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 **Aakruti 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**[1], Joanna Aizenberg[2] and Bernice Feuer[1], (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

10:00		Introductory Remarks
10:05	**35**	Seeing Chemistry Non-visually; Using Talking Lab Tools to Assist a Blind Student's Ambitions in the Laboratory **Cary A Supalo**, Pennsylvania State University
10:45	**36**	Robotics as a Vehicle to Achievement, Entrepreneurship and Higher Education **Peter Kieselbach**, Pharmacopeia Drug Discovery, Inc
11:15		Break
11:30	**37**	Non-Engineering Mentoring **Kathie Kentfield**, Co-Founder, NEMO (Non-Engineering Mentor Organization), FIRST Robotics
12:00		Lunch
1:00	**38**	FIRST Robotics in the classroom **David Beck**, Palisades High School
1:30	**39**	There's No Wrong Way To Get Involved **Sabrina Marie Varanelli**, Pope John XXIII Regional High School
2:00		Break
2:15	**40**	Student Mentorship of FIRST LEGO League **Rebecca Kieselbach**, Palisades High School
2:45	**41**	Life skills learned through FIRST robotics **Patrick Bogard**, Johns Hopkins University

Sunday, 22 May 2005, 1:00 PM – 2:00 PM

Teambuilding Workshop

Room 207 (Science & Engineering Resource Center)

Presider: Kathie Kentfield

1:00	**42**	Teambuilding - Getting Your Introverts to Work Together! **Kathie Kentfield**, FIRST Robotics Team 173 - East Hartford and Rockville High Schools

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

10:00	**43**	Volcanoes of the Deep Sea: An IMAX Film **Richard Lutz and Peter rona**, Rutgers University

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 Break

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

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

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

8:30	**77**	Stealth Polymeric Nanoparticles for Drug Delivery Devices **Emmanuel O Akala**, Oluyomi Okunola and Gaofeng Pan, School of Pharmacy, Howard University
9:00	**78**	Encapsulation of Drug Nanoparticles in Self-Assembled Macromolecular Nanoshells **Michael Pishko**, Alisar Zahr and Cheryl Rumbarger, Penn State University
9:30	**79**	Polymersomes & related Nanotransforming Carriers for Drug Delivery **Dennis Discher**, Univ Pennsylvania

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 Yildiz[1], Elise Lorenceau[2], Andrew S Utada[2], David A Weitz[2], Robert K Prud'homme[1] and **Douglas H Adamson**[1], (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 Chen**[1], Latha M Santhakumaran[2], Sandhya K Nair[2], Thresia Thomas[2], T J Thomas[2] and Huixin He[1], (1)Rutgers University, (2)UMDNJ-Robert Wood Johnson Medical School
11:45	**85**	Synthesis and Characterization of Collagen Mimetic Peptide Conjugated Gold Nanoparticles **Xiao Mo**, Yoojin An, Allen Y Wang and Michael S Yu, The Johns Hopkins University

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

8:50		Introductory Remarks
9:20	**92**	Understanding the folding mechanism of beta-hairpins **Feng Gai**, University of Pennsylvania
9:00	**93**	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
10:00		Break
10:30	**94**	Two dimensional infrared spectroscopy of biologically relevant systems **Robin M Hochstrasser**, University of Pennsylvanie
11:30	**95**	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

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

9:00	**96**	Density and Coulomb's Law: Two Under-Utilized Concepts in General Chemistry **Parinbam (RAJ) K Thamburaj**, Ohio University- Zanesville
9:25	**97**	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
9:50	**98**	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
10:15	**99**	Microscale Experiments for the General Chemistry Laboratory **Arden P Zipp**, Marcia Bonneau and Irene Maffetore, SUNY College at Cortland
10:40	**100**	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
11:05	**101**	Using Software to Simplify Grading Labs and Making Pre-Labs **Charles H Mahler**, Lycoming College
11:30	**102**	Economies of Scale: Bio, Materials, and Environmental Sections of General Chemistry Lab **Joseph T Keiser**, Penn State University

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 Yuan**[1], Diane Shevell[1], Peter S Linsley[2], Patricia A Detmers[1] and John R Thompson[1], (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 Ding**[1], Mitch Kostich[2], Luquan Wang[3], Ping Qiu[1], Jonathan Greene[1] and Marco Hernandez[1], (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 Yurke**[1], David C Lin[2] and Noshir A Langrana[2], (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

9:05 **122** Development of Aniline amides Containing Alternative Cores as Orally Active P38 MAP kinase Inhibitors **Katerina Leftheris**, John Hynes, Jr, Alaric Dyckman, Tianle Li, Shuqun Lin, Stephen T Wrobleski, 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

9:35 **123** Inhibitors of mitogen-activated protein (MAP) kinases synthesized by parallel solution- and solid-phase methods **Jeremy Green**, Vertex Pharmaceuticals

