatile Organic Compounds on Proximate Plants Nidhi Jain, JFK Memorial High School
31 Gender Aggression in Crayfish Kerima Burdette, The Young Women's Leadership
32 High School Fitness Assessment Alycia K Ryan, The Health and Medical Science Academy at Morristown High School
33 Aloe Vera: the Green Wonder Plant Andrij O Kuzyszyn, Woodbridge High School
34 The Effects of Bathroom Cleaners on Mold Nina E Babeu, JFK Memorial High School
**Sunday, 22 May 2005, 10:00 AM - 3:30 PM**
Technology and Robotics in the High School Curriculum
**Using Technology to Inspire Students, Teachers and Mentors**

Room 117 (Science & Engineering Resource Center)
Organizer: Peter Kieselbach, Pharmacopeia Drug Discovery, Inc

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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</thead>
<tbody>
<tr>
<td>10:00</td>
<td>Introductory Remarks</td>
</tr>
<tr>
<td>10:05</td>
<td>Seeing Chemistry Non-visually; Using Talking Lab Tools to Assist a Blind Student’s Ambitions in the Laboratory <strong>Cary A Supalo</strong>, Pennsylvania State University</td>
</tr>
<tr>
<td>10:45</td>
<td>Robotics as a Vehicle to Achievement, Entrepreneurship and Higher Education <strong>Peter Kieselbach</strong>, Pharmacopeia Drug Discovery, Inc</td>
</tr>
<tr>
<td>11:15</td>
<td>Break</td>
</tr>
<tr>
<td>11:30</td>
<td>Non-Engineering Mentoring <strong>Kathie Kentfield</strong>, Co-Founder, NEMO (Non-Engineering Mentor Organization), FIRST Robotics</td>
</tr>
<tr>
<td>12:00</td>
<td>Lunch</td>
</tr>
<tr>
<td>1:00</td>
<td>FIRST Robotics in the classroom <strong>David Beck</strong>, Palisades High School</td>
</tr>
<tr>
<td>1:30</td>
<td>There's No Wrong Way To Get Involved <strong>Sabrina Marie Varanelli</strong>, Pope John XXIII Regional High School</td>
</tr>
<tr>
<td>2:00</td>
<td>Break</td>
</tr>
<tr>
<td>2:15</td>
<td>Student Mentorship of FIRST LEGO League <strong>Rebecca Kieselbach</strong>, Palisades High School</td>
</tr>
<tr>
<td>2:45</td>
<td>Life skills learned through FIRST robotics <strong>Patrick Bogard</strong>, Johns Hopkins University</td>
</tr>
</tbody>
</table>

**Sunday, 22 May 2005, 1:00 PM – 2:00 PM**
Teambuilding Workshop

Room 207 (Science & Engineering Resource Center)
Presider: Kathie Kentfield

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:00</td>
<td>Teambuilding - Getting Your Introverts to Work Together! <strong>Kathie Kentfield</strong>, FIRST Robotics Team 173 - East Hartford and Rockville High Schools</td>
</tr>
</tbody>
</table>

**Sunday, 22 May 2005, 10:00 AM - 4:15 PM**
Volcanoes of the Deep Sea

Room 118 (Science & Engineering Resource Center)
Presider: Richard Lutz, Rutgers University

<table>
<thead>
<tr>
<th>Time</th>
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<tbody>
<tr>
<td>10:00</td>
<td>Volcanoes of the Deep Sea: An IMAX Film <strong>Richard Lutz and Peter rona</strong>, Rutgers University</td>
</tr>
</tbody>
</table>

**Sunday, 22 May 2005, 11:00 AM - 12:00 PM**
Food Science

Room 208 (Science & Engineering Resource Center)

11:00 44 Food Science and Technology Geetha Ghai and Mukund Karwe, Rutgers University

Sunday, 22 May 2005, 11:00 AM - 1:00 PM
Marine and Coastal Sciences

Room 204 (Science & Engineering Resource Center)

11:00 45 The Seascape - Then and Now Gregory Mountain, Rutgers University
12:00 46 Earth System Science: In the World & In Our Classrooms Missy Holzer, NJ Earth Science Teachers Association

Sunday, 22 May 2005, 11:00 AM - 12:00 PM
Women in Pharmacy

Room 205 (Science & Engineering Resource Center)

11:00 47 Women in Pharmacy: The Pioneers Geoff W Rayner-Canham and Marelene F Rayner-Canham, Sir Wilfred Grenfell College

Sunday, 22 May 2005, 12:00 PM - 3:00 PM
Chemagination Contest

Room 210 (Science & Engineering Resource Center)
Workshop Leader: Allene Johnson, NJACS-TA

12:00 48 Chemagination Poster Allene Johnson, ACS-Teachers Affiliates

Sunday, 22 May 2005, 12:00 PM - 4:00 PM
Chemistry I

Room 208 (Science & Engineering Resource Center)

12:00 49 From Willow Bark to PolyAspirin: Discovery and Invention Kathryn E Uhrich, Rutgers University
1:00 50 From Banknotes to Diamonds: Applications of Micro Analytical Chemistry in Forensic Science Gene Hall, Rutgers University
2:00 51 Chemistry Chronicles: the life and times of undergraduate and graduate Eve L Berger, Rutgers University

Sunday, 22 May 2005, 12:00 PM - 3:00 PM
Chemistry II: Joseph Priestley in Person

Room 206 (Science & Engineering Resource Center)

12:00 52 Putting on Airs: The Life and Work of Joseph Priestley Ronald C Blatchley, Retired high school chemistry teacher
12:45 Break
2:00  53  Joseph Priestley in Person Ronald C Blatchley, Retired HS

Sunday, 22 May 2005, 12:00 PM - 2:00 PM
K-8 Science

Room 205 (Science & Engineering Resource Center)
12:00  54  Science on a Shoe String Linda Lee Smith, Paulsboro Public Schools
1:00  55  Lakewood Prep’s 7th Grade Science Curriculum: Building a Foundation for High School Science Christine Wiamer, Lakewood Prep

Sunday, 22 May 2005, 1:00 PM - 2:00 PM
Engineering

Room 204 (Science & Engineering Resource Center)
Organizer: Norman Zabusky, Rutgers University

1:00  56  The motion of matter and waves, computational science, digital technology and the arts Norman Zabusky, Rutgers University

Sunday, 22 May 2005, 1:00 PM - 7:00 PM
High School Education Posters

Poster Areas (Busch Campus Center)
Organizer: Anita J Brandolini, William Paterson University

57  Can the Health Benefits of Oatmeal be Undone? Michael Kortrey, Woodbridge High School
58  The Effect of Ginkgo Biloba on Inhibiting the Growth of Bacteria (eg bacillus megaterium, bacillus subtilis) Kelly A Bramwell, John F Kennedy HS
59  Infrared Spectroscopic and Calorimetric Analysis of Various Fuels: Structure and Efficiency Karan Chhabra and Mana Ameri, Northern Highlands Regional High School
60  The Effect of Music on Plants Infected With TMV Apurva B Sanghvi, John F Kennedy Memorial High School
61  The Effects of Different Concentrations of Pesticides on Onion DNA Payal A Patel, John F Kennedy Memorial High School

Sunday, 22 May 2005, 1:00 PM - 5:10 PM
Tech to Great

Room 203 (Science & Engineering Resource Center)
Organizer: Mary Virginia Orna, College of New Rochelle
Presider: Mary Virginia Orna, College of New Rochelle

1:00  Introductory Remarks
1:05  62  Michael Faraday, Technician Extraordinaire Mary Virginia Orna, College of New Rochelle
1:35  63  From Technician to Discoverer: the Scientific Career of Marguerite Perey  
Janan M Hayes, Merced College and Patricia Perez, Mt San Antonio College

2:05  

2:25  64  Edward Hart, from Laboratory Assistant to Editor of JACS Roger A Egolf,  
Pennsylvania State University

2:55  65  Joseph X Labovsky: a Technician at the Frontier of Polymer Chemistry Mark  
Michalovic, Chemical Heritage Foundation

3:25  66  NCTA - What Fuels all those Technician Award Winners Elizabeth Poole, Shell  
International Exploration and Production

Sunday, 22 May 2005, 3:00 PM - 4:00 PM  
Chemistry IV: A Wizard in the Classroom

Room 111 (Science & Engineering Resource Center)

3:00  67  Wizards Chemistry Show David Lee, NJACS-Teachers Affiliates

Sunday, 22 May 2005, 4:00 PM - 5:10 PM  
Physics and Astronomy  
Physics: Spectacular Physics Show

AUD (Physics)

4:00  68  Spectacular Physics Show Mark C Croft and David P Maiullo, Rutgers University
### Monday, 23 May 2005

**Monday, 23 May 2005, 8:30 AM - 12:10 PM**
Environmental/Green Chemistry

**Environmental Chemistry**

Room 218 (Science & Engineering Resource Center)

Organizers: Wen-Chung Shieh, Novartis Pharmaceuticals, Sanjay V Malhotra, New Jersey Institute of Technology

<table>
<thead>
<tr>
<th>Time</th>
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<tbody>
<tr>
<td>8:30</td>
<td>Introductory Remarks</td>
</tr>
<tr>
<td>8:35</td>
<td>69 Greening the chemistry curriculum <strong>Mary M Kirchhoff</strong>, American Chemical Society</td>
</tr>
<tr>
<td>9:05</td>
<td>70 Structure-Property Relationships in Ionic Liquids: Rebuilding Chemical Intuition <strong>Mark N Kobrak</strong>, Brooklyn College -- CUNY</td>
</tr>
<tr>
<td>9:25</td>
<td>71 The Greening of the Chemical Engineering Curriculum: From Green Stoichiometry to Life Cycle Assessment <strong>Daniel Fichana</strong>, Robert P Hesketh and C Stewart Slater, Rowan University</td>
</tr>
<tr>
<td>9:45</td>
<td>72 Large Area &quot;Mud Batteries&quot; to Power In-Situ Sensors <strong>Gregory A Konesky</strong>, ATH Ventures, Inc</td>
</tr>
<tr>
<td>10:05</td>
<td>Break</td>
</tr>
<tr>
<td>10:20</td>
<td>73 Analysis of trace elements and heavy metals in fish otoliths as tracers of habitat use <strong>Zikri Arslan</strong>, Jackson State University and David H Secor, University of Maryland Center for Environmental Science</td>
</tr>
<tr>
<td>10:40</td>
<td>74 Model Complexes of Anaerobic Sulfate-Reducing Bacteria <strong>Karen R Hatwell</strong>, Villa Julie College and Jonathon Elmer, Swarthmore College</td>
</tr>
<tr>
<td>11:00</td>
<td>75 Grass Fights Back <strong>Yves A Javier</strong> and Katherine Wysoczanski, Woodbridge High School</td>
</tr>
<tr>
<td>11:20</td>
<td>76 Green Electrical Energy from Marine Microbial Biofuel Cells <strong>Gregory A Konesky</strong>, ATH Ventures, Inc</td>
</tr>
</tbody>
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**Monday, 23 May 2005, 8:30 AM - 12:00 PM**

**Biomaterials and Polymers**

**Symposium: Polymeric Biomaterials**

**Nanoparticles, Microparticles and Vesicles**

Room 205 (Science & Engineering Resource Center)

Organizer: Kathryn E Uhrich, Rutgers University

Presider: Dennis E Discher, University of Pennsylvania

<table>
<thead>
<tr>
<th>Time</th>
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<tr>
<td>8:30</td>
<td>77 Stealth Polymeric Nanoparticles for Drug Delivery Devices <strong>Emmanuel O Akala</strong>, Oluymoi Okunola and Gaofeng Pan, School of Pharmacy, Howard University</td>
</tr>
<tr>
<td>9:00</td>
<td>78 Encapsulation of Drug Nanoparticles in Self-Assembled Macromolecular Nanoshells <strong>Michael Pishko</strong>, Alisar Zahr and Cheryl Rumbarger, Penn State University</td>
</tr>
<tr>
<td>9:30</td>
<td>79 Polymersomes &amp; related Nanotransforming Carriers for Drug Delivery <strong>Dennis Discher</strong>, Univ Pennsylvania</td>
</tr>
</tbody>
</table>
10:00 Break

10:30  80 In Vivo and In Vitro Elution of NSAID and Drugs from Self-Delivering PolyNSAIDs Microspheres Yun H Choe, Zheng Wang, Bryant J Pudil, Michael B Hicks, Suseela Kanamathareddy, Stephen Goodrich and Alan Letton, Polymerix Corporation

10:45  81 Degradable Polymersomes Foster Endosomal Release and Delivery of Cytotoxic Drugs to Cancer Cells Fariyal Ahmed, Goundla Srinivas, Michael L Klein and Dennis Discher, Univ Pennsylvania

11:00  82 Formation of Polymersomes by Microfluidics M Erhan Yildiz1, Elise Lorenceau2, Andrew S Utada2, David A Weitz2, Robert K Prud'homme1 and Douglas H Adamson1, (1)Princeton University, (2)Harvard University

11:15  83 Degradable Polymeric Worm Micelles for Drug Delivery Yan Geng, University of Pennsylvania, Larry Romsted, Rutgers University and Dennis Discher, Univ Pennsylvania

11:30  84 Multifunctional Non-Viral Condensing Agent for Gene Delivery Alex M Chen1, Latha M Santhakumaran2, Sandhya K Nair2, Thresia Thomas2, T J Thomas2 and Huixin He1, (1)Rutgers University, (2)UMDNJ-Robert Wood Johnson Medical School


Monday, 23 May 2005, 8:50 AM - 12:05 PM
Organic Chemistry
Symposium: Bench Top To Pilot Plant
Bench Top to Pilot Plant I

Room 111 (Science & Engineering Resource Center)
Organizers: Ambarish Singh, Bristol-Myers Squibb Company, Shankar Swaminathan, Bristol-Myers Squibb

8:50 Welcoming Remarks

9:00  86 Evolution of Process R&D as we enter the 21st century Mauricio Futran, Bristol-Myers Squibb

9:50  87 Synergy-Chemists and Chemical Engineers From Bench To Scaleup Operations Raghavan Krishnan, Wyeth Research

10:15 88 Micro Reactors: New Technology for Chemical Synthesis and Drug Discovery Paul Watts, University of Hull

10:50 89 Bench Top Flow Reaction Optimization Mike C Hawes, Syrris Ltd

11:15 90 Continuous Processing from Lab to Pilot Plant for Intermediates and API Thomas La Porte, Chenchi Wang and Mourad Hamedi, Bristol-Myers Squibb

11:40 91 Scaling up Microwave Reactions: An Overview of the Advancer Joseph M Pawluczyk, Merck & Co

Monday, 23 May 2005, 8:50 AM - 12:00 PM
Physical Chemistry
Symposium: Spectroscopy of Biomolecules, Interfaces and Materials
Spectroscopy of Biomolecules, Interfaces, and Materials I

Room 207 (Science & Engineering Resource Center)
Organizer: Edward, W Castner, Rutgers University
Presider: Edward, W Castner, Rutgers University

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<tr>
<td>8:50</td>
<td>Introductory Remarks</td>
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<tr>
<td>9:20</td>
<td>Understanding the folding mechanism of beta-hairpins Feng Gai, University of Pennsylvania</td>
</tr>
<tr>
<td>9:00</td>
<td>Wetting and Diffusion Phenomena in Hydrophobic Silica Nanotubes and Nanotube Membranes Karthik Jayaraman, Kenji Okamoto, Sang Jun Son, Charles Luckett, Sang Bok Lee and Douglas English, University of Maryland CollegePark</td>
</tr>
<tr>
<td>10:00</td>
<td>Break</td>
</tr>
<tr>
<td>10:30</td>
<td>Two dimensional infrared spectroscopy of biologically relevant systems Robin M Hochstrasser, University of Pennsylvania</td>
</tr>
<tr>
<td>11:30</td>
<td>Microviscosity and solvation dynamics in non-ionic surfactant PEO-PPO-PEO triblock copolymer aggregates Christian D Grant, Karen Steege, Tania Fadeeva and Edward W Castner Jr, Rutgers, The State University of New Jersey</td>
</tr>
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**Monday, 23 May 2005, 9:00 AM - 12:00 PM**
College Education
Symposium: About the General Chemistry Laboratory
*About the General Chemistry Laboratory I*

Room 209 (Science & Engineering Resource Center)
Organizer: Rudolph W Kluiber, Rutgers University

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<tr>
<td>9:00</td>
<td>Density and Coulomb's Law: Two Under-Utilized Concepts in General Chemistry Parinbam (RAJ) K Thamburaj, Ohio University- Zanesville</td>
</tr>
<tr>
<td>9:25</td>
<td>The Myers-Briggs Type Indicator (MBTI): a matrix for evaluating effective alternative teaching methods with diverse student populations Victoria Finkenstadt, Illinois Heartland ACS and Sheryl L Finkenstadt, Bridgeway Counseling Services</td>
</tr>
<tr>
<td>9:50</td>
<td>Determination of the Ionization Constant of Weak Carboxylic Acids Using Computer Interface Freezing Point Depression Measurements Imranul Haque, Paris Svoronos and Pedro Irigoyen, Queensborough Community College</td>
</tr>
<tr>
<td>10:15</td>
<td>Microscale Experiments for the General Chemistry Laboratory Arden P Zipp, Marcia Bonneau and Irene Maffetore, SUNY College at Cortland</td>
</tr>
<tr>
<td>10:40</td>
<td>A Freshman Level Capstone Experiment with an Environmental Forensic Twist Liina H Ladon, Laurence J Boucher, Alan J Pribula and Joseph J Topping, Towson University</td>
</tr>
<tr>
<td>11:05</td>
<td>Using Software to Simplify Grading Labs and Making Pre-Labs Charles H Mahler, Lycoming College</td>
</tr>
<tr>
<td>11:30</td>
<td>Economies of Scale: Bio, Materials, and Environmental Sections of General Chemistry Lab Joseph T Keiser, Penn State University</td>
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**Monday, 23 May 2005, 9:00 AM - 12:00 PM**
Computers in Chemistry
Symposium: Bioinformatics
*Bioinformatics*

Room 217 (Science & Engineering Resource Center)
Organizer: Nichols Murgolo, Schering-Plough Research Institute
Presider: Nichols Murgolo, Schering-Plough Research Institute

9:00 Welcoming Remarks
9:05 103 Ezetimibe mechanism of action: what did we learn from gene chips? Jeffrey Yuan¹, Diane Shevell¹, Peter S Linsley², Patricia A Detmers¹ and John R Thompson¹,
(1)Merck and Co, Inc, (2)Rosetta Inpharmatics, a wholly owned subsidiary of Merck & Co, Inc
9:45 104 Phylogenetic Analysis and Classification of Human Protein Kinases Targeting the ATP Binding Site Philip W Mui, Glaxo SmithKline
10:25 Break
10:40 105 Phenotype Mapping of Genes Qing Zhang, Schering Plough Research Institute
11:20 106 Identification of tumor associated SNPs based on EST analysis Wei Ding¹, Mitch Kostich², Luquan Wang³, Ping Qiu¹, Jonathan Greene¹ and Marco Hernandez¹,
(1)Schering-Plough Research Institute, (2)Environmental Protection Agency, (3)GenScript Corporate

Monday, 23 May 2005, 9:00 AM - 12:05 PM
Analytical Chemistry Frontiers
Symposium: Biomarkers: Quantification, PK/PD Correlation and Bioanalytical Issues
Room 117 (Science & Engineering Resource Center)
Presider: Michael Hayes, Novartis Pharmaceuticals

9:00 Welcoming Remarks
9:05 107 Navigating the Shoals of Biomarker Assays Brian Swanson, Sanofi Avantis Pharmaceuticals
9:50 108 Discovery, Identification and Quantitation of Biomarkers using iTRAQ™ Reagent Technology Lynn Zieski, Applied Biosystems Corporation
10:35 109 Development and validation of analytical methods to measure biomarkers in drug development Francois Legay, Novartis Pharma AG
11:20 110 Probing Aging in Zucker Rats Using Ultra Performance Liquid Chromatography Coupled to Time of Flight Mass Spectrometry John Shocklor, Waters Corporation

Monday, 23 May 2005, 9:00 AM - 12:45 PM
Biological Chemistry
Symposium: DNA Gadgets: Making Novel Use of the Physico-chemical Properties of DNA
Room 202 (Science & Engineering Resource Center)
Organizers: Nadrian C Seeman, New York University, Wilma K Olson, Rutgers University
Presider: Wilma K Olson, Rutgers University

9:00 111 DNA: Not Merely the Secret of Life Nadrian C Seeman, Shiping Liao, Baoquan Ding, William B Sherman, Tong Wang, Pamela E Constantinou, Jens Kopatsch, Ruojie Sha and Philip S Lukeman, New York University
9:35  112 DNA Machines Chengde Mao, Yi Chen, Ye Tian and Seung-Hyun Lee, Purdue University

10:10  113 Engineering DNA Motors and Sensors Niles A Pierce, California Institute of Technology

10:45  114 Nucleation and Stability of Nanotubes from DNA Tiles Ashish Kumar, Axel Ekani-Nkodo*, Armand Vartanian and Deborah K Fygenson, University of California, Santa Barbara

11:20  115 DNA-crosslinked gels Bernard Yurke1, David C Lin2 and Noshir A Langrana2, (1)Bell Laboratories/Lucent Technologies, (2)Rutgers University

11:55  116 DNA as the Raw Material for General-purpose Electrical Biosensors Dipankar Sen, Richard Fahlman, Carlo Sankar and Edward Leung, Simon Fraser University

Monday, 23 May 2005, 9:00 AM - 12:00 PM
Biomaterials and Polymers
Symposium: Inorganic and Organometallic Polymers
Inorganic and Organometallic Polymers I

Room 206 (Science & Engineering Resource Center)
Organizer: Frieder Jaekle, Rutgers University
Presiders: John B Sheridan, Rutgers University, Bhanu P S Chauhan, Nanomaterials Laboratory of Center for Engineered Polymeric Materials, City University of New York at CSI

9:00  Welcoming Remarks

9:10  117 New Hybrid Polymer Systems and Materials Harry R Allcock, The Pennsylvania State University

9:40  118 Design, Syntheses and Materials Applications of Organodecaborane Polymers Larry G Sneddon, Xiaolan Wei, Mark Pender, Kersten Forsthoefel, Upal Kusari and Chang Won Yoon, University of Pennsylvania

10:10  119 New Routes to Boron Containing Polymeric Lewis Acids Frieder Jäkle, Rutgers University

10:40  Break

11:00  120 Polycarbosilanes – Hybrid Inorganic/Organic Polymers Leonard V Interrante, Rensselaer Polytechnic Institute

11:30  121 Silsesquioxane based Inorganic Organic Hybrid Copolymers E Bryan Coughlin, University of Massachusetts Amherst

Monday, 23 May 2005, 9:00 AM - 12:00 PM
Medicinal Chemistry
Symposium: Kinase / Virtual Screening
Kinase / Virtual Screening

Room 203 (Science & Engineering Resource Center)
Organizer: Robert Goodnow Jr, Hoffmann-La Roche
Presiders: Dorothy Kominos, Sanofi-Aventis, Paul Cox, Sanofi-Aventis