10:05 **124** Design, Synthesis and SAR of Pyrimidopyrimidines, Dual KDR/FGFR TyrosineKinase Inhibitors **Pamela Rossman**, Hoffmann-La Roche

10:35 Coffee Break

11:00 **125** Discovery of BMS-354825, a dual Src/Abl kinase inhibitor with potent anti-tumor activity in preclinical assays **Louis J Lombardo**, Francis Y Lee, Ping Chen, Derek Norris, Joel C Barrish, Kamelia Behnia, Amy Camuso, Stephen Castaneda, Lyndon A M Cornelius, Jag Das, Arthur M Doweyko, Krista Fager, Christine Flefleh, Craig Fairchild, John T Hunt, Ivan Inigo, Kathy A Johnston, Amrita Kamath, David Kan, Herbert Klei, Roger Luo, Punit Marathe, Suhong Pang, Russell Peterson, Sidney Pitt, Gary L Schieven, Robert J Schmidt, John Tokarski, Mei-Li Wen, Robert Wild, John Wityak and Robert M Borzilleri, Bristol-Myers Squibb Pharmaceutical Research Institute

11:30 **126** Discovery of novel p38 MAP kinase inhibitors: **Gulzar Ahmed**, Pharmacopeia Drug Discovery Inc

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

9:00 **127** Overview of Pharmaceutical Profiling in Drug Discovery **Edward H Kerns**, Wyeth Research

9:15 **128** In Silico Model for CYP Inhibition **Roy J Vaz**, Sanofi Aventis Pharmaceuticals

9:55 **129** Deciphering the Role of Drug Transporters in Early Drug Development: Cell Culture Models and Approaches **Patrick Sinko**, Rutgers University

10:35 Break

10:50 **130** Biochemical and Molecular Assays In Early Toxicity Assessments: A Tier Approach **Prathibha S Rao**, sanofi-aventis

11:30 **131** Prediction of P450 Mediated Reactive Intermediate Formation **Ken Korzekwa**, Merck Research Laboratories

Monday, 23 May 2005, 9:00 AM - 12:00 PM
Nano 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
11:00	**135**	Optimized Synthesis, Elucidation of Structures, and Properties for Porous Materials **John B Parise**, State University of New York
11:30	**136**	High Porosity TiO2 via Inorganic- Salt Porogens **Charlie C Torardi**[1], C Roger Miao[1], C Ed Greer[1] and John Gavenonis[2], (1)DuPont Central Research and Development, (2)DuPont Titanium Technologies

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)

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

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

10:20 **145** Preparation of Enamides via Palladium-Catalyzed Amidation of Enol Tosylates **Artis Klapars**, Kevin R Campos, Cheng-yi Chen and Ralph P Volante, Merck & Co, Inc

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 Zhang**[1], Thomas J Emge[2], Rajshekhar Ghosh[2] and Alan S Goldman[2], (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 Gultneh**[1], Yohannes, T Tesema[1], Teshome B Yisgedu[1], Raymond J Butcher[1],

Guang-bin Wang[2] and Gordon Yee[2], (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 Introductory Remarks

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 Rosuvastatin **Liyue Huang**, AstraZeneca

10:45 Break

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 Soroka**[1], István Pelczer[1], Sarah Ralston[2] and Elissa Lappostato[2], (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-Fe_2O_3 Core/Au Shell Nanoparticles as a Means of Selective Magnetic Separations of Mixtures of DNA **Rebecca A Grimme**[1], John N Richardson[1] and Mary Elizabeth Williams[2], (1)Shippensburg University of Pennsylvania, (2)The Pennsylvania State University

165 Interaction of N-methylmesoporphyrin IX NMM with Quadruplex DNA formed from Scerevisae 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**[1], Paris Svoronos[1], Kathryn Emanuele[2] and Vincent DiProssimo[2], (1)Queensborough Community College, (2)Food and Drug Administration

170 Exploring Protein Structure in a Biochemistry Laboratory Experiment **Lisa Christadore**[1], Dean Del Geurcio[2] and Amber Flynn Charlebois[2], (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 Japeth 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**[1], Ralph Stephani[2] and Luis Vargas[1], (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

181 Neighboring Group Carbamate Participation in the Synthesis and Reactions of Dibromo- and Bromo-hydroxy-2-azanorbornanes **Kevin C Cannon**[1], Asha Mathews[1], Nini L Garcia[1], Chirdeep K Patel[1], Ryan A Centafont[2] and Grant R Krow[2], (1)Penn State Abington, (2)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**[1], Jun H Shin[1] and Gopal Subramaniam[2], (1)Queensborough Community College, (2)Queens College

186 Computation of Organic Carbon Acids **Daqing Gao**, Paris Svoronos, Tianchu Xu and Debbie Maddelena, 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 Benzylic Hydrogens **Hector Mavromatis**[1], Sasan Karimi[1], Pedro Irigoyen[1], Paris Svoronos[1] and David Locke[2], (1)Queensborough Community College, (2)Queens College

190 Synthesis of New Types of Quaternary Ammonium Ionic Liquids **Heidi Martinez**[1], Hughton Walker[2], Vanessa Hernandez[1], Robert Engel[2] and Sharon Lall-Ramnarine[1], (1)Queensborough Community College, CUNY, (2)Queens College, CUNY

191 Synthesis of ionic liquids containing ether and hydroxyl substituted cations **Kijana Kerr**[1], Hughton Walker[2], Vanessa Hernandez[1], Robert Engel[2] and Sharon Lall-Ramnarine[1], (1)Queensborough Community College, CUNY, (2)Queens College, CUNY

192 Synthesis and characterization of chiral ionic liquids **Marie Thomas**[1], Jasmine Hatcher[2], Leah Rothman[1], Sharon Lall-Ramnarine[2] and Robert Engel[1], (1)Queens College, CUNY, (2)Queensborough Community College, CUNY

193 Investigation of the Structure/Property Relationship of New Ionic Liquids **Hughton R Walker**[1], Marie Thomas[1], Vanessa Hernandez[2], Sofiya Penkhasova[2], Heidi Martinez[2], Kijana Kerr[2], Jasmine Hatcher[2], Robert Engel[1] and Sharon Lall-Ramnarine[2], (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 Hernandez**[1], Hughton R Walker[2], Sofiya Penkhasova[1], Robert Engel[2] and Sharon Lall-Ramnarine[1], (1)Queensborough Community College, CUNY, (2)Queens College, CUNY

195 Characterization of the physical properties of new ionic liquids **Sofiya Penkhasova**[1], Hughton R Walker[2], Heidi Martinez[1], Jasmine Hatcher[1], Vanessa Hernandez[1], Robert Engel[2] and Sharon Lall-Ramnarine[1], (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 Lammers**[1], S A Gould[2], A B Bocarsly[2] and G A Arbuckle-Keil[1], (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 Loo**[1], Steve Tse[1], Wendy Mays[1], Nicole Loo[2] and Nordulf Debye[1], (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 Nirode, Hofstra University

210 Correlation of the van't Hoff Factor with the Concentration of Inorganic Solutes Using Computer Interface Freezing Point Depression Measurements **Jorge Ubillus**, 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 Czerw[1], **Gregory F Herzog**[2], John Krenos[2], Joseph A Potenza[2], Paul Schueler[1] and Diane C Trainor[3], (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

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

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 Rockerfeller 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 Presbyterian 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**[1], Yi He[2], Yan Zheng[3] and Alexander Van Geen[1], (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
Symposium: Assuring Water Purity
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

3:30 **253** The Utilization of Common Paramater Monitoring as an on-Line Surveillence Tool for Water Security: Identifying Distribution System Incursions through the Use of Interpretive Algorithms **Dan Kroll** and Karl King, Hach Homeland Security Technologies

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 Gallagher**[1], George Preti[1], Russell Bazemore[1], James J Leyden[2], Arlene Foglia[2] and Andrew I Spielman[3], (1)Monell Chemical Senses Center, (2)University of Pennsylvania, (3)NYU

3:30 **259** MHC-related Odorprints in Mice **George Preti**[1], Alan Willse[2], Gary K Beauchamp[1], Kunio Yamazaki[1], Peter Yang[1] and Jon H Wahl[2], (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

1:30 **261** Practical synthesis and crystal structure of GlcNAc-thiazoline **Richard A Huhn**, Thomas J Emge and Spencer Knapp, Rutgers University

1:50 **262** Synthesis and crystal structure of GlcNAc-thiazoline-6-O-tetradecanoate **David Fash**, Thomas J Emge and Spencer Knapp, Rutgers University

2:10 **263** Developing the Structure-Activity Relationships for cADPR: Conformational Analysis of cADPR Analog Agonists and Antagonists **Steven M Graham**, St John's University

2:30 **264** Short route to octosyl nucleosides **Vinay V Thakur**, Machender Madduru, Krishnan Malolanarasimhan and Spencer Knapp, Rutgers University

2:50 **265** 2'-Deoxynucleosides through 2'-thio-S-acetyl participation **Srihari Pabbaraja** and Spencer Knapp, Rutgers University

3:10 **266** Carbohydrate-fused heterocycles: Preparation and further transformations **Cecilia H Marzabadi** and Michael De Castro, Seton Hall University

3:30 **267** Synthesis of 1-C-elaborated GalNAc-thiazolines **Benjamin Amorelli** and Spencer Knapp, Rutgers University

3:50 **268** Vinyl glycosides and carbohydrate vinyl ethers: Synthesis and applications **Robert Giuliano**, Kevin Hughes, Christopher Cummings and Tuan Nguyen, Villanova University

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

1:30 Introductory Remarks

1:40 **269** Molding an Innovation to Market Needs: A Critical Key to a Start-up's Success! **Joe D'Antuono**, ROW2 Techologies, Inc