9:00  Dorothy Kominos & Paul Cox
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<tr>
<td>9:05</td>
<td>122</td>
<td>Development of Aniline amides Containing Alternative Cores as Orally Active P38 MAP kinase Inhibitors <strong>Katerina Leftheris</strong>, John Hynes, Jr, Alaric Dyckman, Tianle Li, Shuqun Lin, Stephen T Wroblewski, Hong Wu, Rosemary Zhang, Kathleen M Gillooly, Derek Loo, Kim W McIntyre, Sidney Pitt, Ding Ren Shen, David J Shuster, Arthur Doweyko, John Sack, Joel Barrish, John Dodd and Gary L Schieven, Bristol-Myers Squipp</td>
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</tr>
<tr>
<td>9:35</td>
<td>123</td>
<td>Inhibitors of mitogen-activated protein (MAP) kinases synthesized by parallel solution- and solid-phase methods <strong>Jeremy Green</strong>, Vertex Pharmaceuticals</td>
<td></td>
</tr>
<tr>
<td>10:05</td>
<td>124</td>
<td>Design, Synthesis and SAR of Pyrimidopyrimidines, Dual KDR/FGFR TyrosineKinase Inhibitors <strong>Pamela Rossman</strong>, Hoffmann-La Roche</td>
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<td>10:35</td>
<td></td>
<td>Coffee Break</td>
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<tr>
<td>11:30</td>
<td>126</td>
<td>Discovery of novel p38 MAP kinase inhibitors: <strong>Gulzar Ahmed</strong>, Pharmacopeia Drug Discovery Inc</td>
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**Monday, 23 May 2005, 9:00 AM - 12:10 PM**
Medicinal Chemistry
Symposium: Pharmaceutical Profiling
**Pharmacetical Profiling I**

Room 118 (Science & Engineering Resource Center)

Organizer: Edward H Kerns, Wyeth Research
Presider: Edward H Kerns, Wyeth Research

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<td>9:00</td>
<td>127</td>
<td>Overview of Pharmaceutical Profiling in Drug Discovery <strong>Edward H Kerns</strong>, Wyeth Research</td>
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<tr>
<td>9:15</td>
<td>128</td>
<td>In Silico Model for CYP Inhibition <strong>Roy J Vaz</strong>, Sanofi Aventis Pharmaceuticals</td>
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<tr>
<td>9:55</td>
<td>129</td>
<td>Deciphering the Role of Drug Transporters in Early Drug Development: Cell Culture Models and Approaches <strong>Patrick Sinko</strong>, Rutgers University</td>
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<td>10:35</td>
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<td>Break</td>
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<tr>
<td>10:50</td>
<td>130</td>
<td>Biochemical and Molecular Assays In Early Toxicity Assessments: A Tier Approach <strong>Prathibha S Rao</strong>, sanofi-aventis</td>
<td></td>
</tr>
</tbody>
</table>
Monday, 23 May 2005, 9:00 AM - 12:00 PM  
Nato and Materials Science  
Symposium: Solid State and Materials Chemistry  
**Solid State and Materials Chemistry I**

Room 204 (Science & Engineering Resource Center)  
Organizers: Jing Li, Rutgers, The State University of New Jersey, Martha Greenblatt, Rutgers, The State University of New Jersey  
Presiders: Jing Li, Rutgers, The State University of New Jersey, Martha Greenblatt, Rutgers, The State University of New Jersey

9:00  132  Chemistry and Physics of Semiconductor Nanocrystals **Louis E Brus**, Columbia University  
9:30  133  Solid state chemistry of biological glass fibers **Joanna Aizenberg**, Bell Labs/Lucent Technologies  
10:00  134  Wide bandgap II-VI nanostructures for intersubband devices **Maria C Tamargo**, The City College of New York  
10:30  Break  
11:30  136  High Porosity TiO2 via Inorganic- Salt Porogens **Charlie C Torardi**¹, C Roger Miao¹, C Ed Greer¹ and John Gavenonis², (1)DuPont Central Research and Development, (2)DuPont Titanium Technologies

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**Monday, 23 May 2005, 9:00 AM - 12:00 PM**  
**Small Chemical Business**  
**Symposium: Strategies for Growth: How a “Small” Company can become a “Big” Player**

Room 212 (Science & Engineering Resource Center)  
Organizers: Mary Catherine Dinunzio, Stroock & Stroock & Lavan LLP  
Presiders: Matthew L Wotiz, Lundbeck, Inc  
Matthew R Rothman, EuclidSR Partners  
Todd Burns, Johnson & Johnson  
Kathleen W Scotto, The University of Medicine and Dentistry of New Jersey

9:00  137  IP Assets – Springboards for Success **Mary Catherine Dinunzio**, Stroock & Stroock & Lavan LLP  
9:45  138  Growing Your Business by Partnering with Industry **Matthew L Wotiz**, Lundbeck, Inc  
10:15  139  Venture Capital – Securing Needed Funds **Matthew R Rothman**, EuclidSR Partners  
10:45  140  Attracting Investment from Large Pharma **Todd Burns**, Johnson & Johnson  
11:15  141  Growing Your Business by Partnering with Universities **Kathleen W Scotto**, The University of Medicine and Dentistry of New Jersey

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**Monday, 23 May 2005, 9:00 AM - 12:00 PM**  
**Organic Chemistry**  
**Total Synthesis/Synthetic Methodology**

Room 216 (Science & Engineering Resource Center)  
Organizer: Cecilia H Marzabadi, Seton Hall University  
Presider: Michael James Konkel, Lundbeck Research, USA
9:00  142  From deep-sea sponge to pilot plant: The large scale total synthesis of the marine natural product (+)-Discodermolide Stuart J Mickel, Novartis Pharma AG

9:40  143  The Furan Approach to the Synthesis of the A-rings of Vitamin D and Calcitriol William H Miles, Katelyn B Connell, Gözde Ulas, Hannah H Tuson, Elizabeth A Dethoff, Varun Mehta and April Thrall, Lafayette College

10:00 144  A Total Synthesis of Epoxomicin Sreenivas Katukojvala, Kristin N Barlett, Stephen D Lotesta and Lawrence J Williams, Rutgers University


10:40 146  Chelation-Controlled Diasteroselective Reduction of 2-Fluoroketones Pramod K Mohanta, Todd A Davis and Robert A Flowers II, Lehigh University

11:00 147  Sequential Birch reduction-allylation/Cope rearrangement for the enantioselective construction of carbocyclic quaternary stereogenic centers William Malachowski, Bryn Mawr College

11:20 148  Improving the Value of HTS Peter Kotsonis, Novartis Institute for Biomedical Research

11:40 149  Process Development and Synthesis of the β-1,3-Glucan Synthase Inhibitor Cancidas® Kevin M Belyk, William R Leonard Jr, David A Conlon, Ji Liu, Dean Bender and David L Hughes, Merck Research Laboratories

Monday, 23 May 2005, 9:00 AM - 12:00 PM
Inorganic Chemistry
Transition Metal Chemistry and Catalysis

Room 208 (Science & Engineering Resource Center)
Organizer: Alan S Goldman, Rutgers University

9:00  150  Steric Effects on the Kinetics of the Reductions of some Tetrakis(arylisocyanide)cobalt(II) complexes by pyridine in Trifluoroethanol Medium Olayinka A Oyetunji, Banyaladzi D Paphane and Clifford AL Becker, University of Botswana

9:20  151  A Series of Iron and Osmium Pincer Complexes Elizabeth M Pelczar, Thomas J Emge and Alan S Goldman, Rutgers, The State University of New Jersey

9:40  152  Selective cleavage of the C-C bond of aminoethyl groups by a pincer iridium complex Xiawei Zhang¹, Thomas J Emge², Rajshekhar Ghosh² and Alan S Goldman², (1)Cornell University, (2)Rutgers University

10:00 153  Mechanistic study of acetylene dimerization: insertion of phenylacetylene into Ir-H versus Ir-C bonds Rajshekhar Ghosh, Xiawei Zhang, Thomas J Emge and Alan S Goldman, Rutgers University

10:20 154  Selective activation of aryl and vinyl C-H bonds adjacent to coordinating groups Not chelation-assisted Xiawei Zhang, Patrick D Achord, Thomas J Emge, Mira Kanzelberger, Karsten Krogh-Jespersen and Alan S Goldman, Rutgers University

10:40 155  Metalloaromaticity: Novel examples and an unexpected role in the site-selective functionalization of C-H bonds by ruthenium complexes Patrick D Achord, Xiawei Zhang, Karsten Krogh-Jespersen and Alan S Goldman, Rutgers University

11:00 156  Coordination Structural Shifts and Oxidation State Control in Dinuclear Complexes Yilma Guiltneh¹, Yohannes, T Tesema¹, Teshome B Yisgedu¹, Raymond J Butcher¹,
Guang-bin Wang³ and Gordon Yee³, (1)Howard University, (2)Virginia Polytechnic Institute and State University

Monday, 23 May 2005, 9:00 AM - 12:00 PM
ADMET at the Crossroads of Drug Discovery
Symposium: Transporters

Transporters

Room 210 (Science & Engineering Resource Center)
Workshop Leader: Jerome H Hochman, Merck and Co

9:00
9:15  157 Perspectives into the Molecular and Functional Characteristics of Intestinal Oligopeptide Transporters Gregory T Knipp, Rutgers, the State University of New Jersey
9:45  158 Application of drug transport studies to drug discovery and development Masayo Yamazaki, Merck and Co
10:15 159 Role of Hepatic Transporters in the Disposition of Rosuvalstatin Liyue Huang, AstraZeneca
10:45
11:00 160 Functional Characterization of a Hepatic Organic Anion Transport Model; OATP1B1 and MRP2 Double Transfected MDCKII cells Kelly Bleasby, Richard Edom and Raymond Evers, Merck and Co
11:30 161 Towards an understanding of organic anion transporters: structure-function relationships Guofeng You, Rutgers University

Monday, 23 May 2005, 9:00 AM - 1:30 PM
College Education
Undergraduate Poster Session

Poster Areas (Busch Campus Center)
Organizer: Susan Ensel, Hood College

Set-up 8:30-9:00
Authors at their posters 11:00 - 1:00

162 Saliva of Humans and Animals as an Alternative Biofluid for NMR-Based Metabonomic Investigations and Diagnostics Teresa A Soroka¹, István Pelczer¹, Sarah Ralston² and Elissa Lappostato², (1)Princeton University, (2)Rutgers University

163 Determining the Preferential Interaction Parameter: A Study of Salt Effects on DNA Oligonucleotides Erica R Bush and A P Williams, Princeton University

164 DNA Oligonucleotide Functionalized γ-Fe₂O₃ Core/Au Shell Nanoparticles as a Means of Selective Magnetic Separations of Mixtures of DNA Rebecca A Grimme¹, John N Richardson¹ and Mary Elizabeth Williams², (1)Shippensburg University of Pennsylvania, (2)The Pennsylvania State University

165 Interaction of N-methylmesoporphyrin IX NMM with Quadruplex DNA formed from Scerevisiae Telomeric Sequences Erum Azeez and Mahrukh Azam, West Chester University
166 Liposomes within Giant Vesicles: Methods of Preparation and Characterization Laura Elbakry, Shaila Zaman, Dwight Campbell and Sergey V Kazakov, Pace University

167 Time Resolved Exchange of Protons in Polymer Networks Korki M Miller and Sergey V Kazakov, Pace University

168 Probing the Interactions of a Guanidinium Ion with Water John Landers and Margaret Mandziuk, Manhattan College

169 Mycotoxin: An FDA Concern Jian Yang, Paris Svoronos, Kathryn Emanuele and Vincent DiProssimo, (1)Queensborough Community College, (2)Food and Drug Administration

170 Exploring Protein Structure in a Biochemistry Laboratory Experiment Lisa Christadore, Dean Del Geurcio and Amber Flynn Charlebois, (1)Loyola College, (2)William Paterson University

171 Synthesis of Amino Acid Derivatives of Flavins Karen R Hatwell, Anthony A Debraccio, Jeanette M Krug and Kimberly L Still, Villa Julie College

172 Amination of a Flavin Compound Karen R Hatwell, Tamara C Ford, Nicole A Hammerbacher and Justin W Young, Villa Julie College

173 Computational Prediction of Spontaneous Thermal Resolution in Racemic Biaryl Atropisomers Japheth Demetria, King Tse and Dale E Vitale, Kean University

174 Electronic and Geometric Effects of the Cyclopropyl Group in Liquid Crystal Formation Gretchen E Repaal and George Lorenzo, Eastern University

175 Reductive Isopropylation of Ethanolamine Followed by Condensation with Aldehydes: Observation of Enantiotopic and Diastereotopic Nuclei in the $^1$H and $^{13}$C NMR Spectra of Achiral and Chiral Oxazolidines Shahrokh Saba, Jennifer Espinal, James A Ciaccio and Courtney E Aman, Fordham University

176 Synthesis and Solution Property Study of Amphiphilic Star-shaped Macromolecules Anthony A Argenti, Kelly Chang, Jinzhong Wang and Kathryn E Uhrich, Rutgers University

177 Alternate Method for the Synthesis of Salicylate-Based Poly(Anhydride-Ester) Precursors Kelly Chang and Kathryn Uhrich, Rutgers University

178 Reactivity of Tri(trimethylsilyl)phosphite: Reaction with alpha-lactam Jian Yang, Ralph Stephani and Luis Vargas, (1)Queensborough Community College, (2)St John’s University

179 The Reaction of Triethylamine with Hexachloroacetone: Synthesis, Structure, Characterization and Mechanistic Study of trans-1,1,1-Trichloro-4-N,N-Dimethylamino-3-Buten-2-One Ji In Kang and Jun H Shin, Queensborough Community College

180 Selectfluor Mediated Rearrangements of Azabicyclic Halides: Ring Size, Halide, and Positional Effects on Neighboring group Participation Ryan A Centafont, Grant Krow and Deepa Rapolu, Temple University


182 Carbamate Pesticide Decomposition Using UV-Vis Spectroscopy Christopher Divito and Clare N Muhoro, Shippensburg University

183 Solvent-Free Malonic Ester Synthesis by Mechanochemical Methods Tristan E Colestock and Joel M Ressner, West Chester University

184 Using NMR Spectroscopy to "Discover" Organic Chemistry Megan James, Holly Haley and Susan Ensel, Hood College

185 Determination of the Isoelectric Point of Various Amino Acids in Aqueous Solutions Using $^{13}$C NMR Spectroscopy Sabrina M Song, Jun H Shin and Gopal Subramaniam, (1)Queensborough Community College, (2)Queens College
186 Computation of Organic Carbon Acids Daqing Gao, Paris Svoronos, Tianchu Xu and Debbie Maddlena, Queensborough Community College

187 Investigation of the Composition of a Prescription Brand Drug vs Its Generic Using HPLC Elizabeth P Crowe, Sarah Crowe and Kathryn A Lysko, Immaculata University

188 Comparison of the Degree of Hotness of Various Hot Peppers using HPLC (High Pressure Liquid Chromatography) Tolulope Falope, Paris Svoronos and Pedro Irigoyen, Queensborough Community College

189 Free Radical Chlorination of Benzyl Hydrogens Hector Mavromatis¹, Sasan Karimi¹, Pedro Irigoyen¹, Paris Svoronos¹ and David Locke², (1)Queensborough Community College, (2)Queens College

190 Synthesis of New Types of Quaternary Ammonium Ionic Liquids Heidi Martinez¹, Hughton Walker², Vanessa Hernandez³, Robert Engel² and Sharon Lall-Ramnarine¹, (1)Queensborough Community College, CUNY, (2)Queens College, CUNY

191 Synthesis of ionic liquids containing ether and hydroxyl substituted cations Kijana Kerr¹, Hughton Walker², Vanessa Hernandez³, Robert Engel² and Sharon Lall-Ramnarine¹, (1)Queensborough Community College, CUNY, (2)Queens College, CUNY

192 Synthesis and characterization of chiral ionic liquids Marie Thomas¹, Jasmine Hatcher², Leah Rothman¹, Sharon Lall-Ramnarine² and Robert Engel¹, (1)Queens College, CUNY, (2)Queensborough Community College, CUNY

193 Investigation of the Structure/Property Relationship of New Ionic Liquids Hughton R Walker¹, Marie Thomas¹, Vanessa Hernandez³, Sofiya Penkhasova², Heidi Martinez², Kijana Kerr², Jasmine Hatcher², Robert Engel¹ and Sharon Lall-Ramnarine², (1)Queens College, CUNY, (2)Queensborough Community College, CUNY

194 Investigation of the effect of anion variation on physical properties of new ionic liquids Vanessa Hernandez¹, Hughton R Walker², Sofiya Penkhasova¹, Robert Engel² and Sharon Lall-Ramnarine¹, (1)Queensborough Community College, CUNY, (2)Queens College, CUNY

195 Characterization of the physical properties of new ionic liquids Sofiya Penkhasova¹, Hughton R Walker², Heidi Martinez¹, Jasmine Hatcher¹, Vanessa Hernandez¹, Robert Engel² and Sharon Lall-Ramnarine¹, (1)Queensborough Community College, CUNY, (2)Queens College, CUNY

196 Synthesis of G3 PPI Dendrimer Encapsulated Ag Nanocomposites and Their Potential Applications in the Condensation of DNA Jowairia Chaudhry Jr, Alex Chen and Prof Huixin He, Rutgers University, Newark Campus

197 Thermal and Infrared Analysis of Cyanogels Kristin Lammers¹, S A Gould², A B Bocarsly² and G A Arbuckle-Keil¹, (1)Rutgers, The State University of New Jersey, (2)Princeton University

198 Origin of Fine-structure in Absorption Spectra of Cyanine Dyes Anna Zarow and Yeung-gyo Shin, Kean University

199 Detecting Phase Transitions in Triblock Copolymers Using Solvatochromic Dyes David J Sierra Jr, Edward W Castner, Jr, Christian D Grant and Hideaki Shirota, Rutgers, The State University of New Jersey

200 Ultra-sensitive Detection of a Neurotransmitter (Dopamine) Shah R Ali, Yufeng Ma and Huixin He, Rutgers University

201 Surface-Enhanced Raman Scattering Studies of Molecules Adsorbed on Gold, Silver and Copper Nanoparticles Boon Loo¹, Steve Tse¹, Wendy Mays¹, Nicole Loo² and Nordulf Debye¹, (1)Towson University, (2)Rice University

202 Reaction pH and the Evolution of Polyaniline Nanofibers Erika Feldeshi and David M Sarno, Queensborough Community College / CUNY
203 Effect of Dopant Cycling on Polyaniline Nanofiber Morphology Adina Hodes and David M Sarno, Queensborough Community College / CUNY

204 Degradation Media Composition Analysis of Salicylic Acid-Based Poly(Anhydride-Esters) Vivian Ng, Almudena Prudencio and Kathryn Uhrich, Rutgers University

205 The PolymIR Library: Development of a Web-Based Resource Anita J Brandolini, Noelle DeStefano, Betsy Huerta and Kevin Lemire, William Paterson University

206 An Indirect Determination of Sulfate by Back-Titration of Barium with EDTA Gregory S Kowalczyk and Christopher P Simpson, Southern Connecticut State University

207 SPE and HPLC Method for the Determination of Aspirin, Acetaminophen, and Caffeine in Aqueous Environmental Samples Scott LeFevre and Stephen C Waller, Fairleigh Dickinson University

208 Statistical Evaluation of Acid Indicators Seth A Elwood, Carolyn Supplee, Jenna Case, Marie Ineus and Lisa Salvemini, Monmouth University

209 Using Differential Scanning Calorimetry (DSC) in a General Chemistry Laboratory Course Ronald P D'Amelia, Thomas Franks and William F Niore, Hofstra University

210 Correlation of the van’t Hoff Factor with the Concentration of Inorganic Solutes Using Computer Interface Freezing Point Depression Measurements Jorge Ubilus, Pedro Irigoyen and Paris Svoronos, Queensborough Community College

211 A Computational Chemistry Research Program at Community College Level Daqing Gao, Sanwal Mushtaq, Hilda Dan-Archibong and Pochou Chen, Queensborough Community College

212 Philadelphia CSI vs CBS CSI Stacy A Gibbs, Community College of Philadelphia

213 Why College Freshman Believe Biology Is Easier Then Chemistry and How to Debunk the Myth Stacy A Gibbs, Community College of Philadelphia

214 Student Affiliate Chapters at Community Colleges Stacy A Gibbs, Community College of Philadelphia

215 Reviving an Ailing Student Affiliate Chapter: Community College of Philadelphia Stacy A Gibbs and Christa Nolsoe, Community College of Philadelphia

Monday, 23 May 2005, 12:00 PM - 1:30 PM
Student Affiliate Chemistry Outreach

Room 260 (Wright Lab)
Workshop Leader: Julius M Johnson, Rutgers University Chemistry Society

12:00 216 Student Affiliate Outreach -Chemical Demonstration Forum Julius M Johnson, Rutgers University Chemistry Society

Monday, 23 May 2005, 1:00 PM - 5:00 PM
College Education Symposium: About the General Chemistry Laboratory About the General Chemistry Laboratory II

Room 209 (Science & Engineering Resource Center)
Organizer: Rudolph W Kluiber, Rutgers University

1:00 217 Keynote Address: Is the Textbook Dead? John C Kotz, SUNY-Oneonta
1:50  218  Does the chemistry teaching laboratory have a future? Melanie M Cooper, Clemson University

2:35  219  Using Technology to Teach: Are Lab Instructors Really Needed? Rudolph W Kluiber, Rutgers University

3:15  220  Million Dollar Data: Students constructing confidence in the laboratory Stephen DeMeo, Hunter College of the City University of New York

3:45  221  Undergraduate Research Center for Chemistry & Closely Allied Fields Margaret Czerw1, Gregory F Herzog2, John Krenos2, Joseph A Potenza2, Paul Schueler1 and Diane C Trainor3, (1)Raritan Valley Community College, (2)Rutgers University, (3)Middlesex County College

4:10  222  A One Semester First Year Seminar: An Interdisciplinary Study of the SARS Virus Julie B Ealy, Penn State University

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Monday, 23 May 2005, 1:00 PM - 5:00 PM
Careers For Chemists
Careers Workshops

Exploring Routes for Becoming a HS/MS Teacher

Room 115 (Busch Campus Center)
Workshop Leader: Anita J Brandolini, William Paterson University

1:00  223  Exploring Routes for Becoming a HS/MS Teacher Panel Discussion Anita J Brandolini, William Paterson University

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Monday, 23 May 2005, 1:00 PM - 4:00 PM
Medicinal Chemistry
Symposium: GPCR / Virtual Screening

GPCR / Virtual Screening

Room 203 (Science & Engineering Resource Center)
Organizer: Robert Goodnow, Hoffmann-La Roche
Workshop Leader: Dr Shawn Erickson, Hoffmann-La Roche

1:00  Introductory Remarks Shawn Erickson

1:05  224  Ligand Twisting and Counterion Switching in Rhodopsin Activation Thomas P Sakmar, The Rockefeller University

1:35  225  Using Designed Peptide Panels for De-risking GPCR Projects Waleed Danho, Hoffmann-La Roche

2:05  226  GPCR Ligands from Enzyme Targeted Libraries Michael Ohlmeyer, Pharmacopeia

2:35  Coffee Break

3:00  227  Discovery and Development of the First Centrally Active mGluR5 Positive Allosteric Modulators Craig Lindsley, Merck & Co, Inc

3:30  228  A LMW CCR5 Antagonist in Combination with CsA Prolongs Graft Survival in Life Supporting Kidney TX Model in Cynomolgus Monkeys Gerhard Thoma, Novartis Pharma AG
Monday, 23 May 2005, 1:10 PM - 5:30 PM
Medicinal Chemistry
Symposium: Pharmaceutical Profiling
Pharmaceutical Profiling II

Room 118 (Science & Engineering Resource Center)
Organizer: Edward H Kerns, Wyeth Research
Presider: Edward H Kerns, Wyeth Research

1:10 229 Preclinical Assessment of QT Liability and Proarrhythmic Risk Paul Levesque, Bristol-Myers Squibb Co
1:50 230 Pharmaceutical Profiling: The Interface between Drug-like Property Prediction and Application for Project Impact Li Di, Edward H Kerns, Susan L Petusky, Susan Q Li and Hong Chen, Wyeth Research
2:30 231 The Application of Pharmaceutical Profiling Data to Lead Identification and Optimization John Ellingboe, Wyeth Research
3:10 Break
3:25 232 The use of in vitro profiling in the optimization of IMPDH inhibitors Murali Dhar, Bristol-Myers Squibb
4:05 233 Strategies and techniques for providing in vivo PK and tissue penetration data for drug discovery Timothy Olah, Bristol-Myers Squibb Co
4:45 Panel Discussion