2:20 **270** From a Eureka Moment to a Clinical Candidate: a Case Study of a PolymerDrug™ **Karen Giroux**, Polymerix Corporation

3:00 Q&A, Discussion I Moderator: Judith Sheft

3:10 Break

3:30 **271** HydroGlobe - Commercializing an Innovative Water Purification Technology **John Schroeder**, Graver Technologies llc, Hydroglobe Div

4:10 **272** Commercialization of Nanocomposite Barrier Coatings **Harris Goldberg**, Inmat, Inc

4:50 Q&A, Discussion II Moderator: Judith Sheft

5:00 Concluding Remarks

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 anticoagulantion blood and it's membrance 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 Norman**[1], Robert Ivkov[2], Jeffrey G Forbes[3] and Sandra C Greer[1], (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 Arnold**[1], Steven Tuske[2], Stefan G Sarafianos[1], Xinyue Wang[2], Brian Hudson[2], E Sineva[2], Jayanta Mukhopadhay[1], Jens J Birktoft[2], Oliver Leroy[2], Sajida Ismail[2], Arthur D Clark Jr[1], Chhaya Dharia[1], Andrew Napoli[1], Oleg Laptenko[3], Jookyung Lee[3], Sergei Borukhov[3] and Richard H Ebright[2], (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 Revyakin[1], Chenyu Liu[1], Terence Strick[2] and **Richard H Ebright**[1], (1)Howard Hughes Medical Institute, Rutgers University, (2)Institut Jacques Monod

4:25 **287** Single-molecule-spectroscopy analysis of transcription **Achillefs Kapanidis**, University of Oxford

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 Romanyshyn, 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 Bessel**[1], Donna Omiatek[1], Susan Thai[1], Georgia C Papaefthymiou[1], Arthur Viescas[1], Douglas A Blom[2] and Lawrence F Allard[2], (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**[1], Kirstan Bowser[1] and Tamara Bell[2], (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

4:15 **307** Optical Switching Properties of Dye Doped Organic/Inorganic Composite Films **Nathan Stevens** and Daniel L Akins, The City College of New York

Monday, 23 May 2005, 1:30 PM - 5:00 PM
Physical Chemistry
Symposium: Spectroscopy of Biomolecules, Interfaces and Materials
Spectroscopy of Biomolecules, Inferfaces 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

4:20 **312** Conformational Dynamics in Triplet Repeat Models of DNA **Benjamin J Lee**, Maryan Barch, Jens Völker, Edward W Castner Jr and Kenneth J Breslauer, Rutgers, The State University of New Jersey

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

313 Today's Chemical Technician –How ACS Can Help Your Career! **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

316 Process Development for Pilot Plant Synthesis of Methyl 2-Bromo-6-chlorobenzoate **Matthew R Hickey**, Shawn P Allwein, Todd D Nelson, Michael H Kress, Osama S Sudah, Mahmoud Kaba, Aaron J Moment and Paul Fernandez, Merck Research Laboratories

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 **Lifen Shen** and Dimuthu Jayawickrama, Bristol Myes Squibb

321 A Novel IGF-IR signaling inhibitor: A Challenge to Process Chemists **Joel S Slade**, Joginder Bajwa, Prasad Kapa, Hui Liu, John Calienni, James Vivelo, David Parker, Guang-Pei Chen and Edwin Villhauer, Novartis Pharmaceutical Corp

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 Guttarla, 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 Sabean, Community College of Denver

325 FAD Synthetase is slightly promiscuous **David M Yearsley**[1], William S McIntire[2] and Robert J Stanley[1], (1)Temple University, (2)Department of Veterans Affairs Medical Center

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

327 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

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

329 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

330 Comparison of Chondroitinase Digestion on Rat Spinal Cord Using Anion Exchange Chromatography **Rohini D'Souza**, William J Dollard, Anthony O Caggiano, Gargi Roy, Yelena G Sheptovitsky, Sarah J Kasperbauer and Elliott Gruskin, Acorda Therapeutics

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

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

333 Electrostatic interaction between supramolecular host-guest assembly and zinc-substituted cytochrome c **Cynthia Pagba**[1], Jane M Vanderkooi[2], Kurt Deshayes[3], Eugene Piatnitski[4] and Piotr Piotrowiak[1], (1)Rutgers University at Newark, (2)University of Pennsylvania, (3)Genentech Incorporated, (4)Imclone Systems

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

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

336 Bromoindoles and Bromotryptophan: Origin and Application of Red-Shifted UV Spectra **Ann E Shinnar**[1], Sevan Ozcetinkaya[2] and Dina C Merrer[2], (1)Lander College, (2)Barnard College

337 Ab initio and Density Functional Calculations of the Nucleic Acid Bases in Free and Watson-Crick Hydrogen-bonded States **A R Srinivasan, PhD**[1], Ronald R Sauers[1], Marcia O Fenley[2], Alexander H Boschitsch[3], Atsushi Matsumoto[4], Andrew V Colasanti[1] and Wilma K Olson[1], (1)Rutgers University, (2)Florida State University, (3)Continuum Dynamics, Inc, (4)Quantum Bioinformatics Group

338 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)

339 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

Presider: Alan S Goldman, Rutgers 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 Venkatasubbaiah**[1], Lev N Zakharov[2], Scott Kassel[2], Arnold L Rheingold[2] and Frieder Jäkle[1], (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 Porphryins, 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 Kim**[1], C A Heyer[1], M Berardini[1], D M Ho[2] and GM Arvanitis[1], (1)The College of New Jersey, (2)Princeton University

356 Copper(II) Complexes of Tetradentate 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

Monday, 23 May 2005, 2:30 PM - 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

358 Synthesis of 3-beta-acyloyloxy-4,6-pregnadiene-6,20-dione derivatives as antiandrogens **Elena Ramirez**[1], Eugene Bratoeff[1], Marisa Cabeza[2], Victor Perez[1], David Valdez[1], Alejandro Orozco[1] and Alejandra Munguia[1], (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-Mensah**[1], Regina Sullivan[1] and Susan A Rotenberg[2], (1)Queensborough Community College, (2)Queens College

361 Analysis and Interpretation of DNA to Metallated and Nonmetallated Tetrapyridino 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 PPAR$\alpha/\delta/\gamma$ 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

369 Synthesis of 3-Substituted Cyclopent[a]pyrrolo[3,4-c]carbazole-5,7-dione Analogs as Potent Cell Permeable Inhibitors of PARP-1 **Allison L Zulli**, James L Diebold, Ron Bihovsky, Edward R Bacon, Jean Husten, Mark Ator and Robert L Hudkins, Cephalon, Inc

370 Developing novel inhibitors of the enoyl reductase from Mycobacterium tuberculosis (InhA): SAR studies of triclosan congeners **Todd J Sullivan**[1], Polina Novichenok[1], James J Truglio[1], Francis Johnson[1], Richard A Slayden[2] and Peter J Tonge[1], (1) Stony Brook University, (2)Colorado State University,

371 Regio- and Stereospecific Syntheses of Syn- and Anti-1,2-Imidazolylpropylamines from the Reaction of 1,1'-Carbonyldiimidazole 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

372 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

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

374 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

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

376 Strategies and Techniques of Major Metabolite Profiling for Structure Optimization in Drug Discovery **Mei-Yi Zhang**, Teresa Kleintop, Natasha Kagan and Edward Kerns, 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

377 Sorption Properties of Pure Silica ITQ-13 **Aleksandra Biedron**[1], Miguel Camblor[2], David Olson[1] and Jing Li[1], (1)Rutgers, The State University of New Jersey, (2)Institute of Materials Science of Madrid (CSIC), Campus Cantoblanco

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

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

380 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

381 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

382 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 $(M_2Q_2)L$ and Mn doped $(M_2Q_2)L$ (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 Whaley**[1], Martha Greenblatt[1], Mark C Croft[2] and Kandalam V Ramanujachary[3], (1)Rutgers, The State University of New Jersey, (2)Rutgers University, (3)Rowan University

388 Synthesis of $SrLaFeO_3H_x$ **Sibel Dikmen**, Viktor V Poltavets and Martha Greenblatt, Rutgers, The State University of New Jersey

389 $Sr_3Fe_{1225}Mo_{0775}O_7$, a Unique n = 2 Ruddlesden-Popper Phase with a Metal-Insulator Transition **Louis W Whaley**[1], Martha Greenblatt[1], Mark C Croft[2], Kandalam V Ramanujachary[3], Maxim Lobanov[1] and Denis Sheptyakov[4], (1)Rutgers, The State University of New Jersey, (2)Rutgers University, (3)Rowan University, (4)Paul Scherrer Institute

390 Isothermal section of the $Na_{03}CoO_2$ - H_2O 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

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 Kapetanaki**[1], Xiangbo Zhao[2], Richard S Magliozzo[2] and Johannes P M Schelvis[1], (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 Piotrowiak[1], **Mykhaylo Myahkostupov**[2], Dong Wang[2], Qian Wei[2] and Elena Galoppini[2], (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

Lecture Theatre (Fiber Optics)

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

8:30 **406** Potential Synergies of Tailored Branching and Intermolecular Interactions: From Gene Transfer Agents to Elastomers and Fibers **Timothy E Long**, Matthew McKee, John Layman, Serkan Unal, Afia Karikari and Casey Elkins, Virginia Tech