Monday, 23 May 2005, 1:20 PM - 5:10 PM
Organic Chemistry
Symposium: Bench Top To Pilot Plant
Bench Top To Pilot Plant II

Room 111 (Science & Engineering Resource Center)
Organizers: Ambarish Singh, Bristol-Myers Squibb Company, Shankar Swaminathan, Bristol Myers Squibb

1:20 234 Case Study: The Approval of Somavert, a Bio-therapeutic Agent Amit Banerjee, Pfizer Global Research and Development
2:10 235 Process Improvements in Synthesis of Therapeutic Oligonucleotides: From Grams to Kilograms Yogesh S Sanghvi, Rasayan Inc
3:00 Break
3:15 236 Palladium Coupling Catalysts for Pharmaceutical Applications Thomas Colacot, Johnson Matthey
3:40 237 Development and Scale-Up of the TACE Inhibitor BMS-561392 Scott A Savage, Bristol-Myers Squibb
4:05 238 The use of SMB as a chiral separation tool from bench to commercial production Emile Farhan, Johnson Matthey Pharmaceutical Material
4:30 239 Preparative supercritical fluid chromatography (SFC) at the kilogram scale William R Leonard Jr, Christopher Welch, Jennifer Albaneze-Walker, Mirlinda Biba, Jimmy DaSilva and Derek Henderson, Merck Research Laboratories
4:55 Concluding Remarks

**Monday, 23 May 2005, 1:30 PM - 5:15 PM**
*Analytical Chemistry Frontiers*

**Analytical**

Room 208 (Science & Engineering Resource Center)

Presider: Duxi Zhang, Bristol-Meyers-Squibb

1:30 Introductory Remarks

1:35 240 Evaluation of a Rapid and Automated Intra Operative Parathyroid Hormone Assay
    **Michael A Pesce**, New York Presbyery Hospital Columbia University Medical Center

1:55 241 Overcoming the LC Bottleneck in ADME Studies **Paren Patel**, Nanostream

2:15 242 Di-(2-Ethylhexyl)-Phthalate and its Metabolites Influence the Expression and Function of Fatty Acid Homeostasis Regulating Proteins in Rat Placental HRP-1 Cells **Yan Xu**, Thomas J Cook and Gregory T Knipp, Rutgers, the State University of New Jersey

2:35 243 Investigation of the Dissociation of Double Stranded Oligodeoxynucleotides in an Ion Trap: Sequence, Length and Charge Level **Su PAN** and Jeehiun K Lee, Rutgers, The State University of New Jersey

2:55 Break

3:05 244 Trascient isotachophoretic (tITP) stacking of in-line generated reactions products in CE **Timothy G Strein**, Rachel Slotcavage, Diana Scheerbaum, Brandi Sanders, Phillip Mason and Derek Schildt, Bucknell University

3:25 245 Clean Chemistry for Trace Metals Analysis **Nimi Kocherlakota** and Ralph H Obenauf, Spex CertiPrep

3:45 246 Analyzing speciation of arsenic in iron rich groundwater and wastewater **Zhongqi Cheng**, Yi He, Yan Zheng and Alexander Van Geen, (1)Lamont Doherty Earth Observatory of Columbia University, (2)John Jay College, City University of New York, (3)Queens College, City University of New York

4:05 247 Quantitative Analysis of Lead (II) Carbonates Using Vibrational Spectroscopy **Christine A Rapach** and Gene S Hall, Rutgers University

4:25 248 Concentrations of Phthalates in Plastic Toys as Determined by ATR-FTIR Spectroscopy **jeannine Matuza**, Rutgers, The State University of New Jersey

**Monday, 23 May 2005, 1:30 PM - 4:10 PM**
*Environmental/Green Chemistry*

**Assuring Water Purity**

Room 218 (Science & Engineering Resource Center)

Presider: Sut Ahuja, Ahuja Consulting

Workshop Leader: Sut Ahuja, Ahuja Consulting

1:30 249 Assuring Water Purity for Human Consumption **Sut Ahuja**, Ahuja Consulting

2:00 250 Poison in the Well: The Crisis of Arsenic in Drinking Water in Bangladesh **Joe Graziano**, Columbia University
2:30  251  Leachability of Arsenic in Water Treatment Residuals Xiaoguang Meng, Chuanyong Jing and Suqin Liu, Stevens Institute of Technology

3:00  252  Development and Deployment of an Arsenic Filter for Groundwater of Bangladesh Abul Hussam, George Mason University and A K M Munir, Sono Diagnostic Center Environment Initiative


4:00  Concluding Remarks: William F Carroll Jr (President ACS)

Monday, 23 May 2005, 1:30 PM - 4:30 PM
Biological Chemistry
Biological Chemistry

Room 217 (Science & Engineering Resource Center)

1:30  254  Automation of Cell Culture to Support Cell-based Assays for Compound Profiling Debra Burdick, Novartis Institute for Biomedical Research

1:50  255  A new factor required for Wnt-mediated cellular motility Melissa Maglaqui, The College of Saint Elizabeth and Raymond Habas, University of Medicine and Dentistry of New Jersey-Robert Wood Johnson Medical School

2:10  256  Investigation of polyamine analogs on the growth of MCF-7 breast cancer cell lines Francis Charles Mayville Jr, Michelle Piel, Kristina Thornburg, Christopher Higgins and Peter Leonard, DeSales University

2:30  257  NMR studies of Liver Fatty Acid-Binding Protein in lipid membrane media Fouad Francis, Ruth Stark, Hsin Wang and Xiaomin Yang, College of Staten Island City University of New York

2:50  Break

3:10  258  Human Skin Odors Michelle Gallagher¹, George Preti¹, Russell Bazemore¹, James J Leyden², Arlene Foglia² and Andrew I Spielman³, (1)Monell Chemical Senses Center, (2)University of Pennsylvania, (3)NYU

3:30  259  MHC-related Odorprints in Mice George Preti¹, Alan Willse², Gary K Beauchamp¹, Kunio Yamazaki¹, Peter Yang¹ and Jon H Wahl¹, (1)Monell Chemical Senses Center, (2)Pacific Northwest National Labs

3:50  260  Characteristic Odor Components in Mouse Urine Jae Kwak, Marcus Jackson, George Preti, Maryanne Curran, Kunio Yamazaki and Gary Beauchamp, Monell Chemical Senses Center

Monday, 23 May 2005, 1:30 PM - 5:00 PM
Organic Chemistry
Carbohydrates

Room 216 (Science & Engineering Resource Center)
Organizer: Cecilia H Marzabadi, Seton Hall University
Presider: Cecilia H Marzabadi, Seton Hall University
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<th>Time</th>
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<th>Title</th>
<th>Authors/Institutions</th>
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<tr>
<td>1:30</td>
<td>261</td>
<td>Practical synthesis and crystal structure of GlcNAc-thiazoline</td>
<td>Richard A Huhn, Thomas J Emge and Spencer Knapp, Rutgers University</td>
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<tr>
<td>1:50</td>
<td>262</td>
<td>Synthesis and crystal structure of GlcNAc-thiazoline-6-O-tetradecanoate</td>
<td>David Fash, Thomas J Emge and Spencer Knapp, Rutgers University</td>
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<tr>
<td>2:10</td>
<td>263</td>
<td>Developing the Structure-Activity Relationships for cADPR: Conformational Analysis of cADPR Analog Agonists and Antagonists</td>
<td>Steven M Graham, St John's University</td>
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<tr>
<td>2:30</td>
<td>264</td>
<td>Short route to octosyl nucleosides</td>
<td>Vinay V Thakur, Machender Madduru, Krishnan Malolanarasimhan and Spencer Knapp, Rutgers University</td>
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<tr>
<td>2:50</td>
<td>265</td>
<td>2'-Deoxynucleosides through 2'-thio-S-acetyl participation</td>
<td>Srihari Pabbaraja and Spencer Knapp, Rutgers University</td>
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<tr>
<td>3:10</td>
<td>266</td>
<td>Carbohydrate-fused heterocycles: Preparation and further transformations</td>
<td>Cecilia H Marzabadi and Michael De Castro, Seton Hall University \</td>
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<tr>
<td>3:30</td>
<td>267</td>
<td>Synthesis of 1-C-elaborated GalNAc-thiazolines</td>
<td>Benjamin Amorelli and Spencer Knapp, Rutgers University</td>
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<td>3:50</td>
<td>268</td>
<td>Vinyl glycosides and carbohydrate vinyl ethers: Synthesis and applications</td>
<td>Robert Giuliano, Kevin Hughes, Christopher Cummings and Tuan Nguyen, Villanova University</td>
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**Monday, 23 May 2005, 1:30 PM - 5:30 PM**
Small Chemical Business
Symposium: Discovery to Commercialization
**Discovery to Commercialization**

Room 212 (Science & Engineering Resource Center)
Organizers: Rhoda Kriesel, Touchstone Marketing, Ed Harris, E B Harris & Assoc

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<th>Authors/Institutions</th>
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<tr>
<td>1:30</td>
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<td>Introductory Remarks</td>
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<tr>
<td>1:40</td>
<td>269</td>
<td>Molding an Innovation to Market Needs: A Critical Key to a Start-up's Success!</td>
<td>Joe D’Antuono, ROW2 Technologies, Inc</td>
</tr>
<tr>
<td>2:20</td>
<td>270</td>
<td>From a Eureka Moment to a Clinical Candidate: a Case Study of a PolymerDrug™</td>
<td>Karen Giroux, Polymerix Corporation</td>
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<td>3:00</td>
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<td>Q&amp;A, Discussion I Moderator: Judith Sheft</td>
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<td>3:10</td>
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<td>Break</td>
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<td>3:30</td>
<td>271</td>
<td>HydroGlobe - Commercializing an Innovative Water Purification Technology</td>
<td>John Schroeder, Graver Technologies llc, Hydroglobe Div</td>
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<tr>
<td>4:10</td>
<td>272</td>
<td>Commercialization of Nanocomposite Barrier Coatings</td>
<td>Harris Goldberg, Inmat, Inc</td>
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<td>4:50</td>
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<td>Q&amp;A, Discussion II Moderator: Judith Sheft</td>
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<td>5:00</td>
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<td>Concluding Remarks</td>
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**Monday, 23 May 2005, 1:30 PM - 5:05 PM**
Biomaterials and Polymers
Symposium: Polymeric Biomaterials
**Engineered and Novel Biomaterials**

Room 205 (Science & Engineering Resource Center)
Organizer: Kathryn E Uhrich, Rutgers University
Presider: Michael S Yu, The Johns Hopkins University

1:30  273  Non-Covalent Modification of Collagen Scaffolds  Michael S Yu, The Johns Hopkins University

2:00  274  Biomimetic Scaffolds for Vascular Tissue Engineering  Joyce Y Wong, Boston University

2:30  275  Electrospun Polymer Nanofibers and Nanospheres for Drug Delivery and Tissue Engineering Scaffolds  John F Rabolt, University of Delaware

3:00 Break

3:30  276  Drug Delivery Vehicles Based on Poly(Oxyethylene Phosphonate)s Kolio Troev, Bulgarian Academy of Sciences and Ivan Gitsov, SUNY College of Environmental Science and Forestry

3:45  277  Artificial Glycopolymers for the Inhibition of Bacterial Toxins  Brian D Polizzotti and Kristi L Kiick, University of Delaware and Delaware Biotechnology Institute

4:00  278  Glycosylation of Multifunctional Alanine-Rich Protein Polymers for Biological Applications  Ying Wang and Kristi L Kiick, University of Delaware and Delaware Biotechnology Institute

4:15  279  A Universal Synthetic Methodology to Prepare Peptide-Polymer Hybrids  Ying Mei, National Institute of Standard and Technology

4:20  280  Protonation/deprotonation in natural (Bacillus subtilis spore) and synthetic (hydrogel) ionic reservoirs  Sergey V Kazakov, Elizabeth M Bonvouloir and Korki Miller, Pace University

4:35  281  Preparation of heparinized polyethersulfone with anticoagulant blood and it’s membrane properties  Changjun Hou, Chongqing University/University of Illinois at Urbana-Champaign and Danqun Huo, Chongqing University

4:50  282  The polymerization of actin: Structural changes from small angle neutron scattering  Alexander I Norman¹, Robert Ivkov², Jeffrey G Forbes³ and Sandra C Greer¹, (1)University of Maryland, (2)Triton Biosystems Inc, (3)Laboratory of Muscle Biology, NIAMS, NIH, DHHS

Monday, 23 May 2005, 1:30 PM - 5:00 PM

Biological Chemistry
Symposium: Gene Expression: Transcription

Gene Expression: Transcription

Room 202 (Science & Engineering Resource Center)

1:30 Welcoming Remarks

1:40  283  Structural studies of bacterial transcription  Seth A Darst, The Rockefeller University

2:15  284  Structure of bacterial RNA polymerase holoenzyme complexed with streptolydigin  Eddy Arnold¹, Steven Tuske², Stefan G Sarafianos¹, Xinyue Wang², Brian Hudson², E Sineva², Jayanta Mukhopadhy¹, Jens J Birktoft², Oliver Leroy², Sajida Ismail², Arthur D Clark Jr¹, Chhaya Dharia¹, Andrew Napoli¹, Oleg Laptenko³, Jooyung Lee³, Sergei Borukhov³ and Richard H Ebright², (1) Rutgers University, (2)Rutgers University, (3)UMDNJ

2:50  285  Complexes of CAP in Transcription Activation  Catherine Lawson, Andrew A Napoli, Brian Benoff, Helen M Berman, Yon W Ebright and Richard H Ebright, Rutgers University
3:25 Break

3:50 286 Direct Observation of Abortive Initiation and Promoter Escape: Single-Molecule DNA Nanomanipulation Andrei Revyakin¹, Chenyu Liu¹, Terence Strick² and Richard H Ebright¹, (1)Howard Hughes Medical Institute, Rutgers University, (2)Institut Jacques Monod


Monday, 23 May 2005, 1:30 PM - 5:00 PM
Biomaterials and Polymers
Symposium: Inorganic and Organometallic Polymers
Inorganic and Organometallic Polymers II

Room 206 (Science & Engineering Resource Center)
Organizer: Frieder Jaekle, Rutgers University
Presiders: Greg Tew, University of Massachusetts, Matthias Wagner, J W Goethe-Universität

1:30 Intermission

2:00 288 Photocontrolled Routes to Functional Metallopolymers Ian Manners, University of Toronto

2:30 289 Hydrosilylation Polymerizations of Metal-Containing Monomers with Dialkynes John B Sheridan, Rutgers University

3:00 290 Nanocluster Catalysis for Regioselective Synthesis of Multifunctional Hybrid Polysiloxanes Bhanu P S Chauhan and Jitendra S Rathore, Nanomaterials Laboratory of Center for Engineered Polymeric Materials, City University of New York at CSI

3:30 Break

3:50 291 Macromolecules for Supramolecular Polymer Science Containing Metal-ligands in the Side Chain Greg Tew, University of Massachusetts

4:20 292 Synthesis and Properties of Rodlike Ruthenium(II) Coordination Polymers Matthias Rehahn, Oliver Schmelz and Steffen Kelch, Darmstadt University of Technology

Monday, 23 May 2005, 1:30 PM - 5:00 PM
Inorganic Chemistry
Symposium on Organometallic-based Catalysis
Organometallic-based Catalysis

Room 117 (Science & Engineering Resource Center)
Organizer: Alan S Goldman, Rutgers University
Presider: Alan S Goldman, Rutgers University

1:30 293 A Synergy between Synthetic Organic and Organometallic Chemistry John F Hartwig, Yale University

2:15 294 Catalytic Asymmetric C-C and C-O Bond Forming Reactions Patrick J Walsh, University of Pennsylvania
3:00  295  Development of New Generation of Asymmetric Hydrogenation Catalysts Xumu Zhang, Penn State University
3:45  296  C-H Bond Functionalization in Complex Organic Synthesis Dalibor Sames, Columbia University Columbia University Columbia University

Monday, 23 May 2005, 1:30 PM - 5:00 PM
ADMET at the Crossroads of Drug Discovery
Symposium: P450 Metabolism Enzymes

Room 210 (Science & Engineering Resource Center)
Presiders: Donglu Zhang, Bristol-Myers Squibb, Leslie Romanyszyn, Merck & Co

1:30  Introductory Remarks
1:45  297  P450 in drug discovery and development - Now and the future Ronald E White, Schering-Plough Research Institute
2:30  298  The Incorporation of Active and Reactive Metabolite Data into the Drug Discovery Process Griffith Humphreys, Bristol Myers Squibb Pharmaceutical Research Institute
3:15  Break
3:30  299  Human Extrahepatic Cytochrome P450 (CYP) Enzymes: Role in Xenobiotic Metabolism and Toxicity Jun-Yan Hong, UMDNJ
4:15  300  Drug-Drug Interactions: P450 Inhibition and Induction Michael W Sinz, Bristol_Myers Squibb

Monday, 23 May 2005, 1:30 PM - 4:30 PM
Nano and Materials Science
Symposium: Solid State and Materials Chemistry
Solid State and Materials Chemistry II

Room 204 (Science & Engineering Resource Center)
Organizers: Jing Li, Rutgers, The State University of New Jersey, Martha Greenblatt, Rutgers, The State University of New Jersey
Presiders: Jing Li, Rutgers, The State University of New Jersey, Martha Greenblatt, Rutgers, The State University of New Jersey

1:30  301  Abalone Nacre: A Perfect Marriage of Soft and Hard Materials Nan Yao, Princeton University
2:00  302  Solution processable semiconductive coordination networks based on large aromatic building blocks Zhengtao Xu, Kunhao Li, Hanhui Xu and Jacqueline M Ryan, The George Washington University
2:30  303  Graphite Nanofibers in Direct Methanol Fuel Cell Electrodes Carol A Bessel1, Donna Omiatek1, Susan Thai1, Georgia C Papaefthymiou1, Arthur Viescas1, Douglas A Blom2 and Lawrence F Allard2, (1)Villanova University, (2)Oak Ridge National Laboratory
3:00  304  Hydrogen Storage on Metal Organic Frameworks Jeffrey T Culp, US DOE National Energy Technology Laboratory
3:30  305  Preparation and characterization of zinc titanate nano-crystal powders via sonochemical synthesis **Feng Chen**, Kirstan Bowser and Tamara Bell, (1)Rider University, (2)George School

4:00  306  Infrared Fluorescence Emission Characteristics of Chalcogenide-Bound Erbium Complexes and their Fluoropolymer Composites **Santanu Banerjee**, Anna Kornienko, John G Brennan, GA Kumar and Richard E Riman, Rutgers, The State University Of New Jersey


**Monday, 23 May 2005, 1:30 PM - 5:00 PM**

**Physical Chemistry**

Symposium: Spectroscopy of Biomolecules, Interfaces and Materials

**Spectroscopy of Biomolecules, Interfaces and Materials II**

Room 207 (Science & Engineering Resource Center)

Organizer: Edward, W Castner, Rutgers University

Presider: Edward, W Castner, Rutgers University

1:30  308  Probing Photophysical Processes by Time-Resolved Linear Dichroism Spectroscopy **Dustin Levy** and Bradley R Arnold, University of Maryland Baltimore County

1:50  309  Single molecule studies of protein conformational dynamics **David S Talaga**, Rutgers University

2:30  310  Ultrasensitive binding and transport studies of model membrane-active peptides at bilayer interfaces **Douglas S English**, Xiang Wang and Nikolai Sinkov, University Of Maryland, College Park

3:10  Break

3:40  311  Fast Long-range Electron Injection at Molecule-Nanoparticle Interfaces **Piotr Piotrowiak**, Rutgers University at Newark


**Monday, 23 May 2005, 2:00 PM - 3:00 PM**

**Careers For Chemists**

**Careers Workshops**

**Career Enhancement for Chemical Technicians**

Room 120B (Busch Campus Center)

Workshop Leader: George J O'Neill, Consultant

Monday, 23 May 2005, 2:30 PM - 7:00 PM  
Organic Chemistry  
Symposium: Bench Top To Pilot Plant  
Bench Top to Pilot Plant Posters  

Poster Areas (Busch Campus Center)  
Organizers: Anita J Brandolini, William Paterson University, A Singh, Bristol-Myers Squibb Company, Shankar Swaminathan, Bristol Myers Squibb  

314 Membrane Pervaporation Process for Diacetone Alcohol – Water Separations Timothy Schurmann, Joshua MacMillan, Angela Zimarowski and C Stewart Slater, Rowan University  

315 Nucleophilic displacement at suitably activated secondary benzylic alcohol by a sulfonamide-Development and scale-up for the preparation of an intermediate in the synthesis of a drug candidate in Alzheimer's disease Ming Yang, M Saindane, C Nilsen, A Staab, K Gesenberg, K Wong, T Vu, Z Shi, J Fan, G Crispino, Y Pendri, Siva J Prasad and A Singh, Bristol-Myers Squibb Company  


317 Implementation of HPLC Automation for the Analysis and Purification of Chiral Molecules Craig K Esser, Regina M Black and Derek Von Langen, Merck Research Laboratories  

318 Photodegradant of Razaxaban: Structure Characterization Using 15N NMR Techniques Qingmei Ye, Yande Huang, Liya Tang, Scott Miller, Charles Pathirana and VP Palaniswamy, Bristol-Myers Squibb  

319 Solvent swap tracking using an in-situ Foss Near-IR probe Charles Van Kirk, Elias Mattas, Ehrlic Lo, Scott Savage and Shih-Ying Chang, Bristol-Myers Squibb  

320 Solvent and Temperature Mediated Pharmaceutical Polymorphic Transformation Lifeng Shen and Dimuthu Jayawickrama, Bristol Myes Squibb  


322 Assessing Feasibility of Supercritical Reaction Processes Using Benchtop Laboratory Equipment Kenneth J James and Kenneth R Krewson, Supercritical Fluid Technologies Inc  

Monday, 23 May 2005, 2:30 PM - 7:00 PM  
Biological Chemistry  
Biological Chemistry Posters  

Poster Areas (Busch Campus Center)  
Organizer: Anita J Brandolini, William Paterson University  
Presider: Wilma K Olson, Rutgers University  

323 Purification and Characterization of Ricin from Castor seed Srinivas VS Chakravartula, New York Medical College and Nagaraj Guttalra, Directorate of Oilseeds Research  

324 Effects of phytoplankton and eelgrass uptake on bioavailability of toxic trace metals in marine environments Peter R Pascucci and Steven W Sasean, Community College of Denver
FAD Synthetase is slightly promiscuous David M Yearsley1, William S McIntire2 and Robert J Stanley1, (1)Temple University, (2)Department of Veterans Affairs Medical Center

Biochemical properties of Ricin in Immature Castor seed Srinivas VS Chakravartula, New York Medical College and Nagaraj Gutterla, Directorate of Oilseeds Research

Spin-Labeling and Characterization of DNA Oligonucleotides Joseph J Schramm III, Christopher Tuohy, Heather Skiff and Dr Donald J Hirsh, The College of New Jersey

Sequence-dependent Cyclization of Short DNA Sequences Luke F Czapla and Wilma K Olson, Rutgers University

Oxygen Binding and Cooperativity in a De Novo Designed Heme Protein Ronald L Koder, Christopher S Moser, A Joshua Wand and P Leslie Dutton, The Johnson Foundation and the University of Pennsylvania


The Influence of Abasic Sites on the Self-Assembly of DNA Quadruplexes Cosimo Antonacci and Richard D Sheardy, Seton Hall University

The role of proline in the folding of alpha-conotoxins H Reyna Herold, Amy K Croskey and Balazs Hargittai, Saint Francis University