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 Talanov**[1], Hisataka Kobayashi[1], Marcelino Bernardo[1], Moinuddin Hassan[2], Amir H Gandjbakhche[2], Peter L Choyke[1] and Martin W Brechbiel[1], (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 Ludescher**, 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 Funston[1], Tomasz Szreder[1], Edward W Castner Jr[2], Hideaki Shirota[2] and Tania Fadeeva[2], (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 Funston[2], James F Wishart[2] and Edward W Castner Jr[1], (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 McMorrow[1] and Matthew C Beard[2], (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 Winnik[2], B Buckley[2] and TJ Cook[1], (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 Zheng[2], Zhongqi Cheng[3] and David C Locke[2], (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-Drowos[1], Linda Betz[2], Justin Miscavige[1], **Nisreen Madhoun**[1] and Joe Di Bussolo[3], (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 Martin**[1], Kristin L Main[1], Amy K Pyles[1] and David M Loveless[2], (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

433 Vibrational Circular Dichroism: Absolute Configuration Determination **Linda M Phillips**, Jack Z Gougoutas, Stephen K Gozo and Michael Galella, Bristol-Myers Squibb

434 Fuzzy relational clustering of molecular conformations using novel features based on DNA base-pair step parameters **Milind Misra**[1], Deepa Pai[1], Rohan Woodley[1], Amit Banerjee[1], Rajesh N Davé[1], Liang-Yu Shih[1], Xiang-Jun Lu[2], A R Srinivasan, PhD[2], Wilma K Olson[2] and Carol A Venanzi[1], (1)New Jersey Institute of Technology, (2)Rutgers University

435 Comparative Study of Docking Programs GLIDE and GOLD for Virtual Screening **Zhiyong Zhou**[1], Anthony K Felts[2], Matt Repasky[3], Ronald M Levy[2] and Richard A Friesner[1], (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 Lee**[1], Mark E Tuckerman[1] and Glenn Martyna[2], (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 Szalewicz**[1], Alston J Misquitta[1], Rafal Podeszwa[1] and Bogumil Jeziorski[2], (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 Faassen**[1], Robert van Leeuwen[1], Kieron Burke[2] and Paul L de Boeij[1], (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

9:30 **449** New Technologies for the Sample Preparation of Organic Compounds **Ronald E Majors**, Agilent Technologies, Inc

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

11:10 **452** Ultra-High Pressure Liquid Chromatography and Pharmaceutical R&D Laboratories **Kelly Swinney**, Johnson & Johnson Pharmaceutical Research & Development LLC and Adam M Fermier, Johnson & Johnson Pharmaceutical Research & Development, LLC

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 Triphenyltins 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 Hausner**[1], Daniel R Strongin[1] and Richard J Reeder[2], (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 Usher**[1], Daniel R Strongin[1] and Martin A A Schoonen[2], (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 Hao**[1], Daniel R Strongin[1], Eelin Lim[1] and Martin A A Schoonen[2], (1)Temple University, (2)State University of New York at Stony Brook

461 Pyrite oxidation in the environment and the effect of bacteria **Jun Hao**[1], Daniel R Strongin[1], Eelin Lim[1], Martin A A Schoonen[2] and David Vuong[1], (1)Temple University, (2)State University of New York at Stony Brook

Tuesday, 24 May 2005, 9:00 AM - 1:30 PM
Graduate
Graduate Posters
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**[1], JA Gamboa[1], A Sundararaman[1], F Jakle[1], Arnold L Rheingold[2] and Lev Zakharov[2], (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**[1], Grant Krow[1], Ryan A Centafont[1] and Kevin C Cannon[2], (1)Temple University, (2)Penn State Abington

465 Synthetic Studies Towards Ustiloxin Natural Products **Cory D Evans**, Pixu Li and Madeleine M Joullié, 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 **Lubabalo 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 Unviversity, (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
10:55	**486**	Maraviroc (UK-427,857) The Process chemists tale **Jens Ahman**, Sarah J Haycock-Lewandowski, Nicola Mawby, Alex Wilder and Steve Challenger, Pfizer

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 BH_3 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 Staen 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 Piotrowiak 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 Caulfield
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 Burns[1], Madeley Alcala[2], Syeda Islam[2] 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 Chauhan[1], **Wayne Narain**[1], Umar Latif[2] and Bhanu PS Chauhan[3], (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 Hydrosilylation of Alkenes and Alkynes Bhanu PS Chauhan[1], Moni Chauhan[2], **Gilchris O Burton**[2] and Umar Latif[3], (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 nano-patterned 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 Jiang**[1], Eric Garfunkel[1], Nikolai Zhitenev[2] and Zhenan Bao[3], (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, Kimloan 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 Arnold**[1], Yulia Frenkel[2], Arthur D Clark Jr[1], Kaylan Das[2], Yuh-Hwa Wang[3], Paul J Lewi[4] and Paul A J Janssen[2], (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 **Shiby 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 Tribe, 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 Clement**[1], Manfred Philipp[1] and Christian Matthaeus[2], (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 Assembeld 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 Rivillon**[1], Kenneth A Bratland[1], Yves J Chabal[1], Fabrice Amy[2], Antoine Kahn[2] and Marek P Boleslawski[3], (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 Goncharova**[1], Dmitri Starodub[1], Robin Barnes[1], Eric Garfunkel[1], Torgny Gustafsson[1], Genadii Bersuker[2], Brendan Foran[2] and Pat Lysaght[2], (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 Bozzelli[1], **Eric E Moore**[1] and John T Farrell[2], (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 Sun**[1], Joseph W Bozzelli[2] and Chung K Law[1], (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
9:15	**576**	Protein Ensemble Docking: A Robust, General Strategy for Greatly Enhanced Lead Docking **Daniel L Cheney** and Luciano Mueller, Bristol-Myers Squibb PRI
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**[1], P Nordlander[2] and Emily A Carter[1], (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
3:05	**584**	Structure in Self-Assembled Organic Thin Films: Chirality, Nano-patterns, and Interaction Energies **Steven L Bernasek**[1], Feng Tao[1] and Yuguang Cai[2], (1)Princeton University, (2)Brookhaven National Laboratory

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
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 Suleiman**[1], Hoa Chau[1] and Marshall L Fishman[2], (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 TiO_2 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 Bundens**, 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 Diarylmethanol 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 Chauhan**[1], Richard Pantano[1], Gilchris Burton[1], Jitendra S Rathore[2] and Bhanu P S Chauhan[2], (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 Sundararaman**[1], Resmi Varughese[2], Maria Victor[1] and Frieder Jäkle[1], (1)Rutgers University, Newark, (2)Rutgers Newark

2:40 **622** Functionalilzed Polyaniline/Carbon Nanotube Composite for Sensitive Biosensor Applications Yufeng Ma[1], Jianming Zhang[2], ali Shah[3], Afua S Dodoo[3] and **Huixin He**[1], (1)Rutgers University, (2)Rutgers University, Newark Campus, (3)chemistry department,newark campus, rutgers university

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

2:10 **625** Potent, low-calcemic, selective inhibitors of CYP24 hydroxylase: 24-sulfone analogs of the hormone 1α,25-dihydroxyvitamin D_3 Gary H Posner, Kenneth R Crawford, Hong Woon Yang, Mehmet Kahraman, Heung Bae Jeon, Hongbin Li, Jae Kyoo Lee, Byung Chul Suh, Mark A Hatcher, Tanzina Mirza, **Aimee Usera**, Patrick M Dolan and Thomas W Kensler, The Johns Hopkins University

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 Ahmed**[1], S M K R Zaidi[2], NU Khan[2] and KC Singhal[2], (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 D_3** Mehmet

Kahraman[1], **Sandra Sinishtaj**[1], Patrick M Dolan[1], Thomas W Kensler[1], Sara Peleg[2] and Gary H Posner[1], (1)The Johns Hopkins University, (2)The University of Texas

3:10 **628** Structure-based Design of a Barbiturate Containing Inhibitor of MMP-13 **William Pitts**, Soong-Hoon Kim, Andrew Pudzianowski, Kenneth J Leavitt, Joseph Barbosa, Patricia A McDonnell, Bruce M Rankin, Richard Liu, Wayne Vacarro, William Metzler, Steven Sherriff and Bruce Jacobson, Bristol-Myers Squibb

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 Das**[1], Arthur D Clark[1], Yulia Volovik Frenkel[1], Paul J Lewi[2], Jan Heeres[2], Marc R de Jonge[2], Lucien M H Koymans[2], Paul AJ Janssen[2], Donald W Ludovici[3], Bart De Corte[3], Robert W Kavash[3], Chih Y Ho[3], Hong Ye[3], Mark A Lichtenstein[3], Michael J Kukla[3], Rudi Pauwels[4], Koen Andries[4], Marie-Pierre de Béthune[4], Stephen H Hughes[5] and Eddy Arnold[6], (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-Toung, Warren Li, Michael Spino and Khashayar Karimain, 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

2:15 **637** Current Developments in Federal Circuit Court Decisions on Patent Law: What Scientists Need to Know **Jay M Brown**, The Eclipse Group

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

2:20 **643** The Camille and Henry Dreyfus Foundation **Gerard L Brandenstein III**, The Camille and Henry Dreyfus Foundation, Inc

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 Bozzelli, New Jersey Institute of Technology

Presider: Joseph W Bozzelli, 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 Bozzelli, 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 Bozzelli, 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

1:50 **660** A Comparison of the Doctoral Achievement Rates in STEM Fields: Does Gender Affect the Yields? **Valerie J Kuck**, Buckner Janine P, Marzabadi Cecilia H and Nolan Susan A, Seton Hall University