Electrostatic interaction between supramolecular host-guest assembly and zinc-substituted cytochrome c Cynthia Pagba1, Jane M Vanderkooi2, Kurt Deshayes3, Eugene Piatnitski4 and Piotr Pietrowiak1, (1)Rutgers University at Newark, (2)University of Pennsylvania, (3)Genentech Incorporated, (4)Imclone Systems

Biochemical characterization of the amino-terminus of the capsaicin receptor, TRPV1 Christopher Jones, Marta Jimenez, Barry Selinsky and Joseph Rucker, Villanova University

Incorporation of the capsaicin receptor, TRPV1, into retroviral particles Panagiotis Maniatis and Joseph Rucker, Villanova University

Bromoindoles and Bromotryptophan: Origin and Application of Red-Shifted UV Spectra Ann E Shinnar1, Sevan Ozchetinkaya2 and Dina C Merrer2, (1)Lander College, (2)Barnard College

Ab initio and Density Functional Calculations of the Nucleic Acid Bases in Free and Watson-Crick Hydrogen-bonded States A R Srinivasan, PhD1, Ronald R Sayers1, Marcia O Fenley2, Alexander H Boschitsch3, Atsushi Matsumoto4, Andrew V Colasanti1 and Wilma K Olson1, (1)Rutgers University, (2)Florida State University, (3)Continuum Dynamics, Inc, (4)Quantum Bioinformatics Group

Structure-based design, structure-conformation and structure-activity relationships of DPhe(D/L-Tic)-Pro-DArg-P1'-CONH2 tetrapeptides with inhibitory activity for thrombin Cristina C Clement and Manfred Philipp, Lehman College, City University of New York (CUNY)

Different translesion bypass of guanine-N2 monoadducts of mitomycin C and guanine-N7 monoadducts of 2,7-diaminomitosene by eta, Klenow exo-, Klenow exo+ and T7 exo- DNA polymerases Cristina C Clement and Maria Tomasz, Hunter College, City University of New York (CUNY)

Monday, 23 May 2005, 2:30 PM - 7:00 PM
Inorganic Chemistry
Inorganic and Organometallic Posters

Poster Areas (Busch Campus Center)
Organizer: Anita J Brandolini, William Paterson University
340 Exploring the Chemistry of Aqueous Ionic Zinc for Various Applications Sabrina G Sobel, William F Nirode, Tracy Concepcion and Allison Haigney, Hofstra University

341 One-Pot Synthesis of Acyclic Epoxy Alcohols and Allylic Epoxy Alcohols Ann Rowley Kelly, Alice E Lurain and Patrick J Walsh, University of Pennsylvania

342 In Vitro Studies on Solubilizing Tattoo Pigments Lisa Sibley, Raymond Nocon, M Gerety and S A Katz, Rutgers University

343 The Interactions of Simple Co(III) Complexes with DNA Oligomers Jaime M Ferreira and Richard D Sheardy, Seton Hall University

344 Investigation of trimetallic light absorbing complexes that photocleave DNA Matthew T Mongelli, Mark Elvington, David Zigler, Jerita Dubash, Matthew Jeletic, Brenda S J Winkel and Karen J Brewer, Virginia Tech

345 The Effect of Spacer Chain Length in Phosphine-Imidazolium Compounds on the Catalytic Hydrogenation of Polymeric Materials Richard J Rosso, Nawras Harsouni, Christi Gandham, Aman Deep and Vicky Choda, St John's University

346 First Isolation, Characterization, and Binding Studies of a 1,2-Diborylated Ferrocene Dimer Krishnan Venkatasubbaiah¹, Lev N Zakharov², Scott Kassel², Arnold L Rheingold² and Frieder Jäkle¹, (1)Rutgers university-Newark, (2)University of California at San Diego

347 Imidazolium porphyrins as precursors to porphyrin arrays Virginia W C Seng, Rukya Ali, Xiulan Wang, Farah Charles-Pierre, Weici Fang and Alison G Hyslop, St John's University

348 Phosphorous Substituted Porphyrins, Synthesis and Characterization Salome Bhagan and Alison G Hyslop, St John's University

349 Organic polymer frameworks that become fully-conjugated upon metallation Donald W Carpenetti II and Alan Grubb, Marietta College

350 The Hexakis(thiocyanato)ferrate(III) Ion: a Coordination Chemistry Classic Reveals an Interesting Geometry Pattern for the Thiocyanate Ligands Anthony W Addison, Drexel University, Vitaly V Pavlishchuk, Institute of Physical Chemistry, Raymond J Butcher, Howard University, Laurence K Thompson, Memorial University, Zoltan Homonnay, Eötvös Loránd University and Michael J Prushan, LaSalle University

351 Effect of lanthanum and neodymium incorporation on oxygen storage capacity of ceria-zirconia mixed oxides Donald W Carpenetti II and Eric Seabright, Marietta College

352 Synthesis and Characterization of Mixed Ligand Rhodium(III) Complexes Stephanie R Ovalles and Elise G Megehee, St John's University

353 Synthesis and Characterization of Luminescent Osmium (II) Halide and Phosphine Complexes Pantea Menhaji and Elise G Megehee, St John's University

354 Synthesis and Characterization of New Luminescent Osmium(II) Polypyridyl Complexes Irma N Tertulien and Elise G Megehee, St John's University

355 Characterization of biologically active bis-(hinokitiolato)copper(II) complexes S Y Kim¹, C A Heyer¹, M Berardini¹, D M Ho² and GM Arvanitis¹, (1)The College of New Jersey, (2)Princeton University

356 Copper(II) Complexes of Tetridentate Thioether-Oxime Ligands Michael J Prushan, LaSalle University, Anthony W Addison, Drexel University, Raymond J Butcher, Howard University and Laurence K Thompson, Memorial University

357 Dehydrogenation of aliphatic polymers (polyolefins) catalyzed by pincer-ligated iridium complexes Amlan Ray and Alan S Goldman, Rutgers University
Poster Areas (Busch Campus Center)
Organizers: Anita J Brandolini, William Paterson University, Robert Goodnow Jr, Hoffmann-La Roche

358 Synthesis of 3-beta-acyloxyloxy-4,6-pregnadiene-6,20-dione derivatives as antiandrogens Elena Ramirez1, Eugene Bratoeff1, Marisa Cabeza2, Victor Perez1, David Valdez1, Alejandro Orozco1 and Alejandra Munguia1, (1)National University of Mexico City, (2)Metropolitan University of Mexico City-Xochimilco

359 Bicyclic Hydantoins as Androgen Receptor Antagonists Weifang Shan, Aaron Balog, Mark Salvati, Donna Wei, Greg Vite, Jack Hunt, Leslie Leith, Arvind Mathur, Ricardo Attar, Jieping Geng, Cheryl Rizzo, Marco Gottardis, Robert Weinmann, Stanley Krystek and John Tokarski, Bristol-Myers Squibb Company

360 Reduced FAK Phosphorylation and Migration Observed in Murine Melanoma Cells after Transfection with a Kinase-defective PKC alpha Yaw Amo-Mensah1, Regina Sullivan1 and Susan A Rotenberg2, (1)Queensborough Community College, (2)Queens College

361 Analysis and Interpretation of DNA to Metallated and Nonmetallated Tetrapyrindino Porphyrazines Melanie Bozza and Richard D Sheardy, Seton Hall University

362 Template-Assembled Peptide Models of the N-Peptide Helix Bundle from HIV-1 Gp41 Weiming Xu and John W Taylor, Rutgers University

363 Discovey Of PPARα/δ/γ Pan-agonists: Ligand Conformational Constraint and Selectivity Daniel J Miller, Hiroo Koyama, Joel P Berger, Karen L MacNaul, Thomas W Doebber, Margaret Wu, David E Moller and Soumya P Sahoo, Merck Research Laboratories

364 Discovery and Structure-Activity Relationship of Potent CC Chemokine Receptor-3 (CCR3) Antagonists Qing Shi, Patricia K Welch, Eric A Wedman, Soo S Ko and George V De Lucca, Bristol-Myers Squibb Pharmaceutical Research Institute

365 Synthesis and Lipid Lowering Effects of Acyl-Carnitines Kyle C Pillitteri, Rider University

366 Investigation of the effect that different drying methods have on the mechanism of theophylline release from microcrystalline cellulose beads Francis Charles Mayville Jr, Kristin Kurek and Kathryn Smith, DeSales University

367 Switching the configuration from L to D of P1’substituents is increasing inhibitory activity for thrombin of peptides D-Phe-Pro-D-Arg-P1'-CONH2 Cristina C Clement and Manfred Philipp, Lehman College, City University of New York (CUNY)

368 Influence of Miswak on the Binding of Polyphenols to Protein Pellicle Dina M Alhelawe, JFK Memorial High School


370 Developing novel inhibitors of the enoyl reductase from Mycobacterium tuberculosis (InhA): SAR studies of triclosan congeners Todd J Sullivan1, Polina Novichenok1, James J Truglio1, Francis Johnson1, Richard A Slayden2 and Peter J Tonge1, (1) Stony Brook University, (2)Colorado State University,

371 Regio- and Stereosepecific Syntheses of Syn- and Anti-1,2-Imidazolypropylamines from the Reaction of 1,1’-Carboxyldimidazole with Syn- and Anti-1,2-Aminoalcohols Mark J Mulvihill,
Anthony I Nigro, Cara Cesario, Vanessa Smith, Patricia Beck and Kathryn M Stolz, OSI Pharmaceuticals

Potent and Selective 2,6-Disubstituted Naphthalenes as Retinoic Acid Metabolic Blocking Agents (RAMBAs) Mark J Mulvihill, Julie L C Kan, Andrew Cooke, Patricia Beck, Shripad Bhagwat, Mark Bittner, Cara Cesario, Carrie Ecker, David M Keane, Anthony I Nigro, Christy Nillson, Suzanne Russo, Vanessa Smith, Mary Srebernak, Feng-Lei Sun, Michael Vrkljan, Shannon L Winski, Arlindo L Castelhano, David Emerson and Neil W Gibson, OSI Pharmaceuticals

Monday, 23 May 2005, 2:30 PM - 7:00 PM
Medicinal Chemistry
Symposium: Pharmaceutical Profiling
Pharmaceutical Profiling Posters

Poster Areas (Busch Campus Center)
Organizers: Anita J Brandolini, William Paterson University, Edward Kerns, Wyeth Research

Applications of Microsomal Stability Assays in Drug Discovery Susan Q Li, Li Di and Edward H Kerns, Wyeth Research

Comparison of PAMPA Methodology using Iso-pH and Multiple-pH Gradient Methods: Applications in Drug Discovery Research Susan L Petusky, Li Di and Edward Kerns, Wyeth Research

Pharmacetical Profiling and Medicinal Chemistry Collaboration for Project Impact Edward Kerns, Li Di and Guy Carter, Wyeth Research


Monday, 23 May 2005, 2:30 PM - 7:00 PM
Nano and Materials Science
Symposium: Solid State and Materials Chemistry
Solid State and Materials Chemistry Posters

Poster Areas (Busch Campus Center)
Organizers: Anita J Brandolini, William Paterson University, Jing Li, Rutgers, The State University of New Jersey, Martha Greenblatt, Rutgers, The State University of New Jersey

Sorption Properties of Pure Silica ITQ-13 Aleksandra Biedron1, Miguel Camblor2, David Olson1 and Jing Li1, (1)Rutgers, The State University of New Jersey, (2)Institute of Materials Science of Madrid (CSIC), Campus Cantoblanco

Structural modifications of extended metal-organic frameworks Ren Zhang and Jing Li, Rutgers, The State University of New Jersey

Gas sorption studies of 3D supermicroporous metal organic frameworks Jeongyong Lee and Jing Li, Rutgers, The State University of New Jersey

Versatile Metal-Organic Frameworks Synthesized Using Several Long Pan, Brett Parker, Xiaoying Huang, David Olson and Jing Li, Rutgers, The State University of New Jersey

Synthesis and characterization of ZnO-L (L= ethylenediamine, aniline) materials Min Wu, Hyun-Kyung Rhee, Xiaoying Huang and Jing Li, Rutgers, The State University of New Jersey

Modification of extended metal-organic structures
383 Synthesis of Microporous Materials containing Light Metals by Hydrothermal/Solvothermal Routes Sanhita Pramanik, Long Pan and Jing Li, Rutgers, The State University of New Jersey

384 New Routes of II-VI Semiconductors and Hybrid Thin Film Fabrication Wooseok Ki and Jing Li, Rutgers, The State University of New Jersey

385 (M₂Q₃)L and Mn doped (M₂Q₃)L (M = Zn, Cd, Q = S, Se, L = n-propylamine, n-butylamine, n-hexylamine): A class of promising multifunctional inorganic-organic hybrid II-VI Xiaoying Huang and Jing Li, Rutgers, The State University of New Jersey

386 Crystal Engineering with the Uranyl Cation: Use of Multiple Ligands as a Route to Novel Structures Lauren A Borkowski and Christopher L Cahill, The George Washington University

387 SrFe1/4Re3/4O3: A metallic ferromagnetic double perovskite with an uncommon octahedral tilt as revealed by high-resolution synchrotron powder X-ray diffraction Louis W Whaley¹, Martha Greenblatt¹, Mark C Croft² and Kandalam V Ramanujachary³, (1)Rutgers, The State University of New Jersey, (2)Rutgers University, (3)Rowan University

388 Synthesis of SrLaFeO₃Hₓ Sibel Dikmen, Viktor V Poltavets and Martha Greenblatt, Rutgers, The State University of New Jersey

389 Sr₃Fe₁₂₂₅Mo₀₇₇₅O₇₉, a Unique n = 2 Ruddlesden-Popper Phase with a Metal-Insulator Transition Louis W Whaley¹, Martha Greenblatt¹, Mark C Croft², Kandalam V Ramanujachary³, Maxim Lobanov¹ and Denis Sheptyakov⁴, (1)Rutgers, The State University of New Jersey, (2)Rutgers University, (3)Rowan University, (4)Paul Scherrer Institute

390 Isothermal section of the Na₀₃CoO₂ - H₂O system phase diagram at 22°C from 11 to 100% relative humidity Viktor V Poltavets and Martha Greenblatt, Rutgers, The State University of New Jersey

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Monday, 23 May 2005, 2:30 PM - 7:00 PM
Physical Chemistry
Symposium: Spectroscopy of Biomolecules, Interfaces and Materials
Spectroscopy of Biomolecules Posters

Poster Areas (Busch Campus Center)

Organizers: Edward W Castner Jr, Rutgers, The State University of New Jersey, Anita J Brandolini, William Paterson University

391 Time-Resolved UV Resonance Raman Studies of Polyriboadenylic Acid and DNA Alison P Williams, Princeton University and Ishita Mukerji, Wesleyan University

392 Resonance Raman investigation of the structural/functional role of the unusual adduct in Mycobacterium tuberculosis catalase-peroxidase KatG Sofia M Kapetanaki¹, Xiangbo Zhao², Richard S Magliozzo² and Johannes P M Schelvis¹, (1)New York University, (2)Brooklyn College and the Graduate Center of the City University of New York

393 Time-resolved Resonance Raman Spectroscopy of Tryptophans and Flavins Ullas Gurudas and Johannes PM Schelvis, New York University

394 Probing the Interaction Between Proteins and Some Small Molecules Using Fluorescence Spectroscopy Rosa Patricia Rosales, Queensborough Community College and Ruel Desamero, York College

395 Ultrafast Electron Injection in Dye Sensitizer / Semiconductor Systems Piotr Piotrowiak¹, Mykhaylo Myakhkostupov², Dong Wang², Qian Wei² and Elena Galoppini², (1)Rutgers University at Newark, (2)Rutgers-Newark

396 Formulating a Mechanism of Amyloid Growth using Single Molecule Spectroscopy Jason T Giurleo, Troy C Messina, Hiyun Kim, Jongjin Jung and David Talaga, Rutgers University
397  Ultrafast Folding of Trp-cage Mutants Michelle R DeRitter, Xi Yang, Jeffrey Saven and Feng Gai, University of Pennsylvania

398  Trans/Cis Proline Isomerization in Different Solvents Studied by Fluorescence Quenching due to Intramolecular Electron Transfer Youssef Issa, David S Talaga, Edward W Castner and Stephan S Isied, Rutgers University

399  A Stark Spectroscopic Study of Semiquinone FAD in DNA Photolyase Goutham Kodali, M Salim Siddiqui and Robert J Stanley, Temple University

400  Solvent Transport inside Surface Modified Silica Nanotubes Charles Luckett, Karthik Jayaraman, Kenji Okamoto, Sang Jun Son, Sang Bok Lee and Douglas English, University of Maryland CollegePark

401  Single Molecule Measurement of Fast Folding Proteins Using Fluorescence Resonance Energy Transfer Confocal Microscopy Jongjin Jung, Hiyun Kim, Troy C Messina, Jason T Giurleo and David S Talaga, Rutgers University

Monday, 23 May 2005, 3:00 PM - 5:00 PM
Student Affiliate Program
Eminent Scientist Lecture

Lecture Theatre (Fiber Optics)

3:00  402  What’s New In The New World Of Astrochemistry Yorke Rhodes, New York University

Monday, 23 May 2005, 7:00 PM - 8:15 PM
Keynote Presentation
Age-related Macular Degeneration (AMD)

Center Hall (Busch Campus Center)

7:00  403  Age-related Macular Degeneration (AMD) Koji Nakanishi, Columbia University

Monday, 23 May 2005, 7:00 PM - 8:30 PM
Keynote Presentation
Enterprise 2015: Chemistry at the Crossroads of Science
Enterprise 2015: Chemistry at the Crossroads of Science

Presider: William F Carroll Jr, Occidental Chemical Corporation

7:00  Introductory Remarks

7:15  404  A Future Outlook for the Chemistry Enterprise: A Pharmaceutical Industry Perspective Magid Abou-Gharbia, Wyeth Research

7:35  405  Changing Face of Chemistry and Implications for ACS Madeleine Jacobs, American Chemical Society

8:05  Enterprise 2015: An Academic Perspective Ken Breslauer, Rutgers University

8:25  Concluding Remarks
Tuesday, 24 May 2005

Tuesday, 24 May 2005, 8:30 AM - 12:00 PM
Biomaterials and Polymers
Symposium: Polymeric Biomaterials
Stars, Branched, Graft and Dendritic Polymers

Room 205 (Science & Engineering Resource Center)
Organizer: Kathryn E Uhrich, Rutgers University
Presider: Kristi L Kiick, University of Delaware and Delaware Biotechnology Institute


9:00  407 Assembly of Polysaccharide-Derivatized Star Polymers for Protein Delivery Applications Kristi L Kiick, University of Delaware

9:30  408 Preparation of Biocompatible and Biodegradable Nanobrushes from Cellulose and Hydroxyapatite Nanocrystals Ivan Gitsov, SUNY College of Environmental Science and Forestry, Anne Kathrine Overgaard, Technical University of Denmark and Bhushan Hole, Syracuse University

10:00 Break

10:30  409 Dendrimers for Dual Imaging Modalities: Combining Magnetic Resonance and Optical Fluorescent Imaging Vladimir S Talanov¹, Hisataka Kobayashi¹, Marcelino Bernardo¹, Moinuddin Hassan², Amir H Gandjbakhche³, Peter L Choyke¹ and Martin W Brechbiel¹, (1)National Cancer Institute, NIH, (2)National Institute of Child Health and Human Development, NIH

10:45  410 Fluorescence Probing of Drug Delivery Polymers Karen Steege, Jinzhong Wang, Kathryn E Uhrich and Edward W Castner, Jr, Rutgers, The State University of New Jersey

11:00  411 Conjugation of folic acid on Amphiphilic Scorpion like Macromolecules for targeting drug delivery Jinzhong Wang, Li Tao and Kathryn Uhrich, Rutgers, The State University of New Jersey

11:15  412 Phosphorescence Probes of Mobility and Site Heterogeneity in Amorphous Biomaterials Richard D Luderscher, Linda Pravinata, Sonali Shirke, Thomas Nack, Kasi Sundaresan, Rashmi Tiwari, Yumin You and Kristine Lukasik, Rutgers University

11:30  413 Amphiphilic Graft Copolymers for Interfacial Assembly, Encapsulation, and Controlled Release Kurt Breitenkamp, Bryan Parrish, Rebecca Breitemkamp and Todd Emrick, University of Massachusetts Amherst

Tuesday, 24 May 2005, 8:55 AM - 12:00 PM
Physical Chemistry
Symposium: Spectroscopy of Biomolecules, Interfaces and Materials
Spectroscopy of Biomolecules, Interfaces and Materials III

Room 207 (Science & Engineering Resource Center)
Organizer: Edward W Castner Jr, Rutgers, The State University of New Jersey
Presider: Edward W Castner Jr, Rutgers, The State University of New Jersey

8:55  Introductory Remarks

9:00  414 Solvation Dynamics of Excess Electrons in Ionic Liquids **James F Wishart**¹, Alison M Funston¹, Tomasz Szreder¹, Edward W Castner Jr², Hideaki Shirota² and Tania Fadeeva², (1)Brookhaven National Laboratory, (2)Rutgers, The State University of New Jersey

9:40  415 Dynamic Probing of Microviscosity and Solvation in Ionic Liquids **Tania Fadeeva**¹, Alison M Funston², James F Wishart² and Edward W Castner Jr¹, (1)Rutgers, The State University of New Jersey, (2)Brookhaven National Laboratory

10:00  Break

10:30  416 Dynamics in Ionic Liquids: Silyl vs Alkyl Cation Side Groups **Hideaki Shirota**, Rutgers, The State University of New Jersey

11:10  417 Thz-TDS and fs-Raman Probes of Intermolecular Interactions **William T Lotshaw**¹, Dale McMorrow¹ and Matthew C Beard², (1)Naval Research Lab, (2)National Renewable Energy Lab

Tuesday, 24 May 2005, 9:00 AM - 1:30 PM
Analytical Chemistry Frontiers
Analytical Posters

Poster Areas (Busch Campus Center)
Organizer: Anita J Brandolini, William Paterson University

418  Isotope Effects in the Chromatographic Behavior of Hemicarceplexes **Yong Liu**, Merck Research Laboratories and Ralf Warmuth, Rutgers University

419  Application of Orthogonal Signal Correction and Partial Least Square for the Simultaneous Determination of Aspirin, Caffeine and Acetaminophen based on UV Spectra **Hugh Zhang**, Weng Li Yoon, Janet Mashkovich, Benjamin Costa and John Sienkiewicz, GlaxoSmithKline

420  Bridging Institutions through Shared Instrumentation (NSF Award #0088392) **Rebecca DeRosa**, **Garrett J McGowan**, Michele M Hluchy and Jean Cardinale, Alfred University

421  Examination of Yeast Cell Parameters Using Optical Techniques **Julio Cesar Romero**, Jessenia Burges, Karen Leon, Alvaro Castellanos, Tak Cheung, Alex Flamholz and Patricia Schneider, Queensborough Community College

422  Simultaneous Determination of Sulforaphane and its Major Metabolites with Liquid Chromatography-Tandem Mass Spectroscopy **S Agrawal**¹, B Winnik², B Buckley² and TJ Cook³, (1)Ernest Mario School of Pharmacy, Rutgers, The State University of New Jersey, (2)Rutgers, The State University of New Jersey

423  Helium: Effect on Wisconsin Fast Plants **Mitesh R Patel**, John F Kennedy Memorial High School

424  Water Quality Experiment **Rafay Abbasi** and Michael Kreisel, Woodbridge High School

425  A Pilot Study of Arsenic Speciation and Its Bioaccessibility in Rice **Yi He**¹, Yan Zheng², Zhongqi Cheng³ and David C Locke², (1)John Jay College, City University of New York, (2)Queens College, City University of New York, (3)Lamont Doherty Earth Observatory of Columbia University