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 Program[SM] **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 **Mozhgan 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 Zhang**[1], Neepa T Maitra[2], Robert J Cave[3] and Kieron Burke[1], (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 Bach**[1], Raymond A Baylouny[2], Edgar Leone[3] and Willis B Hammond[3], (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 ^{15}N 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 Tierney**[1], Linda M Mascavage[2] and Christopher Dieterick[2], (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 Hutnick**[1], Lynn M Bradley[1] and David A Hunt[2], (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 Hsiao[1], **Nelo R Rivera**[1], Thorsten Rosner[1], Shane W Krska[1], Eugenia Njolito[1], Fang Wang[1], Yongkui Sun[1], Joseph D Armstrong III[1], Edward J J Grabowski[1], Richard D Tillyer[1], Felix Spindler[2] and Christophe Malan[2], (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, StJohn's University, Luis Vargas, Queensborough Community College and Ralph Stephani, St John's University

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

719 S-Benzyl thioglycosidic 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 Green[1], **Francesca Khani**[1], Lynn M Bradley[1] and David A Hunt[2], (1)The College of New Jersey, (2)Albany Molecular Research

723 Sythesis and Characterization of a Naphthoquinone Derived Amino Acid **Bruce R Lichtenstein**[1], Ronald L Koder[2] and P Leslie Dutton[2], (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 spirodiepoxides **Stephen D Lotesta**, Sreenivas Katukojvala, Sezgin Kiren, R R Sauers and Lawrence J Williams, Rutgers University

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

726 Stereoselective Synthesis of Alpha-hydroxy Ketones: Addition of Carbon Nucleophiles to Spirodiepoxides **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 Witczak** 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 Shah**[1], Shannon Dugan[2], Shannon Verissimo[2], Melissa Zastrow[2] 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-scoripion 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-biotin 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 Goryanova**[1], Kolio Troev[2] and Ivan Gitsov[1], (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/PMMA 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/PMMA Thermal Blends **Kim-Phuong N Le**, Richard L Lehman and James D Idol, AMIPP Advanced Polymer Center -- Rutgers University

746 Using Supercritical CO_2 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		Gene Hall, presider
9:05	**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 Bartick**[1], Diane K Williams[1], Heather L Peters[1], Rebecca L Schwartz[1], Nicole J Crane[2], Rohit Bhargava[3], Daniel Fernandez[3], Scott W Huffman[3] and Ira Levin[3], (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 Rothhaar**[1], Jimmy Oxley[2], Dor Ben-Amotz[3], Dongmao Zhang[3], Yong Xie[3], Corasi Ortiz[3] and Jo Davisson[3], (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

9:15 **775** A Unique Approach towards the Design of Nano-Materials: Hybrid Inorganic-Organic Semiconductors with Tunable Structures and Properties **Jing Li**, Rutgers, The State University of New Jersey

9:45 **776** Time Resolved Decay Dynamics and Mechanism of Energy Transfer in Undoped and Mn2+ Doped ZnSe Nanoparticles **Christian D Grant**[1], Edward M Olano[2], Thaddeus J Norman Jr[3], Edward W Castner Jr[1] and Jin Z Zhang[2], (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 Ma[1], Jianming Zhang[2] and **Huixin He**[1], (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

11:15 **785** Reversible Binding of Collagen Mimetic Peptide Derivatives to Collagen Films Effects Cell Adhesion and Spreading Behaviors **Allen Y Wang**, Jared S Hierman, Chang-Soo Yun and Michael S Yu, The Johns Hopkins University

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 Mukhopadhyay[1], E Sineva[2], YW Ebright[1], V Mekler[1], A Volkov[1], A Srivastava[1], A Kravets[1], D Wang[1], X Wang[1], S Ismail[1], S Sarafianos[2], S Tuske[2], B Hudson[2], A Clarke[2], J Birktoft[2], C Dharia[2], M Bayro[2], GVT Swapna[2], J Huang[2], LC Ma[2], J Knight[2], O Laptenko[3], J Lee[3], S Borukhov[3], H Berman[2], E Arnold[2], G Montelione[2], R Levy[2] and **RH Ebright**[1], (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 Syntheses
Enantioselective Reactions and Syntheses

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 Adar**[1], Sergey Mamedov[1], Andrew Whitley[1] and Luc Brazeau[2], (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

2:10 **807** Artemisinin Antimalarials: Mode of Action and Potent Analogs **Jared Cumming**, Schering-Plough Research Institute and Gary H Posner, The Johns Hopkins 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 Sophorolipids by Candida Bombicola Using Industrial Fatty Acid Residues and Its Anti-HIV/Spermicidal Activity **Vishal Shah**[1], Arthur Felse[1], Gustavo F Doncel[2] and Richard A Gross[1], (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 Shah**[1], P Arthur Felse[1], Gustavo F Doncel[2] and Richard Gross[1], (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 Zhou**[1], Chang Xu[1], Jun Wang[1], Wei Gao[2], Rena Akhverdiyeva[2], Vishal Shah[2] and Richard Gross[2], (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

2:55 **822** The History of African American Women Chemist Project **Jeannette E Brown**, 2004 Société Fellow Chemical Heritage Foundation

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