426  Characterization of Unsaturated Perfluoro-Carboxylic Acids Shirley Fischer-Drowos¹, Linda Betz², Justin Miscavige¹, **Nisreen Madhoun**¹ and Joe Di Bussolo², (1)Widener University, (2)Widener University and West Chester University, (3)Cohesive Technologies
Tuesday, 24 May 2005, 9:00 AM - 11:05 AM
Computers in Chemistry

Room 211 (Science & Engineering Resource Center)
Organizer: Wendy D Cornell, Merck & Co

9:00 Welcoming Remarks

9:05 427 Relative Strengths of Se-N,O Interactions: Implications for GPx-like Activity Craig A Bayse, Old Dominion University

9:45 428 Advances in Conformational Sampling and Free Energy Calculations via Adiabatic Dynamics Jerry B Abrams, Lula Rosso and Mark E Tuckerman, New York University

10:25 429 Combined use of local and global models for improving the accuracy of in silico ADME/Tox prediction Michelle D’Souza, Gregory Banik, Yann Bidault, Jeff Oakes, Kevin Scully and Deborah Kernan, Bio-Rad Laboratories

Tuesday, 24 May 2005, 9:00 AM - 1:30 PM
Computers in Chemistry
Computers in Chemistry Posters

Poster Areas (Busch Campus Center)
Organizers: Wendy D Cornell, Merck & Co, Anita J Brandolini, William Paterson University

430 Conformational Analysis of Piperazine and Piperidine analogs of GBR12909: Effect of Force Field and Solvent Deepangi Pandit, William Roosma, Milind Misra, Kathleen M Gilbert, William Skawinski and Carol A Venanzi, New Jersey Institute of Technology

431 Computation of Through-Space NMR Shielding Effects in Peptides Ned H Martin¹, Kristin L Main¹, Amy K Pyles¹ and David M Loveless², (1)UNCW, (2)Duke University

432 Rebuilding the Computer-Instrument Interface of an ESR Spectrometer Kathleen Hummel and Dr Donald J Hirsh, The College of New Jersey


434 Fuzzy relational clustering of molecular conformations using novel features based on DNA base-pair step parameters Milind Misra¹, Deepa Pai¹, Rohan Woodley¹, Amit Banerjee¹, Rajesh N Davé¹, Liang-Yu Shih¹, Xiang-Jun Lu², A R Srinivasan, PhD³, Wilma K Olson² and Carol A Venanzi¹, (1)New Jersey Institute of Technology, (2)Rutgers University

435 Comparative Study of Docking Programs GLIDE and GOLD for Virtual Screening Zhiyong Zhou¹, Anthony K Felts², Matt Repasky³, Ronald M Levy² and Richard A Friesner¹, (1)Columbia University, (2)Rutgers University, (3)Schrodinger LLC

436 Modeling of triclosan analogs for enoyl reductase inhibition Jeffrey P Wolbach, Jonilyn Longenecker and Paul Schettler, Juniata College

437 Investigating targets of antibacterial cysteine protease inhibitors Jeffrey P Wolbach and Leslie Vogt, Juniata College

438 Molecular docking and analysis of conformation adopted by tetrapeptide inhibitors into active site of thrombin Cristina C Clement and Manfred Philipp, Lehman College, City University of New York (CUNY)
Tuesday, 24 May 2005, 9:00 AM - 12:30 PM
Physical Chemistry
Symposium: Electronic Structure in Chemistry
Electronic Structure in Chemistry I

Room 209 (Science & Engineering Resource Center)
Organizers: Kieron Burke, Rutgers University, Karsten Krogh-Jespersen, Rutgers University
Presider: Kieron Burke, Rutgers University

9:00 Welcoming Remarks
9:05  439 Keynote Address: The H-bond Network in Water Roberto Car, Princeton University
9:50  440 MAME water model: Coulomb, induction and dispersion interactions in water dimer Eugene V Tsiper, George Mason University and Naval Research Lab
10:05 441 Ab Initio MD studies of hydrogen bonding in water and peptidic fragments Glenn Martyna, IBM Research
10:35 442 Efficient evaluation of nonlocal pseudopotentials via Euler exponential spline interpolation Hee-Seung Lee¹, Mark E Tuckerman¹ and Glenn Martyna², (1)New York University, (2)IBM Research
10:50 Break
11:00 443 Spatial and coupling constant scaling in time dependent current density functional theory Maxime Dion and Kieron Burke, Rutgers University
11:15 444 Density-functional-based methods for calculations of intermolecular forces Krzysztof Szalewicz¹, Alston J Misquitta¹, Rafal Podeszwa¹ and Bogumil Jezierski², (1)University of Delaware, (2)University of Warsaw
11:45 445 Undoing static correlation: long-range charge transfer in time-dependent density functional theory Neepa T Maitra, Hunter College of CUNY
12:15 446 Time-dependent current-density-functional theory: excitation and response properties of polymers Meta van Faassen¹, Robert van Leeuwen¹, Kieron Burke² and Paul L de Boeij³, (1)University of Groningen, (2)Rutgers University

Tuesday, 24 May 2005, 9:00 AM - 12:00 PM
Analytical Chemistry Frontiers
Symposium: Enabling Technologies in the Analytical Lab
Enabling Technologies in the Analytical Laboratory

Room 208 (Science & Engineering Resource Center)
Organizer: Bruce A Weber, Johnson & Johnson Pharmaceutical Research & Development, LLC
Presider: Adam M Fermier, Johnson & Johnson Pharmaceutical Research & Development, LLC

9:00  447 Introduction Adam M Fermier, Johnson & Johnson Pharmaceutical Research & Development, LLC
9:05  448 General Principles & Challenges in Automated Sample Preparation for Pharmaceutical Analysis (or: Robots Save the World!) Mark J Dryfoos, Novartis Pharmaceuticals Corp
9:55  450  New Column Technologies - Looking beyond C18 Matthew Przybyciel, ES Industries
10:20  Break
10:45  451  Small Particle Technologies Luis A Colon, University at Buffalo
11:35  453  A Software Automation Strategy for the Analytical Laboratory Eric Milgram, Advanced Chemistry Development, Inc (ACD/Labs)

Tuesday, 24 May 2005, 9:00 AM - 1:30 PM
Environmental/Green Chemistry
Environmental/Green Chemistry Posters

Poster Areas (Busch Campus Center)
Organizer: Anita J Brandolini, William Paterson University
Presiders: Wen-Chung Shieh, Novartis Pharmaceuticals, Sanjay V Malhotra, New Jersey Institute of Technology

454  Using Mössbauer Spectroscopy to Study the Effects of Salinity on the Speciation of Tributyl- and Triphenyltin in Anacostia River Anaerobic Sediments Xueqing Song, Alejandra Zapata and George Eng, University of the District of Columbia

455  Identification and quantitative determination of Polychlorinated Biphenyls in the Urban New York City areas Queen Golder, Manhattan Center for Science and Mathematics

456  The Effect of Nitrogen Fixing Bacteria on Light Absorption in Plants Arvind Srinivasan, John F Kennedy Memorial High School

457  Pb and Cd based recrystallized phases on calcite surfaces Douglas B Hausner¹, Daniel R Strongin¹ and Richard J Reeder², (1)Temple University, (2)State University of New York, Stony Brook

458  Mechanistic Aspects of Pyrite Oxidation in an Oxidizing Gaseous Environment: an In Situ HATR-IR Isotope Study Courtney R Usher¹, Daniel R Strongin¹ and Martin A A Schoonen², (1)Temple University, (2)State University of New York at Stony Brook

459  Synthesis of Beta-Amino alcohols in Pyridinium-based Ionic Liquid Sanjay V Malhotra and Richard P Andal, New Jersey Institute of Technology

460  Pyrite oxidation in the environment: the effect of bacteria Jun Hao¹, Daniel R Strongin¹, Eelin Lim¹ and Martin A A Schoonen², (1)Temple University, (2)State University of New York at Stony Brook

461  Pyrite oxidation in the environment and the effect of bacteria Jun Hao¹, Daniel R Strongin¹, Eelin Lim¹, Martin A A Schoonen² and David Vuong¹, (1)Temple University, (2)State University of New York at Stony Brook
Tuesday, 24 May 2005, 9:00 AM - 1:30 PM
Graduate Posters

Poster Areas (Busch Campus Center)
Organizers: Anita J Brandolini, William Paterson University, Yorke Rhodes, New York University
Presider: Yorke Rhodes, New York University

462 Cooperative binding of 1,2 substituted ferrocene based bidentate Lewis acids R Boshra, JA Gamboa, A Sundararaman, F Jakle, Arnold L Rheingold and Lev Zakharov, (1)Rutgers Univ, (2)University of California at San Diego

463 Current Efforts Towards the Preparation of 2’-Aminotaxol Hengqun Shen and Guillermo Moyna, University of the Scineces in Philadelphia

464 Neighboring Group Participation in the Syntheses and Reactions of 4-X-exo-8-anti-Iodo-6-azabicyclo[321]octanes (X=F, Cl, OH) Selectfluor and Mercuric Fluoride as Nucleofuges Deepa Rapolu, Grant Krow, Ryan A Centafoent and Kevin C Cannon, (1)Temple University, (2)Penn State Abington

465 Synthetic Studies Towards Ustiloxin Natural Products Cory D Evans, Pixu Li and Madeleine M Joullie, University of Pennsylvania

466 Solvent-Dependent Chemoselectivities in Ce(IV)-Mediated Oxidations of 2,4-Diketones: Fragmentations Vs Intramolecular Cyclizations Yang Zhang, Jingliang Jiao and Robert A Flowers II, Lehigh University

467 Synthesis and Novel Homolagation Reactions of 1,2-Cyclopropanated Carbohydrates Cecilia H Marzabadi and Jamie Talisman, Seton Hall University

468 Synthesis of novel nucleosides as potential anti-tumor or antibiotic drugs Irene Negrete and Dr Cecilia H Marzabadi, Seton Hall University

469 Asymmetric Transfer Hydrogenation of Allylic Compounds: a Novel Reaction with Homogeneous Chiral Ruthenium Catalysts Marie G Beauchamps and John Sowa Jr, Seton Hall University

470 Protodeboronation investigation in Heterogenously catalyzed Suzuki-Miyaura cross-coupling reaction Lubabal T Bululu and Dr John R Sowa, Seton Hall University

471 MFCC-DM: An Approximate QM Method to Study Large Biomolecules Xihua Chen, Yingkai Zhang and John ZH Zhang, New York University

472 Controlling the Crystal Growth of Polymorphs with 2-Dimensional Templates Rupa Hiremath, Stephen W Varney, Joseph A Basile, Megan J Carroll and Jennifer A Swift, Georgetown University

473 Study of pH-response of Bacillus subtilis spores Elizabeth M Bonvouloir and Sergey V Kazakov, Pace University

474 Sonication and Electrodeposition of Rhodium: Effects on Surface Morphology and Cathode Efficiency Michael D Hatton Jr, Robert Hesketh and Stephanie Farrell, Rowan University

475 Synthesis and NO-related Properties of Cycloadducts of C-Nitroso Compounds Harinath Chakrapani and Eric J Toone, Duke University

476 Electron Deficient C-Nitroso Compounds as Donors of Nitrosonium (NO+) David M Gooden and Eric J Toone, Duke University
Tuesday, 24 May 2005, 9:00 AM - 11:40 AM
Graduate Symposium: Graduate Presentations

Graduate Presentations

Lecture Theatre (Fiber Optics)
Organizer: Yorke Rhodes, New York University
Presider: Yorke Rhodes, New York University

9:00  477 Enantioselective Synthesis of Majusculone M Inthikhab Sikkander, University of Delaware

9:25  478 The Effect of Fuel Type and Aftertreatment Devices on Mobile School Bus Emissions from Diesel Powered School Buses Andrew Toback, Sarina Colligan, Anthony J Marchese and Robert P Hesketh, Rowan University

9:50  479 Influence of Bead Size on Activity and Distribution of Candida Antarctica Lipase B (CAL-B) Adsorbed on Macroporous Polyacrylic Beads Bo Chen and Richard Gross, Polytechnic University

10:15 480 New Fluorogenic Calix[4]arene-bis-crown-6 Ether for Selective Recognition of Cs\(^+\) Ebony D Roper\(^1\), Galina G Talanova\(^1\), Maryna G Gorbunova\(^2\), Richard A Bartsch\(^3\) and Vladimir S Talanov\(^4\), (1)Howard University, (2)Oak Ridge National Laboratory, (3)Texas Tech University, (4)National Cancer Institute, NIH

10:40 481 Removal of Depleted Uranium from Water Using Titanium Dioxide Christine Chin Choy, Mahmoud Wazne and Xiaoguang Meng, Stevens Institute of Technology

11:05 482 A New Biological Fluorescent Probe: PheCN Matthew J Tucker and Feng Gai, University of Pennsylvania

Tuesday, 24 May 2005, 9:00 AM - 12:00 PM
Environmental/Green Chemistry Symposium: Green Chemistry

Green Chemistry I

Room 117 (Science & Engineering Resource Center)
Organizers: Wen-Chung Shieh, Novartis Pharmaceuticals, Sanjay V Malhotra, New Jersey Institute of Technology
Presider: Sanjay V Malhotra, New Jersey Institute of Technology

9:00  Introductory Remarks

9:05  483 A Green Future for HMPA? Peter Wipf, University of Pittsburgh

9:35  484 Development of an environmentally sound process for production of the new carbapenem antibiotic ertapenem sodium J Michael Williams, Merck Research Laboratories

10:05 485 Development of a 2nd generation process for Gleevec® Mark Meisenbach, Novartis Pharma AG

10:35  Break

11:25  487  Green Chemistry: Current Status and Future Challenges  David Highfield, American Chemical Society

Tuesday, 24 May 2005, 9:00 AM - 12:00 PM
Analytical Chemistry Frontiers
Symposium: In-Line Analytics for Reaction Monitoring
In-Line Analytics for Reaction Monitoring

Room 202 (Science & Engineering Resource Center)
Organizers: John A Grosso, Bristol-Myers Squibb Co, John Wasylyk, Bristol Myers Squibb Co

9:00  488  Building Process Knowledge Through the Use of In-line/On-line Reaction Monitoring - Case Studies Srinivas Tummala, Simon Leung, Ehrlic Lo, John Shabaker and San Kiang, Bristol Myers Squibb

9:40  489  Process Development and Scale-Up with In-Line FTIR Monitoring  George Zhou, Merck and Co

10:15  490  Development and Implementation of an In-Line Quantitative Raman Method for In-Process Pharmaceutical Monitoring  Robert G Wethman, Charles Ray and John Wasylyk, Bristol-Myers Squibb Company

10:50  491  Development of a Laboratory Crystallization System with In-line Sensors  Boris Gordonov and Benoit Vanasse, sanofi-aventis

11:25  492  Real Time, On-Line Analysis of Flow Reactions using Impedance  Mike C Hawes, Syrris Ltd

Tuesday, 24 May 2005, 9:00 AM - 12:00 PM
Biomaterials and Polymers
Symposium: Inorganic and Organometallic Polymers
Inorganic and Organometallic Polymers III

Room 206 (Science & Engineering Resource Center)
Organizer: Frieder Jaekle, Rutgers University
Presiders: Robert B Grubbs, Dartmouth College, Qiao-Sheng Hu, City University of New York-College of Staten Island

9:00  493  Reactive Organometallic Polymers Containing Metallacyclopentadiene Repeating Units in the Main Chain  Ikuyoshi Tomita, Tokyo Institute of Technology

9:30  494  Polymerisation of Ferrocenylboranes via BH3 Elimination or Hydroboration Reactions  Matthias Wagner, Matthias Scheibitz and Julia B Heilmann, J W Goethe-Universität

10:00  495  Synthesis of Ferrocenylmethylphosphine-Containing Polymers for Transition Metal Catalysis  Qiao-Sheng Hu, Cheng-Guo Dong, Yong Lu, Hanako Hirosi, Elizabeth Plocher and Zhen-Yu Tang, City University of New York-College of Staten Island

10:30  Break

10:50  496  Synthetic approaches to hybrid polymer/small-molecule materials for solution processed organic light emitting diode (OLED) devices  Nora S Radu, Norman Herron, Frank Uckert, Eric Smith and Dan LeCloux, DuPont Co

11:20  497  Luminescent Organoboron Quinolate Polymers  Yang Qin, Cynthia Pagba, Piotr Piotrowski and Frieder Jäkle, Rutgers University at Newark
Tuesday, 24 May 2005, 9:00 AM - 12:00 PM
Medicinal Chemistry
Symposium: Ion Channels

Ion Channels

Room 203 (Science & Engineering Resource Center)
Organizer: Robert Goodnow, Hoffmann-La Roche
Presider: Thomas J Caufield, Sanofi-Aventis

9:00    Introductory Remarks Thomas Caufield
9:05    498 Blocking Ion Channel KCNN4 Alleviates the Symptoms of Experimental Autoimmune Encephalomyelitis in Mice Chuan-Chu Chou, Eva-Pia Reich, Long Cui, Lily Yang, Catherine Pugliese-Sivo, Andrei Golovko, Mary Petro, Galya Vassileva, Inhou Chu, Amin A Nomeir, Li-Kang Zhang, Xian Liang, Joseph A Kozlowski, Satwant K Narula and Paul J Zavodny, Schering-Plough Research Institute
9:40    499 Ion Channel Modulation: Can it Enhance Neurotransmission, Conduction, and Myelination for New Therapeutic Interventions? Craig P Smith, Sanofi-Aventis
10:10   Coffee Break
10:25   500 De novo design of potent T-type calcium channel blockers Daniel L Cheney, Jon Hangeland, Todd Friends and Paul Levesque, Bristol-Meyers Squibb PRI
11:10   501 Identification of Ion Channel Modulators Maria L Garcia, Merck Research Laboratories

Tuesday, 24 May 2005, 9:00 AM - 1:00 PM
College Education
Symposium: Laboratory Experiences in the Undergraduate Curriculum
Laboratory Experiences in the Undergraduate Curriculum

Room 204 (Allison Road Classroom Building)
Organizer: Christine M Ingersoll, Muhlenberg College

9:00    Introductory Remarks
9:05    502 Quantitative NMR Experiments Kurt Rublein, Lock Haven University
9:25    503 Introducing Statistics and Nonlinear Least-Squares into the Physical Chemistry Lab Carl Salter, Moravian College
9:45    504 Academic Choice Coupled to Open-Ended Exercises in the Analytical Chemistry Lab Thomas A Betts, Kutztown University of PA
10:05   505 An Interdepartmental Offering in Instrumental Analysis Donald Mencer Jr and J Michael Case, Wilkes University
10:25   506 Molecule Day: Laboratory Projects Based on an Interdisciplinary Theme Christine M Ingersoll, Muhlenberg College
10:45   Break
11:05   507 Maximize your research: Teach it! Olivier J-C Nicaise, Southern Connecticut State University
11:25  508  Does the Solvent Affect the Relative Nucleophilic Strength of Halide Ions in an SN2 Type Reaction? **Terrence P Sherlock**, Ralph Fleming, Ryan Oesterle and Jared Styer, Burlington County College

11:45  509  Development of Inexpensive Nucleic Acid Kinetics Experiments Jamie Burns¹, Madeley Alcala², Syeda Islam² and **Amber Flynn Charlebois**³, (1)Montclair Kimberley Academy, (2)JFK High School, (3)William Paterson University

12:05  510  Advantages of Microwave-Enhanced Reactions in the Organic Lab **Marsha R Baar**, Danielle Falcone and Christopher Gordon, Muhlenberg College

**Tuesday, 24 May 2005, 9:00 AM - 7:00 PM**
*Medicinal Chemistry*

**Medicinal Chemistry Posters**

Poster Areas (Busch Campus Center)
Organizers: Anita J Brandolini, William Paterson University, Robert Goodnow Jr, Hoffmann-La Roche

**Tuesday, 24 May 2005, 9:00 AM - 1:30 PM**
*Nano and Materials Science*

**Symposium: NanoScience and Technology**

**NanoScience and Technology Posters**

Poster Areas (Busch Campus Center)
Organizers: Anita J Brandolini, William Paterson University, Yves J Chabal, Rutgers University, Eric Garfunkel, Rutgers University

511  Simulations of Thiol Terminated Dendrimers **Shyam Vyas**, Accelrys Inc

512  Formation of Nano-sized Lead Sulfide and Cadmium Sulfide by Using Ionomers **Kayla A Lu**, Roshan Deen and Masanori Hara, Rutgers University

513  Molecular Self-Assembly Processes between Vesicles and Nanotubes for Device Fabrications **Ipsita A Banerjee**, Stephanie Colleti and Rose L Spear, Fordham University

514  Probing the Intrinsic Electrical Properties of Individual Nanowires With Electric Force Microscopy **Jianming Zhang**, Oleh Taratula, Jowairia Chaudhry and Huixin He, Rutgers University, Newark Campus

515  Generation and Stabilization of Copper Nanoparticles Moni Chauhan¹, **Wayne Narain**¹, Umar Latif² and Bhanu PS Chauhan³, (1)Queensborough Community College, (2)bNanomaterials Laboratory of Center for Engineered Polymeric Materials, Department of Chemistry and Graduate Center, City Univer, (3)Nanomaterials Laboratory of Center for Engineered Polymeric Materials, Department of Chemistry, City University of New York

516  Functionalized Polyaniline/Carbon Nanotube Composite for Sensitive Detection of Glucose by a Non-Enzymatic Approach **Yufeng Ma**, Ali Shah and Huixin He, Rutgers University

517  Platinum and Rhodium Nanoclusters as Catalyst in Hydroisilylation of Alkenes and Alkynes Bhanu PS Chauhan¹, Moni Chauhan², **Gilchris O Burton**² and Umar Latif³, (1)Nanomaterials Laboratory of Center for Engineered Polymeric Materials, Department of Chemistry, City University of New York, (2)Queensborough Community College, (3)bNanomaterials Laboratory of Center for Engineered Polymeric Materials, Department of Chemistry and Graduate Center, City Univer
518  Synthesis and Characterization of Iron Oxide Nanoparticles Derived from Ferritin Gang Liu, Hazel-Ann Hosein, Sudeep Debnath, Douglas Hausner and Daniel R Strongin, Temple University

519  The Literature of Nanoscience Howard M Dess, Rutgers University

520  Substrate-Assisted Phase Transitions of Au Nanorods Oscar R Miranda and Temer S Ahmadi, Villanova University

521  Electroanalytical study of anti-S aureus enterotoxin B and enterotoxin B reaction on nanopatterned aluminum surface Changhoon Chai and Paul Takhistov, Rutgers, The State University of New Jersey

522  Metal-molecule nano-junctions with organic self-assembled monolayers Weirong Jiang1, Eric Garfunke1, Nikolai Zhitenev2 and Zhenan Bao3, (1)Rutgers University, (2)Bell Laboratories, Lucent Technology, (3)Stanford University

523  Substitutions of the amino-capped aniline trimer and potential applications in nanotechnology Matthew CR Zagorski, Amber J Reilly and Yen Wei, Drexel University

524  Water Intrusion: A New Technique to Characterize Hydrophobic Porous Surfaces and Wetting in Nano-Confinement Roy Helmy and Alexander Y Fadeev, Seton Hall University

Tuesday, 24 May 2005, 9:00 AM - 12:00 PM
Analytical Chemistry Frontiers
Symposium: Novel Instrumentation and Applications of Mass Spectrometry in ADME studies
Novel Instrumentation and Applications of Mass Spectrometry in ADME studies
Room 210 (Science & Engineering Resource Center)
Presider: Dr Walter Korfmacher, Schering Plough Research Institute

9:00  525  Special Applications of MS for Metabolite Identification as Part of Drug Development Ragu Ramanathan and Swapan Chowdhury, Schering-Plough Research Institute

9:30  526  Novel LC-MS Applications for Preclinical ADME/PK Assays Ron Kong, Dahai Dong, Kimloang Nguyen, Martha Vallejo and Gamini Chandrasena, Lundbeck Research USA

10:00  527  Rapid Pharmacokinetic Analysis in Drug Discovery Utilizing Ultra Performance Liquid Chromatography coupled with the Micromass Quattro Premier Cymbelene Nardo, Dr Sam Wainhaus and Dr Walter Korfmacher, Schering Plough Research Institute

10:30  528  On-line Sample Preparation Techniques for Faster LC-MS/MS Assays of Preclinical Samples Voon S Ong, Memory Pharmaceuticals

11:00  529  APPI-MS: Applications and Use in a Drug Discovery Environment Ganfeng Wang and Yunsheng Hsieh, Schering-Plough Research Institute

11:30  530  Drug ADME analysis, including tissue metabolite profiling, in a few rats using a combination of microplate scintillation counting, capillary LC/MS, and whole-body autoradiography Mingshe Zhu, Bristol-Myers Squibb Pharmaceutical Research Institute

Tuesday, 24 May 2005, 9:00 AM - 4:00 PM
Chemical Engineering
Pharmaceutical Engineering Fundamentals Workshop
Pharmaceutical Engineering Fundamentals (Workshop)
Room 260 (Wright Lab)
9:00  531 Pharmaceutical Engineering Fundamentals Workshop Hugo Fernandez, Skanska Pharmaceutical Group

Tuesday, 24 May 2005, 9:00 AM - 12:00 PM
ADMET at the Crossroads of Drug Discovery
Symposium: Pharmacokinetics
Pharmacokinetics in Drug Discovery and Development

Room 118 (Science & Engineering Resource Center)
Presider: Dennis Scott, Pfizer

9:00  Introductory Remarks
9:10  532 Nonspecific brain binding as an indirect tool to assess CNS penetration Tristan Maurer, Pfizer
9:40  533 Human dose projection from pre clinical CNS models: Lundbeck experience Gamini Chandrasena, Lundbeck US Research
10:10 Break
10:25  534 Application of Physiologically-Based Models in Drug Discovery and Development David Plowchalk, Pfizer
10:55  535 Hydrophobic Drug Aggregates: Structure and Biology Eddy Arnold¹, Yulia Frenkel², Arthur D Clark Jr³, Kaylan Das⁴, Yuh-Hwa Wang⁵, Paul J Lewi⁶ and Paul A J Janssen⁷, (1) Rutgers University, (2)Center for Advanced Biotechnology and Medicine, and Rutgers University, (3)UMDNJ, (4)Center for Molecular Design
11:25  536 In Silico Prediction of ADME Properties: Current Status of Predictive Models Terry Stouch, Editor-in-Chief

Tuesday, 24 May 2005, 9:00 AM - 1:30 PM
Physical Chemistry
Physical Chemistry Posters

Poster Areas (Busch Campus Center)
Organizer: Anita J Brandolini, William Paterson University

537 Evaluation of shelf stability of food emulsions by Electrochemical Impedance Spectroscopy Shibly Paul and Paul Takhistov, Rutgers, The State University of New Jersey
538 Mechanistic interpretation of molecular interactions of tetracycline with clay and organic matter Pankaj Kulshrestha, HS Atreya, Dinesh Sukumaran, Rossman F Giese and Troy Wood, University at Buffalo, The State University of New York
539 Adsorption of Glyphosate on Montmorillonite, a Theoretical Study George A Khoury and Lorena Triibe, Penn State Berks
540 Detection of residues of tetracycline antibiotics in soil fertilized with manure and wastewater using Enzyme Linked Immunosorbent Assay Pankaj Kulshrestha, Rossman F Giese and Troy D Wood, University at Buffalo, The State University of New York
541 Potential Energy Surface for ArHCN Rudolph C Mayrhofer, Kutztown University
542 Simulations of Methane in Liquid Water using ab initio force fields Omololu Akin-Ojo and Krzysztof Szalewicz, University of Delaware
543 The Solubility of Chiral Enantiomers and Racemates as a Function of Enthalpy Differences in the Crystalline solids and Activity Coefficients in the Solution S Alex Studniarz, Penn State University

544 Molecular modeling, circular dichroism and FTIR studies of conformation adopted by tetrapeptides with inhibitory activity for thrombin Cristina C Clement¹, Manfred Philipp¹ and Christian Matthaeus², (1)Lehman College, City University of New York (CUNY), (2)Hunter College, City University of New York (CUNY)

545 Scattering of Propanol off Ionic Melts: a Theoretical Study Barbara E Graves and Lorena Tribe, Penn State Berks

546 Molecular Dynamics Calculations of Mg-Cu Alloys Andrew J Modzelewski and Lorena Tribe, Penn State Berks

547 Solvation and Solvation Dynamics in Room-Temperature Ionic Liquids Mark N Kobrak, Brooklyn College -- CUNY

Tuesday, 24 May 2005, 9:00 AM - 12:00 PM
Organic Chemistry
Physical Organic

Room 216 (Science & Engineering Resource Center)
Organizer: Cecilia H Marzabadi, Seton Hall University
Presider: Simon Leung, Bristol Myers Squibb

9:00 548 Efficient Acylation of Benzimidazoles with Esters and Identification of a Tetrahedral Hemiacetal Alkoxide Intermediate Kenneth J Fitch, Merck Research Labs

9:20 550 Polysulfane Natural Products as Evolved Chemical Warfare Agents Edyta M Brzostowska and Alexander Greer, The City University of New York (CUNY), Brooklyn College

9:40 551 Does nature preferably select macrocycles based upon ring size? Aaron R Frank, Nicola S Farina, Orrette R Wauchope, Mo Qi and Alexander Greer, The City University of New York (CUNY), Brooklyn College

10:00 Break

10:15 552 UV-Visible Absorption of 10-Chloro-9-Anthraldehyde as a Probe of Hydrogen Bonding in Bioorganic Systems Josette Crout Seibles, Manhattanville College

10:35 553 The Concept of Protobranching and its Paradigm Shifting Implications Matthew D Wodrich and Paul V R Schleyer, The University of Georgia

10:55 554 Effects of Introducing a Rigid Spacer into Gemini Surfactants: Reversal of the Hofmeister Series and Evidence of Ch•••X- Hydrogen Bonding Brian P Regler and Laurence S Romsted, Rutgers University

11:15 555 Determining the distribution of an antioxidant between the oil, interfacial and aqueous regions of food-like emulsions stabilized by C12E6 Krishnan Gunaseelan and Laurence S Romsted, Rutgers University

11:35 549 Withdrawn
Tuesday, 24 May 2005, 9:00 AM - 11:50 AM
Nano and Materials Science
Symposium: Surface and Interface Science
Surface and Interface Science I

Room 204 (Science & Engineering Resource Center)
Organizers: Yves J Chabal, Rutgers University, Theodore E Madey, Rutgers, The State University of New Jersey
Presiders: Yves J Chabal, Rutgers University, Theodore E Madey, Rutgers, The State University of New Jersey

9:00  556  Biochemical Surface Modification of Self Assembled Monolayers Susan C D'Andrea
       and Alexander Y Fadeev, Seton Hall University

9:20  557  Chemical Control of Surface Morphology: Taming Instabilities in Silicon Etching
       Melissa A Hines, Simon P Garcia and Hailing Bao, Cornell University

10:05 558  Wet chemistry on germanium (100) for high-κ dielectric growth Sandrine Rivillon¹,
       Kenneth A Bratland¹, Yves J Chabal¹, Fabrice Amy², Antoine Kahn² and Marek P
       Boleslawski³, (1)Rutgers University, (2)Princeton University, (3)SAFC

10:25 559  Silicon Surface Functionalization for High-κ Dielectrics Growth Yu Wang, Ming-Tsung
       Ho, Leszek Wielunski, Lyudmila Goncharova, Torgny Gustafsson and Yves Chabal,
       Rutgers University

10:45 560  Buried Interfaces in Thin Molecular Films and Colloids Hai-Lung Dai, University of
       Pennsylvania

11:30 561  The Potentiometric response during Layer-by-Layer Deposition Manju Manju
       and Kalle Levon, Polytechnic University

Tuesday, 24 May 2005, 9:00 AM - 1:30 PM
Nano and Materials Science
Symposium: Surface and Interface Science
Surface and Interface Science Posters

Poster Areas (Busch Campus Center)
Organizers: Anita J Brandolini, William Paterson University, Yves J Chabal, Rutgers University,
Theodore E Madey, Rutgers, The State University of New Jersey

562  Faceting of O/Re (1 2 -3 1 ): a model system for catalytic study Hao Wang, Wenhua Chen,
      Ally SY Chan and Theodore E Madey, Rutgers, The State University of New Jersey

563  Ion scattering study of oxygen diffusion and reactions in high-κ dielectric films on Si Lyudmila
      Goncharova¹, Dmitri Starodub¹, Robin Barnes¹, Eric Garfunkel¹, Torgny Gustafsson¹, Genadii
      Bersuker², Brendan Foran² and Pat Lysaght², (1)Rutgers University, (2)International Sematech

564  Characterization of Wettability of Hydrophobic Dispersed and Porous Solids and A Model-Free
      Method to Determine Macroscopic Contact Angles for Hydrophobic Powders Jeffrey J
      McElwee, Roy Helmy and Alexander Y Fadeev, Seton Hall University

565  Reactive, thin copper foils are readily prepared by controlled chemical etching of rotating disks
      of heavier copper sheet Karen Root Caldwell, Pace University -- Westchester
566 Structure sensitivity in oxidation of CO and decomposition of NH3 over Ir surfaces: relevance to environmental applications of Ir catalysts Wenhua Chen, Ivan Ermanoski and Theodore E Madey, Rutgers, The State University of New Jersey

567 Displacement of Organosilicon Monolayers Supported on Si Joseph W Krumpfer and Alexander Y Fadeev, Seton Hall University

Tuesday, 24 May 2005, 9:00 AM - 11:55 AM
Physical Chemistry
Symposium: Gas-phase Thermochemistry
Thermochemistry and Chemical Kinetics I

Room 218 (Science & Engineering Resource Center)
Organizer: Joseph W Bozzelli, New Jersey Institute of Technology
Presider: Joseph W Bozzelli, New Jersey Institute of Technology

9:00 Welcoming Remarks
9:05 568 Thermochemical and Kinetic Analysis of CH3S + O2 Li Zhu and Joseph Bozzelli, New Jersey Institute of Technology
9:30 569 Experimental and Computational Studies of the Kinetics of Chlorinated Hydrocarbon Radicals Vadim D Knyazev, The Catholic University of America
9:55 570 Reaction Pathways and Kinetic Analysis on Xylene Radical dissociation Joseph W Bozzelli¹, Eric E Moore¹ and John T Farrell², (1)New Jersey Institute of Technology, (2)ExxonMobil Research and Engineering
10:20 Break
10:40 571 Reaction Paths to Gas Phase Perfluoropropene Formation: A CASMP2 Investigation Edward Ritter, William Kohler and Dorothy Skaf, Villanova University
11:05 572 Thermochemical and Kinetic Analysis on Tertiary Alkyl Radicals with Oxygen: 2-Hydroxy-1,1-Dimethylethyl and 1,1-Dimethylpropyl Radicals Hongyan Sun¹, Joseph W Bozzelli² and Chung K Law¹, (1)Princeton University, (2)New Jersey Institute of Technology
11:30 573 Experimental and Computational Study on Preignition Chemistry of SI Primary Reference Fuels in a Pressurized Flow Reactor Xiaohui Gong, David L Miller and Nicholas P Cernansky, Drexel University

Tuesday, 24 May 2005, 9:00 AM - 5:00 PM
Organic Chemistry
Symposium: Visions In Chemistry
Visions in Chemistry I

Room 111 (Science & Engineering Resource Center)
Organizers: Philip Wientraub, sanofi aventis, Tahir N Majid, sanofi aventis

9:00 Introductory Remarks
9:15 574 Lewis Base Activation of Lewis Acids: New Concepts and Applications Scott E Denmark, University of Illinois, Urbana-Champaign
10:15 575 Peptidoconjugates as cellular and molecular probes of DNA damage Shana Kelley, Boston College
Tuesday, 24 May 2005, 9:10 AM - 12:05 PM
Computers in Chemistry
Symposium: Molecular Modeling throughout the Drug Discovery Process
**Molecular Modeling Throughout the Drug Discovery Process I**

Room 217 (Science & Engineering Resource Center)
Organizers: Wendy D Cornell, Merck & Co, Prabha Karnachi, Johnson & Johnson PRD
Presider: Wendy D Cornell, Merck & Co

9:10                  Introductory Remarks
9:55                  577 Critical Assessment of Docking Programs and Scoring Functions **Greg Warren**, GlaxoSmithKline Pharmaceuticals
10:35                 Intermission
10:45                 578 Rapid and Accurate Protein Side-Chain Prediction **Michael Bower**, Incyte Pharmaceuticals
11:25                 579 An Ab Initio Method for Predicting the Stereochemistry of Drug Intermediates Using NMR **Keith W Wiitala**, Christopher J Cramer and Thomas R Hoye, University of Minnesota

Tuesday, 24 May 2005, 1:20 PM - 5:35 PM
Nano and Materials Science
Symposium: Surface and Interface Science
**Surface and Interface Science II**

Room 204 (Science & Engineering Resource Center)
Organizers: Yves J Chabal, Rutgers University, Theodore E Madey, Rutgers, The State University of New Jersey
Presiders: Yves J Chabal, Rutgers University, Theodore E Madey, Rutgers, The State University of New Jersey

1:20                  580 Water-Hydrophobic Interface at the Nanoscale: Wetting Study Indicates That Water is Separated From the Hydrophobic Walls by the Vapor Gap **Alexander Y Fadeev**, Seton Hall University
1:40                  581 First Principles Resonance Widths and Energies for Ions Scattering off Surfaces: Neutralization Predictions for Scattered Ions **Keith Niedfeldt**, P Nordlander and Emily A Carter, (1)Princeton University, (2)Rice University
2:00                  582 Manipulation of nanoparticles growth on surfaces **Jan Hrbek**, Brookhaven National Laboratory
2:45                  583 Orbital-specific model for chemisorption **Sara E Mason**, Ilya Grinberg and Andrew M Rappe, University of Pennsylvania
3:50   585 Second Harmonic Generation Probe of Dye Molecules Chemically Bonded to Colloidal Particles Jun Han, Holly Hofer, Eric Meggers and Hai-Lung Dai, University of Pennsylvania

4:10   586 Self-Organizing Aromate Films: Architecture and Domain Evolution Janice Reutt-Robey, Bo Xu, Hui Li, Diane Evans, Chenggang Tao and Ellen Williams, University of Maryland

4:55   587 TPR and TEM Study of the Reduction of Cobalt-Silica Catalyst Precursors Roger Barth, West Chester University

Tuesday, 24 May 2005, 1:30 PM - 5:00 PM
Analytical Chemistry Frontiers
Symposium: Applications of LC-MS in Drug Discovery/Development
Applications of LC-MS in Drug Discovery/Development

Room 118 (Science & Engineering Resource Center)
Presider: Guodong Chen, Schering-Plough Research Institute

1:30   Introductory Remarks

1:35   588 Overview of LC/MS in Drug Discovery and Development Birendra N Pramanik, Schering-Plough Research Institute

2:05   589 Applications of Small Molecule Mass Spectrometry in Drug Discovery Manish Soni, Sanofi-Aventis

2:35   590 LC/MS Characterization of Intact Proteins: Open Access and High Throughput Applications Bingbing Feng, GlaxoSmithKline

3:05   Break

3:15   591 Identification of Impurities and Degradation Products in Pharmaceutical Development and Pharmaceutical Products Using LC-MS and LC-MS/MS Jason X Tang, Wyeth Research

3:45   592 LC/MS Degradation Studies in Pharmaceutical Development Charles Pan, Frances Liu and Richard Vivilecchia, Novartis

Tuesday, 24 May 2005, 1:30 PM - 5:00 PM
ADMET at the Crossroads of Drug Discovery
Symposium: Biotransformations

Room 210 (Science & Engineering Resource Center)
Workshop Leader: Vinod Ramachandran, GlaxoSmithKline

1:30   Welcoming Remarks

1:45   593 Minimizing the Potential for Metabolic Activation as an Integral Part of Drug Design David C Evans, Merck

2:15   594 Recent Advances in Extrapolating Preclinical ADME Data to Humans Keith Ward, GlaxoSmithKline

2:45   Break

3:15   595 Cytochrome P450 Reaction Phenotyping Study of Hp184 in Human Liver Microsomes Lijuan Wang, Yongqing Huang and Peter S King, sanofi-aventis
3:45  596  Glucuronosyltransferases (UGTs): Several recent examples in drug development
Donglu Zhang, Bristol-Myers Squibb

Tuesday, 24 May 2005, 1:30 PM - 5:00 PM
Analytical Chemistry Frontiers
College Student Award Symposium sponsored by the Chromatography Forum of Delaware Valley

Room 202 (Science & Engineering Resource Center)
Organizer: Marshall L Fishman, East Reg Res Ctr, ARS, USDA

1:30  597  Headspace SDME Using a Single Solvent: An Application to Residual Solvents Analysis
Derrick C Wood and James M Miller, Drew University

1:55  598  Microwave Extraction of Pectin and Characterization using High Performance Size
Exclusion Chromatography Halla Suleiman1, Hoa Chau1 and Marshall L Fishman2,
(1)USDA/ARS/ERRC, (2)East Reg Res Ctr, ARS, USDA

2:20  599  Thin Layer Chromatography to Separate Triglyceride Lipase Products Ang Bian,
Kavitha Sompalli and Peter M Oelkers, Drexel University

2:45  600  Effects of Echinostoma caproni larval trematode infection on lipids in the medically
important snail Biomphalaria glabrata as determined by HPTLC Sharon R Bandstra,
Bernard Fried and Joseph Sherma, Lafayette College

3:10  601  Effect of Pseudostationary Phase on Fluorescence Intensity in Electrokinetic
Chromatography Stephanie A Schuster and Joe P Foley, Drexel University

3:35  602  Chiral Separations in Microemulsion Electrokinetic Chromatography (MEEKC) Utilizing
a Chiral Surfactant and Chiral Co-Surfactant Kimberly A Kahle and Joe P Foley,
Drexel University

4:00  603  Separation of Metals from Water using Collagen Dispersion Christopher S Cohen,
Widener University

Tuesday, 24 May 2005, 1:30 PM - 5:00 PM
Physical Chemistry
Symposium: Electronic Structure in Chemistry
Electronic Structure in Chemistry II

Room 209 (Science & Engineering Resource Center)
Organizers: Kieron Burke, Rutgers University, Karsten Krogh-Jespersen, Rutgers University
Presider: Karsten Krogh-Jespersen, Rutgers University

1:30  604  Ab Initio electronic structure calculations for N-aromatic assemblies Diane Evans
and Janice Reutt-Robey, University of Maryland

1:45  605  Organic molecules on the Si(100) surface: theory of reactivity and electronic
conductance Doug Doren, Jeff Frey and Zareh Darakjian, University of Delaware

2:15  606  First-principles studies of TiO₂ surfaces, their interactions with water and other small
molecules, and their sensitization by molecular dyes Annabella Selloni, Princeton
University
2:45  607  On the fly orbital localization in ab initio molecular dynamics and its application in
the reaction of organic molecules with semiconductor surfaces Mark E Tuckerman,
New York University

3:15  Break

3:30  608  Temperature effects on magnetic resonance parameters from first principles Daniel
Sebastiani and Jochen Schmidt, Max-Planck Institute for Polymer Research

3:45  609  Implications of Symmetry Rules for the Aromaticity of Inorganic Clusters Clémence
Corminboeuf, R Bruce King and Paul v R Schleyer, University of Georgia

4:00  610  High pressure phase diagram of diamond from first principle molecular dynamics
Xiaofei Wang and Roberto Car, Princeton University

4:15  611  DFT studies of the active center in hydrogenase enzymes Silviu Zilberman, Edward I
Stiefel, Morrel H Cohen and Roberto Car, Princeton University

4:30  612  Modeling NQ-based molecular switch structures: A conformation-energy analysis
Jeanne W Bundsen, Eastern University

Tuesday, 24 May 2005, 1:30 PM - 5:05 PM
Environmental/Green Chemistry
Symposium: Green Chemistry
Green Chemistry II

Room 117 (Science & Engineering Resource Center)
Organizers: Sanjay V Malhotra, New Jersey Institute of Technology, Wen-Chung Shieh, Novartis
Pharmaceuticals
Presider: Wen-Chung Shieh, Novartis Pharmaceuticals

1:30  Introductory Remarks

1:35  613  Microwave-promoted synthesis in water and an investigation of microwave effects in
synthetic chemistry using simultaneous cooling Nicholas Leadbeater, University of
Connecticut

2:05  614  Breaking the Petroleum Feedstock Paradigm: 1,3-Propanediol Production from
Renewable Feedstock Mark H Emptage, DuPont

2:35  615  Ionic Liquids on a Large Scale How They Can Improve Chemical Processes Calvin J
Emanuel, BASF Corporation

3:05  Break

3:20  616  Development of a Green Synthesis for Taxol® Manufacture via Plant Cell
Fermentation and Extraction Jonathan C Walker, Bristol-Myers Squibb Company

3:50  617  Shades of Green Chemistry in Selected Pharmaceutical Processes Shankar
Swaminathan, Bristol Myers Squibb

4:20  618  The Use of TADDOls and Other Diaryl(methanol Derivatives in Enantioselective
Synthesis Dieter Seebach, Eidgenössische Technische Hochschule Zürich - ETH
Hönggerberg
**Tuesday, 24 May 2005, 1:30 PM - 5:00 PM**  
Biomaterials and Polymers  
Symposium: Inorganic and Organometallic Polymers  
**Inorganic and Organometallic Polymers IV**

Room 206 (Science & Engineering Resource Center)  
Organizer: Frieder Jaekle, Rutgers University  
Presider: Frieder Jaekle, Rutgers University

1:30 619 Hybrid metallic nanoparticle/block copolymer systems **Robert B Grubbs**, Liliana A Miinea, Laura B Sessions, David S Glueck and Benjamin R Cohen, Dartmouth College

2:00 620 Oligosiloxycynoureates Mediated Approach to Novel Metal Nano Particles and Their Catalytic Applications **Moni Chauhan¹**, Richard Pantano¹, Gilchris Burton¹, Jitendra S Rathore² and Bhanu P S Chauhan², (1)Queensborough Community College, (2)Nanomaterials Laboratory of Center for Engineered Polymeric Materials, City University of New York at CSI

2:20 621 Synthesis and binding properties of borylated oligo- and polythiophenes **Anand S Sundararaman¹**, Resmi Varughese², Maria Victor¹ and Frieder Jäkle¹, (1)Rutgers University, Newark, (2)Rutgers Newark

2:40 622 Functionalized Polyaniline/Carbon Nanotube Composite for Sensitive Biosensor Applications **Yufeng Ma¹**, Jianming Zhang¹, ali Shah³, Afua S Dodo² and **Huixin He¹**, (1)Rutgers University, (2)Rutgers University, Newark Campus, (3)chemistry department,newark campus, rutgers university

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**Tuesday, 24 May 2005, 1:30 PM - 5:00 PM**  
Medicinal Chemistry  
**Medicinal Chemistry**

Room 216 (Science & Engineering Resource Center)  
Presider: Joel S Freundlich, Jacobus Pharmaceutical Company

1:30 623 Epoxybergamottin as a bioactive compound for functional foods applications **Samineh Madani** and Jack N Losso, Louisiana State University

1:50 624 Synthesis of small molecules designed to complement disease-associated thyroid hormone receptor mutants **A Quamrul Hassan** and John T Koh, University of Delaware


2:30 626 Exploration of the Potential Antifilarial Activity of the Fruit, Leaf and Stem Extracts of Melia azedarach Linn on Cattle Filarial Parasite Setaria Cervi **Qamar U Ahmed¹**, S M K R Zaidi², NU Khan² and KC Singhai², (1)International Islamic University Malaysia, (2)Aligarh Muslim University

2:50 627 Potent, Selective and Low-Calcemic Inhibitors of CYP 24 Hydroxylase: 24-Sulfoximine Analogues of the Hormone 1α,25-Dihydroxyvitamin D₃ **Mehmet**
Kahraman¹, Sandra Sinishtaj¹, Patrick M Dolan¹, Thomas W Kensler¹, Sara Peleg² and Gary H Posner¹, (1)The Johns Hopkins University, (2)The University of Texas


Tuesday, 24 May 2005, 1:30 PM - 5:15 PM
Computers in Chemistry
Symposium: Molecular Modeling throughout the Drug Discovery Process

Molecular Modeling throughout the Drug Discovery Process II

Room 217 (Science & Engineering Resource Center)
Organizers: Wendy D Cornell, Merck & Co, Prabha Karnachi, Johnson & Johnson PRD
Presider: Wendy D Cornell, Merck & Co

1:30  629 Targeting Protein Kinases in Drug Discovery Beth Lunney, Pfizer Global R&D
2:10  630 Design of New AIDS Drugs: A Multi-disciplinary Attack on the Problem of Drug Resistance Kalyan Das¹, Arthur D Clark¹, Yulia Volovik Frenkel¹, Paul J Lewi², Jan Heeres², Marc R de Jonge², Lucien M H Koymans², Paul AJ Janssen², Donald W Ludovici³, Bart De Corte³, Robert W Kavash³, Chih Y Ho³, Hong Ye³, Mark A Lichtenstein³, Michael J Kukla³, Rudi Pauwels³, Koen Andries³, Marie-Pierre de Béthune³, Stephen H Hughes³ and Eddy Arnold⁶, (1)Center for Advanced Biotechnology and Medicine, and Rutgers University, (2)Center for Molecular Design, (3)Janssen Research Foundation, (4)Tibotec, (5)HIV Drug Resistance Program, (6)Rutgers University

2:50  Intermission
3:05  631 Cardiac Ion Channel Pharmacology and Structure-Function Analysis Chris Culberson, Merck & Co, Inc
3:45  632 Patenting 3D Structural Information in the Aftermath of the Trilateral Project Alicia Russo, FITZPATRICK, CELLA, HARPER & SCINTO
4:25  Break
4:35  Panel Discussion -- Career Opportunities in Drug Discovery Molecular Modeling

Tuesday, 24 May 2005, 1:30 PM - 3:05 PM
Medicinal Chemistry
Symposium: Proteinase

Room 203 (Science & Engineering Resource Center)
Organizer: Robert Goodnow Jr, Hoffmann-La Roche
Workshop Leader: Michael Angelastro, Sanofi-Aventis

1:30  Introductory Remarks Michael Angelastro
1:35  633 A Novel Class of Non-Covalent Cathepsins Inhibitors Tae-Seong Kim, Amgen Inc
2:05  634 The Discovery and Development of Non-Covalent Cathepsin S Inhibitors James P Edwards, Johnson & Johnson Pharmaceutical Research and Development
2:35   635 Medicinal Chemistry and Properties of 1,2,4-Thiadiazoles Tim Fat Tam, Regis Leung-Young, Warren Li, Michael Spino and Khashayar Karimian, ApoPharma Inc

Tuesday, 24 May 2005, 1:30 PM - 5:00 PM
Chemistry and the Law
Symposium: Regulatory and Patent Law
Regulatory and Patent Law – the Scientist’s Perspective
Room 212 (Science & Engineering Resource Center)
Organizers: Leticia Quinones, Bristol-Myers Squibb, Jay M Brown, The Eclipse Group
Presiders: Jay M Brown, The Eclipse Group, Leticia Quinones, Bristol-Myers Squibb

1:30    Introductory Remarks
1:35   636 Title: Strategies for Writing Effective Global Patent Applications and Developing Technology Rosemary M Miano, Pfizer Inc
2:55    Break
3:10   638 Contrasting GMP and GLP Requirements for Pharmaceutical Development API Supplies David Kunzinger, Proctor and Gamble Pharmaceuticals
3:50   639 FDA and PhRMA's Current Thinking on Starting Materials Sandeep, P Modi, Bristol-Myers Squibb

Tuesday, 24 May 2005, 1:30 PM - 5:00 PM
College Education
Symposium: Research Funding Opportunities
Research Funding Opportunities
Room 204 (Allison Road Classroom Building)
Organizer: Alexander Grushow, Rider University
Presider: Alexander Grushow, Rider University

1:30    Introductory Remarks
1:35   640 Writing excellent research proposals Edward J J Grabowski and Robert H Rich, American Chemical Society
1:50   641 NSF Chemistry Division programs supporting undergraduate research at predominantly undergraduate institutions Richard D Foust Jr, National Science Foundation
2:05   642 NSF update: What's new at DUE? Kathleen A Parson, Susan Hixson, Harry Ungar and Herbert H Richtol, National Science Foundation
2:35   644 Funding opportunities for faculty at predominantly undergraduate institutions Raymond Kellman, Research Corporation
2:50    Intermission
3:00    Panel Discussion
Tuesday, 24 May 2005, 1:30 PM - 5:00 PM
Physical Chemistry
Symposium: Spectroscopy of Biomolecules, Interfaces and Materials

Spectroscopy of Biomolecules, Interfaces and Materials IV

Room 207 (Science & Engineering Resource Center)
Organizer: Edward W Castner Jr, Rutgers, The State University of New Jersey
Presider: Edward W Castner Jr, Rutgers, The State University of New Jersey

1:30  645  Tracking Amyloid Formation by Single Molecule Spectroscopy Troy C Messina, Jason T Giurleo, Hiyun Kim, Jongjin Jung and David S Talaga, Rutgers University
1:50  646  Molecules at Aqueous Interfaces Kenneth B Eisenthal, Columbia University
2:50  Break
3:20  647  The Influence of Surface Charge on Interfacial Polarity: Does It Matter? Robert A Walker, Carmen Huffman, Milton Liu and Daniel Burden, University of Maryland
4:00  648  Intermediates in Light-driven DNA Repair by Photolyase Robert J Stanley, Zhanjia Hou, Madhavan Narayaran and Goutham Kodali, Temple University
4:40  649  Single-molecule Polyproline Isomerization by Fluorescence Quenching due to Short-range Electron Transfer Hiyun Kim, Youssef Issa, Troy Messina, Jongjin Jung, Jason T Giurleo, Stephen S Isied and David Talaga, Rutgers University

Tuesday, 24 May 2005, 1:30 PM - 5:00 PM
Physical Chemistry
Symposium: Gas-phase Thermochemistry

Thermochemistry and Chemical Kinetics II

Room 218 (Science & Engineering Resource Center)
Organizer: Joseph W Bozelli, New Jersey Institute of Technology
Presider: Joseph W Bozelli, New Jersey Institute of Technology

1:30  650  Assessing the impact of accuracy of ab initio calculations in describing chemically activated systems Ioannis P Androulakis, Rutgers University, Joseph Bozelli, New Jersey Institute of Technology and Timothy A Barckholtz, ExxonMobil Research and Engineering
1:55  651  Complete particle nucleation and growth model: Comparison with the classical nucleation theory Evgeni N Chesnokov, Andrei V Chernyshev and Lev N Krasnoperov, New Jersey Institute of Technology
2:20  652  Development of adaptive chemistry model for combustion simulation Marianthi Ierapetritou and Ipsita Banerjee, Rutgers University
2:45  Break
3:05  653  An Experimental and Theoretical Study of the Gas-Phase Properties of the Natural Base Cytosine and the Damaged Base O-Methylguanine F Sedinam Amegayibor, Yunlin Fu and Jeehiun K Lee, Rutgers University
3:30  654  Thermochemistry, Kinetics and Kinetic Modeling on Atmospheric Reactions of the Benzene-OH Adduct with O2 Chiung-Chu Chen and Joseph W Bozelli, New Jersey Institute of Technology
3:55  655  Comparison of the Ignition Quality of Propane and Dimethyl Ether Timothy A Barckholtz, ExxonMobil Research and Engineering and Xiaoqing You, University of Southern California

4:20  656  Laminar flame speeds and kinetic mechanism predictions for C2 hydrocarbons John T Farrell, ExxonMobil Corporate Research

Tuesday, 24 May 2005, 1:30 PM - 5:00 PM  
Organic Chemistry  
Symposium: Visions In Chemistry  
Visions in Chemistry II

Room 111 (Science & Engineering Resource Center)  
Organizers: Philip Wientraub, sanofi aventis, Tahir N Majid, sanofi aventis

1:30  657  Development of New Tools and Methods for Organic Synthesis Steven V Ley, University of Cambridge

2:30  658  Carbanion-mediated Strategies for Synthetic Aromatic Chemistry Victor Snieckus, Queen's University

3:30  Break

3:50  659  Calcium Channels as Drug Targets: Why Some ARE and Some Are NOT David Triggle, State University of New York at Buffalo

4:50  Concluding Remarks

Tuesday, 24 May 2005, 1:45 PM - 5:00 PM  
Women in Science  
Symposium: Nature/Nurture: Women in Academe  
Nature/Nurture: Women in Academe

Center Hall (Busch Campus Center)  
Organizers: Valerie J Kuck, Seton Hall University, Dr Cecilia H Marzabadi, Seton Hall University  
Presider: Dr Cecilia H Marzabadi, Seton Hall University

1:45  Introductory Remarks


2:20  661  Gender patterns in training and career paths of doctoral students from top-ranked chemistry departments Cecilia H Marzabadi, Janine P Buckner, Susan A Nolan and Valerie J Kuck, Seton Hall University

2:50  662  A Gender Analysis of Employment Trends in Academic Chemistry Janel Kasper-Wolfe, American Chemical Society

3:20  Break

3:30  663  Investigating the role of institution-specific training practices in shaping the early career perceptions and paths of graduates from top-ranked chemistry departments Janine P Buckner, Cecilia H Marzabadi, Susan A Nolan and Valerie J Kuck, Seton Hall University
4:00  664  Leaving Science: Occupational Exit from Scientific Careers Anne Preston, Haverford College  
4:30  665  Coaching Women for Success Sally Chapman, Barnard College  

Tuesday, 24 May 2005, 2:00 PM - 3:30 PM  
Celebrating The Contributions of Chemists  
Symposium: Waksman Celebration  
ACS Waksman Landmark: Discovery of the Actinomycete Antibiotics, An Oral History  
Martin Hall, Cook Campus  

Tuesday, 24 May 2005, 2:00 PM - 4:00 PM  
Careers For Chemists  
Careers Workshops  
Becoming a Teacher at a College/Community College (Panel Discussion)  
Room 120B (Busch Campus Center)  
Workshop Leader: Anita J Brandolini, William Paterson University  

2:00  666  Becoming a Teacher at a College/Community College Panel Discussion Anita J Brandolini, William Paterson University  

Tuesday, 24 May 2005, 2:00 PM - 5:20 PM  
High School Education  
Symposium: Journal Of Chem Ed  
Catalyzing Student Excitement in Chemistry/Science  
Room 203 (Allison Road Classroom Building)  
Organizer: Bettyann Howson, Chatham HS  

2:00  667  Using the Journal as a resource Diana Mason, University of North Texas  
2:25  668  DigiDemos Ed Vitz, Kutztown University  
2:50  669  Odyssey: DiscoveryBased learning with Molecular Simulations Nathan Dacuycuy, Wavefunction  
3:15  670  New Ideas in Interactive Animations and Multimedia Conrad N Trumbore, University of Delaware  
3:40  671  Using Peer Review and Competition to Motivate Learners Diane, L Marturano, Wayne Valley High School  
4:05  672  Young Science Achievers ProgramSM Bobbi Gorman, North Brunswick Township High School  
4:30  673  Chemagination: Write a future feature article for ChemMatters Magazine Marisa Burgener, American Chemical Society  
4:55  674  Chemistry Clubs and Special Activities John Dantoni, Wayne Valley High School
Tuesday, 24 May 2005, 2:00 PM - 4:30 PM
High School Education
Symposium: AP Chemistry
Pedagogical Mnemonics: AP, POGIL, Etc

Room 207 (Allison Road Classroom Building)
Organizer: Bettyann Howson, Chatham HS

2:00  675  AP Chemistry Test Development Process John Gelder, Oklahoma State University
2:25  676  AP Grader Remarks Karen L Galley, West Windsor-Plainsboro High School South
2:50  677  POGIL: A Student-Centered Approach to Teaching Chemistry Richard S Moog, Franklin & Marshall College
3:15  678  Laboratory Activities to Reinforce Concepts for Advanced Placement Chemistry NJACS Teacher Affiliates, c/o Diane Krone
3:40  679  POGIL: Guided Inquiry Laboratory Experiments for the General Chemistry Laboratory Richard S Moog, Franklin & Marshall College
4:05  680  Mathematics in Biology: Nothing to Fear and Much to Gain L Charles Biehl and Dr Thomas C Fleetwood, The Charter School of Wilmington

Tuesday, 24 May 2005, 2:00 PM - 3:30 PM
High School Education
Symposium: PowerPoint in Education
PowerPoint in Education

Room 308 (Allison Road Classroom Building)
Organizer: Bettyann Howson, Chatham HS
Workshop Leader: Patricia Duncan, High Point HS

2:00  681  Powerpoint Presentations in Chemistry Patricia Duncan, High Point HS

Tuesday, 24 May 2005, 2:30 PM - 7:00 PM
ADMET at the Crossroads of Drug Discovery
ADMET Posters

Poster Areas (Busch Campus Center)
Organizers: Anita J Brandolini, William Paterson University, Donglu Zhang, Bristol-Myers Squibb

682  Distribution of Periodontopathic Bacteria Among Asian Indians Shari Smith, Elizabeth Pelaez, Raji Subramaniam and Patricia Schneider, Queensborough Community College

683  Essential Fatty Acid Metabolizing Enzymes Expression in the Developing Rat Placenta and Trophoblastic Models Yan Xu, Gregory T Knipp and Thomas J Cook, Rutgers, the State University of New Jersey

684  Preliminary Oral Pharmacokinetics of the Potential Chemopreventive Agents Farnesol and Geraniol Joseph G Desiderio, Harold Newmark and Thomas J Cook, Rutgers, the State University of New Jersey
Tuesday, 24 May 2005, 2:30 PM - 7:00 PM
College Education
College Education Posters

Poster Areas (Busch Campus Center)

685 First-Year Organic Problems that Promote Student Reasoning Ray A Gross Jr, Prince George's Community College

686 Synthesis and Study of Silver Nanoparticles Sally D Solomon, adviser and principle author Solomon Sally II, Aravindan V Jeyarajasingam and Mozghan Bahadory, Drexel University

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

688 Development of laboratory experiments for the undergraduate forensic biochemistry laboratory Francis Charles Mayville Jr, William Farina, Derick Siegel and Edward Fleming, DeSales University

689 Development of laboratory experiments for the undergraduate forensic biochemistry laboratory Francis Charles Mayville Jr and Nicole Beyer, DeSales University

690 A POGIL- and Project-Based Approach to Chemical Literacy for Non-Science Majors A Bryan Lees, Kean University

691 The Use of Chiral Oxazolidinones in an Advanced Instructional Synthesis Lab S Shaun Murphree and Matthew P Betush, Allegheny College

Tuesday, 24 May 2005, 2:30 PM - 7:00 PM
Physical Chemistry
Symposium: Electronic Structure in Chemistry
Electronic Structure Posters

Poster Areas (Busch Campus Center)

Organizer: Anita J Brandolini, William Paterson University

692 Rydberg excitation energies from LDA Adam Wasserman and Kieron Burke, Rutgers University

693 Negative ions on the verge of ionization Kieron Burke and Vazgen Shekoyan, Rutgers University

694 Double excitations in density functional theory Fan Zhang¹, Neepa T Maitra², Robert J Cave³ and Kieron Burke¹, (1)Rutgers University, (2)Hunter College of CUNY, (3)Harvey Mudd College

695 Computational Studies of Benzyl-Substituted Halonium Ions Ronald R Sauers, Rutgers University and Howard Haubenstock, The City University of New York, The College of Staten Island

696 Computational Machinery of Nuclear Shielding Keith W Wiitala, University of Minnesota

697 Charge Transfer Energies and Electronic Coupling across Peptides with Different Dihedral Angles: Ramachandran Electronic Coupling Surfaces for Different Peptides Youssef Issa, Karsten Krogh-Jespersen and Stephan Isied, Rutgers University
Tuesday, 24 May 2005, 2:30 PM - 7:00 PM
Organic Chemistry
Organic Posters II

Poster Areas (Busch Campus Center)
Organizers: Anita J Brandolini, William Paterson University, Cecilia H Marzabadi, Seton Hall University

698 Ligand-Free Palladium-Catalyzed Cyanation of Aryl Halides Steven Weissman, Daniel Zewge
and Cheng Chen, Merck

699 Synthesis of a Merck NK-1 receptor antagonist Jason J Kowal, Merck & Co

700 Addition Of Cuprates To Spirodiepoxides Derived From Allenes: A Concise Stereocontrolled
Synthesis Of α-Hydroxyketones Partha Ghosh and Lawrence J Williams, Rutgers University

701 Preparation of 2-benzamidoindanone semicarbazone derivatives as insecticides Elizabeth G
Rowley, Daniel H Cohen, Ellen M Crawford, Louis V LaFrance, Ernest L Plummer and David M
Roush, FMC Corporation

702 Preparation and reactions of chiral 2-oxazolinyloxy-substituted carbanions Lesley-Ann Nelson
and Sasan Karimi, Queensborough C C

703 A Geminal Chlorolactone Reaction Andrew T Bach¹, Raymond A Baylouny², Edgar Leone³ and
Willis B Hammond³, (1)Novartis Pharmaceuticals, (2)Fairleigh Dickinson University (College at
Florham), (3)Honeywell Corporation

704 Synthesis and Biophysical Studies of c-di-GMP Zhaoying Zhang, Barbara L Gaffney and Roger
A Jones, Rutgers, The State University of New Jersey

705 Preparation and reactions of 2-imidazolinyloxy-substituted carbanions Shazim Mobin and
Sasan Karimi, Queensborough Community College

706 A Practical One-Pot Preparation of 7-Hydroxyquinoline R Scott Hoerrner, Mark Cameron,
Shawn Springfield, James McNamara and Ulf Dolling, Merck & Co

707 Improved Method for Synthesis of DNA and RNA Containing a Thioalkyl Tether in the Minor
Groove at Guanine for Crosslinking to Protein Xiaorong Hou, Gang Wang, Barbara L Gaffney
and Roger A Jones, Rutgers University

708 Major Differences in RNA Metal Biding Motifs Determined by ¹⁵N NMR Yupeng Fan, Barbara L
Gaffney and Roger A Jones, Rutgers, the State University of New Jersey

709 Substituent Effects for Two Series of Substituted N-Benzylideneanilines Using NMR
Spectroscopy John Tierney¹, Linda M Mascavage² and Christopher Dieterick², (1)Pennsylvania
State University, (2)Arcadia University

710 Efficient Preparation of Acyclic Amidinium Salts by Orthoester Exchange and Amidinium Salt
Transamination Shahrokh Saba, Adeline Kojtari, Marinda M Rivera, Peter D’Amico, Dana
Canuso and Moses K Kaloustian, Fordham University

711 An approach to syntheses of tetrahydroisoquinoline compounds Bradley M Hutnick¹, Lynn M
Bradley¹ and David A Hunt², (1)The College of New Jersey, (2)Albany Molecular Research

712 Synthesis and Reactions of Bicyclic Cyclopropylamines from Intramolecular Cylopropanation
of Amino Acid Derivatives Catherine A Faler and Madeleine M Joullie, University of Pennsylvania

713 Synthesis of new cyclin dependent kinase 2 inhibitors Ayana Moses and Kwesi Amoa, Medgar
Evers College
714 Assignment of 13C Chemical Shifts to Ring Carbons of Acetophenones Donald D Clarke, Fordham University

715 Structure-based design, synthesis and structure-activity relationship of peptide libraries containing Phe analogs as reversible inhibitors for thrombin Cristina C Clement and Manfred Philipp, Lehman College, City University of New York (CUNY)

716 Highly Efficient Synthesis of b-Amino Acid Derivatives via Asymmetric Hydrogenation of Unprotected Enamines Yi Hsiao1, Nelo R Rivera1, Thorsten Rosner1, Shane W Kraska1, Eugenia Njolito1, Fang Wang1, Yongkui Sun1, Joseph D Armstrong III1, Edward J J Grabowski1, Richard D Tillyer1, Felix Spindler2 and Christophe Malan2, (1)Merck Research Laboratories, (2)Solvias

717 Reactivity Of Tris(Trimethylsilyl)Phosphite (TMSP): Attempt to prepare the N-mustard-bis phosphonic acid of Bicine Ji Suh, Queensborough Community College, St John's University, Luis Vargas, Queensborough Community College and Ralph Stephani, St John's University

718 "Instant methyliide" modification of the Corey-Chaykovsky cyclopropanation reaction James A Ciaccio, Courtney E Aman and Shahrok Saba, Fordham University

719 S-Benzyl thiglycosidic mycothiol analogue Michael Smerina and Spencer Knapp, Rutgers University

720 P-Glycosyl-phosphonothiate O,O'-diesters Kehinde A Ajayi and Spencer Knapp, Rutgers University

721 The Synthesis of a TMC-95 Intermediate from N-Boc-Tryptophan Ahalya Ramanathan and Leslie, S Jimenez, Rutgers, The State University of New Jersey

722 Study of the Selectivity of the Lithiation of Secondary and Tertiary 3,5-Difluoro-Substituted Benzamides Michael D Green1, Francesca Khani1, Lynn M Bradley1 and David A Hunt2, (1)The College of New Jersey, (2)Albany Molecular Research

723 Synthesis and Characterization of a Naphthoquinone Derived Amino Acid Bruce R Lichtenstein1, Ronald L Koder2 and P Leslie Dutton2, (1)University of Pennsylvania, (2)The Johnson Foundation and the University of Pennsylvania

724 Facile one pot synthesis of heterocycles from allenes and mechanistic insight on the opening of spirodipoxides Stephen D Lotesta, Sreenivas Katukojvala, Sezgin Kiren, R R Sauers and Lawrence J Williams, Rutgers University

725 Thioamides Via Thiatriazolines Robert V Kolakowski, Ning Shanngguan and Lawrence Williams, Rutgers University

726 Stereoselective Synthesis of Alpha-hydroxy Ketones: Addition of Carbon Nucleophiles to Spirodipoxides Jennifer Inghrim and Lawrence J Williams, Rutgers University

727 Studies Towards the Total Synthesis of Psymberin Ning Shangguan, Sezgin Kiren and Lawrence Williams, Rutgers, The State University of New Jersey

728 Stereoselective Synthesis of 1, 5 S-thiodisaccharides from L-Arabinose Enones Zbigniew J Witzczak and David Lorchak, Wilkes University, Nesbitt Schoolof Pharmacy

729 The development of a reliable, highly sensitive technique to determine the metal ion concentration of cells using exciton-coupled circular dichroism Samuel A Simpson, New York University

730 Total Synthesis of Cyclopeptide Alkaloid Hymenocardine Galina V Kapustin, Rao N Nallagancho, Weiying Yang and Madeleine M Joullié, University of Pennsylvania
Tuesday, 24 May 2005, 2:30 PM - 7:00 PM
Biomaterials and Polymers
Symposium: Polymeric Biomaterials
Polymeric Biomaterials Posters

Poster Areas (Busch Campus Center)
Organizers: Anita J Brandolini, William Paterson University, Kathryn E Uhrich, Rutgers University
Presider: Thomas J Cook, Rutgers, the State University of New Jersey

731 Mesoporous Silicate Materials as Carriers for Poorly Water-Soluble Drugs Rupali Shah¹, Shannon Dugan², Shannon Verissimo², Melissa Zastrow² and Isabelle Lagadic*², (1)University of Connecticut, Department of Chemistry, (2)University of Connecticut

732 Electrospinning of porous silica micro/nanofibers containing silver nanoparticles Alpa C Patel and Yen Wei, Drexel University

733 Methacrylate-silica nanocomposite dental materials with low volume shrinkage Zhengfei Sun, Yen Wei, Praveen Solomon and Guoliang Yang, Drexel University

734 The use of carboxymethylcellulose as a drug carrier Megan Nollenberger and Christine Martey-Ochola, Shippensburg University

735 Synthesis and Characterization of Poly(vinyl acetate)-graft-PDMS Copolymers Sarah E Grieshaber and Yadunandan L Dar, National Starch and Chemical Company

736 Amphiphilic-scorpion like macromolecules (ASCMs): efficient carriers for intracellular drug delivery Jelena Djordjevic and Kathryn E Uhrich, Rutgers University

737 Long-circulating cylinder micelles demonstrate the strong effects of morphology on biological transport and interactions Yan Geng, University of Pennsylvania, Paul Dalhaimer, Yale University, Peter Photos, Princeton University and Dennis Discher, Univ Pennsylvania

738 Improved detection sensitivity in ELISAs by multi-labeled enzyme DNA dendrimers conjugated to anti-riboin antibodies Johanna R Mora and Robert C Getts, Genisphere

739 Amphiphilic Star-like Macromolecules for targeted drug delivery yichao Zhang, Rutgers University

740 Synthesis and Hydrolytic Stability of Poly(oxyethylene phosphonate)s with Different Macromolecular Architecture Bogdana Goryanova¹, Kolio Troev² and Ivan Gitsov¹, (1)SUNY College of Environmental Science and Forestry, (2)Bulgarian Academy of Sciences

741 Effect of the Linker Structure on Salicylic Acid-Derived Poly(Anhydride-Esters) Almudena Prudencio, Robert Schmeltzer and Kathryn Uhrich, Rutgers, The State University of New Jersey

742 Microspheres Prepared from Salicylate-Based Poly(anhydride-esters) Brian A Yeagy, Robert Schmeltzer, Almudena Prudencio, Kathryn E Uhrich and Thomas J Cook, Rutgers, The State University of New Jersey

743 Antioxidant-Based Poly(anhydride-esters) : polymer properties and cytotoxicity results Youngmi Kim and Kathryn E Uhrich, Rutgers University

744 Differential Scanning Calorimetry of an Amorphous Phase Formed During Thermal Processing of PLA/PMMC Composites Payal G Patel, Kim-Phuong N Le and Richard L Lehman, AMIPP Advanced Polymer Center, Rutgers University

745 Evidence of an Intermediate Amorphous Phase in PLA/PMMc Thermal Blends Kim-Phuong N Le, Richard L Lehman and James D Idol, AMIPP Advanced Polymer Center -- Rutgers University
746  Using Supercritical CO₂ for polymer/drug formation into microspheres Princy Varughese, Ke Wu and Jing Li, Rutgers, The State University of New Jersey

747  Biodegradable polymer with different morphologies formed by precipitation with super- and sub-critical antisolvent Ke Wu, Jianjun Luo and Jing Li, Rutgers, The State University of New Jersey

748  Rheological Characterization of Hydrogels Assembled via Heparin-Peptide Interactions Le Zhang, Nori Yamaguchi and Kristi L Kiick, University of Delaware

Tuesday, 24 May 2005, 3:30 PM - 5:00 PM
High School Education
Symposium: Computer Simulations
Computer Simulations (Workshop)

Room 308 (Allison Road Classroom Building)
Organizer: Bettyann Howson, Chatham HS

3:30  749  Interactive Web Based Inquiry Labs John Gelder, Oklahoma State University

Tuesday, 24 May 2005, 4:00 PM - 5:00 PM
Celebrating The Contributions of Chemists
Symposium: Waksman Celebration
ACS Waksman Landmark Plaque Presentation

Martin Hall, Cook Campus

Tuesday, 24 May 2005, 4:00 PM - 5:00 PM
High School Education
Symposium: North Jersey American Chemistry Society - Teacher Affiliates
North Jersey American Chemistry Society Teacher Affiliates

Room 205 (Science & Engineering Resource Center)
Organizer: Bettyann Howson, Chatham HS

4:00  750  Odyssey Workshop Nathan Dacuycuy, Wavefunction

Tuesday, 24 May 2005, 7:00 PM - 8:30 PM
High School Education
Chemical Education At It's Best: Keynote Address and Teacher Awards

Room 111 (Science & Engineering Resource Center)
Organizer: Bettyann Howson, Chatham HS

7:00  MARM Teacher of The Year Award

7:15  Recognition of North Jersey Merrill Awardee

7:30  751  Weird Science: A Phenomenological Approach to Teaching Lee Marek, University of Illinois at Chicago [Weird Science, ]
Tuesday, 24 May 2005, 7:00 PM - 8:15 AM
Keynote Presentation

beta and gamma Peptides: Synthesis, Structure and Biomedical Potential D. Seebach

Lecture Theatre (Fiber Optics)
Organizer: Wen-Chung Shieh, Novartis Pharmaceuticals
Presider: Wen-Chung Shieh, Novartis Pharmaceuticals
Wednesday, 25 May 2005

Wednesday, 25 May 2005, 9:00 AM - 12:00 PM
Organic Chemistry
Symposium: Advances In Organic Chemistry
Advances in Organic Synthesis

Room 111 (Science & Engineering Resource Center)
Presider: Spencer Knapp, Rutgers University

9:00  752  Spriodiepoxides: Mechanism, Methods and Applications Lawrence J Williams, Rutgers University
9:45  753  Development and Application of New Synthetic Methods Gary Molander, University of Pennsylvania
10:30  754  Syntheses of Complex, Bioactive Natural Products Erik Sorensen, Princeton University
11:15  755  Synthetic Studies on Heterocyclic Natural Products Marco A Ciufolini, University of British Columbia

Wednesday, 25 May 2005, 9:00 AM - 12:00 PM
Analytical Chemistry Frontiers
Symposium: Applications of Vibrational Spectroscopy in Forensic Science
Applications of Vibrational Spectroscopy in Forensic Science I

Room 210 (Science & Engineering Resource Center)
Organizer: Gene Hall, Rutgers University
Presider: Gene Hall, Rutgers University

9:00  756  IR Microscopes in Forensic Science: Past, Present, and Future John A Reffner, Smiths Detection
9:35  757  Spectrochemical Analysis and Spectral Imaging of Latent Fingerprints and Trace Evidence Included within the Prints Edward G Bartick¹, Diane K Williams¹, Heather L Peters¹, Rebecca L Schwartz¹, Nicole J Crane², Rohit Bhargava³, Daniel Fernandez³, Scott W Huffman³ and Ira Levin³, (1)FBI Laboratory, (2)Oak Ridge Institute for Science and Education (ORISE), (3)National Institutes of Health
10:05  758  Use of Drop Coated Deposition Raman (DCDR) for Detection of Explosives Katia Rothhaar⁴, Jimmy Oxley⁵, Dor Ben-Amotz⁵, Dongmao Zhang⁶, Yong Xie⁶, Corasi Ortiz⁶ and Jo Davisson³, (1)Tienta Sciences, (2)University of Rhode Island, (3)Purdue University
10:35  Morning Break
11:00  759  Applications of Spectroscopy in a Museum Janice H Carlson and Jennifer L Mass, Winterthur Museum
11:30  760  Creation of an ATR-FT-IR Spectral Database of Nail Lacquer Enamel for Use in Forensic Science Laurie E Smith and Gene S Hall, Rutgers University
Wednesday, 25 May 2005, 9:00 AM - 12:00 PM
College Education
Symposium: Forensic Chemistry Education
Forensic Chemistry Education

Room 202 (Science & Engineering Resource Center)
Organizer: Laurence J Boucher, Towson University
Presider: Laurence J Boucher, Towson University

9:00  761  Forensic Science Education Program Accreditation Commission: Accreditation Standards Peter R De Forest, John Jay college of Criminal Justice / CUNY
9:30  762  Challenges of an Undergraduate Forensic Chemistry Curriculum Helen G Reid, West Chester University
9:50  763  Forensic Chemistry at a Community College Ray A Gross Jr, Prince George's Community College
10:10  764  Overview of the Forensic Chemistry and Forensic Science Programs Sherry T Brown, York College of Pennsylvania
10:30  Break
10:40  765  Internships at the New Jersey State Police Crime Laboratory through Partnership Thomas A Brettell, New Jersey State Police
11:00  766  Experiences, Explorations and Research in a Forensic Chemistry Course: Forensic Chemistry at The College of New Jersey John Allison, The College of New Jersey
11:20  767  Forensic Science Education: More Programs, Lower Standards? Lawrence Kobilinsky and Henrietta Margolis-Nunno, John Jay College of Criminal Justice, CUNY
11:40  768  Designing Forensic Science Curriculums to Meet Current and Furture Challenges Brian J Gestring, Pace University

Wednesday, 25 May 2005, 9:00 AM - 12:00 PM
Analytical Chemistry Frontiers
Symposium: Functional Proteomics and Cell Signaling
Functional Proteomics, Cell Signaling and Disease Biomarkers

Room 209 (Science & Engineering Resource Center)
Workshop Leader: Thomas A Neubert, New York University School of Medicine

9:00  769  Novel Multiplexed CSF Biomarkers for Antemortem Alzheimer's Diagnosis Kelvin H Lee, Erin Finehout, Zsofia Franck, Leila Choe and Norman Relkin, Cornell University
9:30  770  Serum peptide signatures of solid tumor cancers Paul Tempst and Josep Villanueva, Memorial Sloan-Kettering Cancer Center
10:00  771  A Mass Spectrometry-Based Quantitative View of Protein Phosphorylation Roland S Annan, Francesca Zappacosta, Dean McNulty, Micheal Huddleston and Therese Sterner, GlaxoSmithKline Pharmaceuticals
10:30  Break
10:45  772  The identification of possible blood proteins as biomarkers for atherosclerotic plaque Stanley A Hefta, Bristol Myers Squibb Co
11:15 773 Functional Proteomics of Ephrin Signaling Thomas A Neubert, Daniel S Spellman and Guoan Zhang, New York University School of Medicine

Wednesday, 25 May 2005, 9:00 AM - 12:00 PM
Nano and Materials Science
Symposium: NanoScience and Technology
NanoScience and Technology
Room 204 (Science & Engineering Resource Center)
Organizers: Yves J Chabal, Rutgers University, Eric Garfunkel, Rutgers University
Presiders: Yves J Chabal, Rutgers University, Eric Garfunkel, Rutgers University

9:00 774 Self-Organization of Nanoscaled Photonic Materials Charles Michael Drain, Hunter College - CUNY


9:45 776 Time Resolved Decay Dynamics and Mechanism of Energy Transfer in Undoped and Mn2+ Doped ZnSe Nanoparticles Christian D Grant¹, Edward M Olano², Thaddeus J Norman Jr³, Edward W Castner Jr¹ and Jin Z Zhang¹, (1)Rutgers, The State University of New Jersey, (2)University of California Santa Cruz, (3)Lawrence Livermore National Laboratory

10:00 777 Nanocrystals and Nanocrystal Assemblies: Building with Artificial Atoms Christopher B Murray, E Shevchenko and D Talapin, IBM Corp, T J Watson Research Center

10:45 778 Supramolecular Extension of pi-Conjugation in Conjugated Oligomers Tsunehiro Sai, Polytechnic University

11:00 779 Integration of Semiconductor Nanowire Array onto Si Chips Using Highly Aligned DNA Strands as Scaffolds Yufeng Ma¹, Jianming Zhang² and Huixin He¹, (1)Rutgers University, (2)Rutgers University, Newark Campus

11:30 780 Formation of nano-particles by rapid expansion of supercritical solutions: In situ characterization by laser scattering Takuya Matsunaga, Andrei V Chernyshev and Lev N Krasnoperov, New Jersey Institute of Technology

11:45 781 The Effect of Polyelectrolytes on the Aggregation of Cyanine Dyes in Langmuir-Blodgett Films and in Aqueous Solution; Some Kinetic Aspects of J-Aggregates Hussein Samha, Southern Utah University

Wednesday, 25 May 2005, 9:15 AM - 12:00 PM
Biomaterials and Polymers
Symposium: Tissue Engineering and Cell-material Interactions
Tissue Engineering and Cell-Material Interactions
Room 205 (Science & Engineering Resource Center)
Organizers: Treena Livingston Arinzeh, New Jersey Institute of Technology, Michael Jaffe, New Jersey Institute of Technology

9:15 782 Protein Biomaterial Communication with Stem Cells to Control Tissue Outcomes David Kaplan, Tufts University
9:45  783 Substrate Elasticity Directs Adult Mesenchymal Stem Cell Differentiation Adam J Engler, Mark F Berry, H Lee Sweeney and Dennis E Discher, University of Pennsylvania

10:15  784 Conformational Behavior of Alanine-Rich Protein Polymers with Varying Functional Group Placement Robin S Farmer, Lindsey M Argust, Jared A Sharp and Kristi L Kiick, University of Delaware

10:45  Break


11:30  787 Neuronal cell guidance and protein adsorption on a melt-crystallized binary polymer blend Andrea Tuckett and Kalle Levon, Polytechnic University

11:45  786 Withdrawn

Wednesday, 25 May 2005, 9:30 AM - 12:30 PM
Celebrating The Contributions of Chemists
Symposium: Waksman Celebration
ACS Waksman Landmark: Celebrating Waksman

Room 117 (Science & Engineering Resource Center)
Presiders: Arnold Demain, Drew University, Douglas Eveleigh, Rutgers University

9:30  Welcoming Remarks

9:45  Plaque presentation to the Waksman Institute: Joachim Messing

10:00  788 Natural product antibiotics from actinomycetes - past, present and (hopefully) future William Strohl, Merck and Company

10:30  789 Why aren't we finding antibiotics as easily as we used to? Julian Davies, University of British Columbia

11:00  790 Soil as a source of genes encoding the production of novel anti-microbials Gerben Zylstra, Boris Wawrik and Jerome J Kukor, Cook College, Rutgers University

11:15  791 Small-molecule inhibitors of bacterial RNA polymerase J Mukhopadhyay1, E Sineva2, YW Ebright1, V Mekler1, A Volkov1, A Srivastava1, A Kravets1, D Wang1, X Wang1, S Ismai1, S Sarafianos2, S Tuske2, B Hudson2, A Clarke2, J Birktoft2, C Dharia2, M Bayro2, GVT Swapna2, J Huang2, LC Ma2, J Knight2, O Laptenko2, J Lee3, S Borukhov3, H Berman2, E Arnold2, G Montelione2, R Levy2 and RH Ebright1, (1)Howard Hughes Medical Institute, Rutgers University, (2)Rutgers University, (3)UMDNJ-Stratford

11:30  792 TB: Global Time bomb Lee Reichman, University of Medicine and Dentistry of New Jersey

12:00  793 Actinomycete secondary metabolites: gifts from the soil Arnold Demain, Drew University

Wednesday, 25 May 2005, 9:30 AM - 11:30 AM
Chemical Engineering
Electrostatic Hazards and the Control Of Dust Explosions
Electrostatic Hazards and the Control Of Dust Explosions (Workshop)

Room 260 (Wright Lab)
9:30  794  Electrostatic Hazards and the Control Of Dust Explosions  Vahid Ebadat, Chilworth Technology, Inc

**Wednesday, 25 May 2005, 1:00 PM - 4:30 PM**  
Organic Chemistry  
Symposium: Enantioselective Reactions and Synthesizes  
**Enantioselective Reactions and Synthesizes**

Room 117 (Science & Engineering Resource Center)  
Organizer: David A Conlon, Merck & Co, Inc

1:00  795  Biocatalysis: Synthesis of Chiral Intermediates for Drugs  Ramesh N Patel, Bristol-Myers Squibb

1:45  796  Stereoselective Synthesis of a Merck Anti-HIV Drug Candidate and Studies in the Development of the Mo-Catalyzed Asymmetric Alkylation Reaction  Michael Palucki, Merck and Co

2:30  797  Strained Silacycles: A Powerful Platform for Asymmetric Reaction Design  James L Leighton, Columbia University

3:15  798  Asymmetric Catalysis in the Synthesis of Stereochemically Complex Targets  Eric N Jacobsen, Harvard University

**Wednesday, 25 May 2005, 1:00 PM - 3:30 PM**  
Chemical Engineering  
**Microreactors and Microreaction Systems**  
**Microreactors and Microreaction Systems for Development and Production (Workshop)**

Room 260 (Wright Lab)  

1:00  799  Microreactors and Micro-reaction Systems for Development and Production  Craig Wurzel, Invenios, Inc and Thomas Dietrich, mikroglas Chemtec GmbH

**Wednesday, 25 May 2005, 1:30 PM - 5:00 PM**  
Analytical Chemistry Frontiers  
Symposium: Applications of Vibrational Spectroscopy in Forensic Science  
**Applications of Vibrational Spectroscopy in Forensic Science II**

Room 210 (Science & Engineering Resource Center)  
Organizer: Gene Hall, Rutgers University  
Presider: Gene Hall, Rutgers University

1:30  800  Novel Method for ATR Microanalysis of Multilayer Paint Chips  Thomas J Tague Jr, Bruker Optics

2:00  801  Applications of Raman Spectroscopy in Forensics Science  Fran Adar¹, Sergey Mamedov¹, Andrew Whitley¹ and Luc Brazeau², (1)Horiba Jobin Yvon, (2)Canada Border Service Agency

2:30  802  Deployment and Use of Infrared Microspectroscopy in Mobile Laboratories: Forensic and Homeland Defense Applications  John A Seelenbinder, Kenneth J, Fredeen and Mark L Norman, Smiths Detection

3:00  Break
3:20  803  Utilization of FT-IR and Raman Spectroscopy in a Crime Laboratory Phil Antoci, NYPD Crime Lab
3:50  804  What Can Raman Spectroscopy Do For the Forensic Scientist? Diane Allen, Renishaw Inc
4:20  805  Use of Vibrational Spectroscopy to Characterize Counterfeit Banknotes and Postage Stamps Gene S Hall, Rutgers University

Wednesday, 25 May 2005, 1:30 PM - 5:00 PM
Organic Chemistry
COPE Scholar Symposium
COPE Scholar Symposium

Room 118 (Science & Engineering Resource Center)
Organizers: Cecilia H Marzabadi, Seton Hall University, R David Crouch, Dickinson College
Presider: R David Crouch, Dickinson College

1:30  806  Hydrocarbon Oxidation Methods for Synthesis M-Christina White, Harvard University
2:50  808  Regiocontrolled Synthesis of substituted 2-pyrones and Their Synthetic Applications Cheon-Gyu Cho, Hanyang University
3:30  809  Synthetic Approaches Towards a Preclinical Target Molecule Todd D Nelson, Merck Research Laboratories
4:10  810  Multicomponent, Sequential Ring-Forming Reactions Gary H Posner, The Johns Hopkins University

Wednesday, 25 May 2005, 1:30 PM - 5:00 PM
Biomaterials and Polymers
Symposium: Catalytic Routes to Novel Biomaterials
Catalytic Routes to Novel Biomaterials

Room 205 (Science & Engineering Resource Center)
Organizer: Richard A Gross, Polytechnic University

1:30  811  Lipase Catalysis: Monomer, Macromer and Polymer Synthesis Richard A Gross, Polytechnic University
2:00  812  Enzymatic Catalysis in Supersaturated Solutions Evgeny N Vulfson, Akzo Nobel Chemicals
2:30  813  Enzyme Immobilization onto Polymeric Supports M Elizabeth Miller, James C Bohling, Marlin K Kinzey, James F Tate, Jr, Mark J VanderHoff and William J Zabrodski, Rohm and Haas Company
3:00  Break
3:30  814  Biosynthesis of Sopholipids by Candida Bombicola Using Industrial Fatty Acid Residues and Its Anti-HIV/Spermicidal Activity Vishal Shah, Arthur Felse, Gustavo F Doncel and Richard A Gross, (1)Polytechnic University, (2)CONRAD
3:45  815 Fermentative Production of Sophorolipids by Candida bombicola Using Industrial Fatty Acid Residues and its Anti-HIV/Spermicidal Activity Vishal Shah¹, P Arthur Felse¹, Gustavo F Doncel² and Richard Gross¹, (1)Polytechnic University, (2)CONRAD

4:00  816 Regioselective Modification of Starch Nanoparticles by CAL-B Soma Chakraborty, Columbia University and Richard Gross, Polytechnic University

4:15  817 Crosslinking/Branching Studies for Polymers Synthesized By Chemical Versus Enzyme-Catalyzed Synthetic Methods Wei Gao, Jun Hu, Ankur S Kulshrestha, Wenchun Xie and Richard A Gross, Polytechnic University

4:30  818 Self-Assembly of Fermentative products from Candida bombicola Shuiqin Zhou¹, Chang Xu¹, Jun Wang¹, Wei Gao², Rena Akhverdiyeva², Vishal Shah² and Richard Gross², (1)CUNY College of Staten Islande, (2)Polytechnic University

Wednesday, 25 May 2005, 1:30 PM - 4:00 PM
Celebrating The Contributions of Chemists
Celebrating Chemists and Chemistry, NJ and Beyond!

Room 211 (Science & Engineering Resource Center)
Organizer: Jeannette E Brown, 2004 Société Fellow Chemical Heritage Foundation
Presider: Jeannette E Brown, 2004 Société Fellow Chemical Heritage Foundation

1:30  Welcoming Remarks

1:35  819 Plumbago, Bamboo, and Goldenrod - Thomas Edison and God’s Almighty Warehouse Kevin Olsen, Montclair State University

1:55  820 Thomas Edison, Chemist Jeannette E Brown, 2004 Société Fellow Chemical Heritage Foundation

2:15  Break

2:35  821 Seven Twists of Fate That Propelled the Explosive 1918-1940 Growth of the US Chemical Enterprise Donald G Hicks, Georgia State University


Wednesday, 25 May 2005, 1:30 PM - 5:00 PM
College Education
Symposium: Process Oriented Guided Inquiry Learning POGIL

Process Oriented Guided Inquiry Learning POGIL

Room 202 (Science & Engineering Resource Center)
Organizer: Richard S Moog, Franklin & Marshall College

1:30  Welcoming Remarks

1:35  823 Process Oriented Guided Inquiry Learning and the POGIL Project Richard S Moog, Franklin & Marshall College

2:00  824 POGIL and PLTL: Contrast and Comparison Thomas H Eberlein, Penn State Schuylkill, The Capital College

2:25  825 POGIL in a Graduate Molecular Spectroscopy Course for High School Chemistry Teachers Susan R Phillips, University of Pennsylvania
2:50  Intermission

3:00  **826** Teaching reasoning process in organic chemistry using electron energies **R Daniel Libby** and Carl Salter, Moravian College

3:25  **827** Student Resistance to POGIL Implementation in an Organic Chemistry Course **Kelly E Butler**, Chestnut Hill College

3:50  **828** The POGIL (Process-Oriented Guided-Inquiry Learning) Laboratory **Frank J Creegan**, Washington College

4:15  Panel Discussion

**Wednesday, 25 May 2005, 3:00 PM - 4:00 PM**
Celebrating The Contributions of Chemists
Team Innovation Award Symposium (Award)

**Regional Industrial Innovation Award Symposium**

Center Hall (Busch Campus Center)
Organizer: Vanessa Johnson-Evans, American Chemical Society
Presider: Vanessa Johnson-Evans, American Chemical Society

3:00  **829** Recognizing scientists behind research & development **Vanessa Johnson-Evans**, American Chemical Society