



120th North Carolina-ACS Sectional Conference
Saturday, April 22, 2006
Mary M. Townes Science Center
North Carolina Central University

TECHNICAL PROGRAM

General Session

NC Distinguished Lecture, Awards,... 11:50 am – 1:10 pm
Lunch* 1:15 pm

Oral Presentations

Analytical Chemistry 9:00 am – 11:20 am
Biochemistry 9:20 am – 11:00 am
**Inorganic & Environmental
Chemistry**..... 9:00 am – 11:00 pm
Nuclear Magnetic Resonance 9:20 am – 11:00 am
**Organic & Physical
Chemistry** 9:00 am – 11:20 am
Polymer Chemistry 8:40 am – 11:20 pm

Poster Presentations

Display Time 8:30 am – 11:40 pm
Presenter Discussion Times 10:00 am – 10:20 am
..... 11:00 am – 11:40 am

Analytical Chemistry
Biochemistry
Inorganic Chemistry
Environmental Chemistry
Nuclear Magnetic Resonance
Organic Chemistry
Physical Chemistry
Polymer Chemistry

ACKNOWLEDGEMENTS

The NC-ACS Local Section gratefully acknowledges the NCCU Chemistry Department for hosting this event, and Dr. John Myers for coordinating the use of the facilities. Many thanks to the other assistants from North Carolina Central University.

GENERAL SESSION

Room 124

11:50 am – 1:10 pm

1:15 pm: Buffet Lunch*

Charles Goss, NC-ACS Chair, Presiding

- ACS President Ann Nalley presentation of an Industrial Sponsor Award to Glaxo-Smith Kline for major support of the ACS Scholars Program
- Presentation of the 2006 NC ACS Distinguished Lecture Award to:

Dr. John Simon

**Department of Chemistry & Biochemistry
Duke University**

Introduction by: **Dr. David Beratan**, Chair
Department of Chemistry
Duke Carolina State University

- Recognition of 50-year ACS members
- Recognition of the 2005 Barbara Whittaker Awardees
- Recognition of the 2005 Undergraduate Scholarship Awardees
- Presentation of the 2005 Chair's Awards to Laura Sremaniac (NCSU) and Keith Levine (RTI)
- Presentation of the Past-Chair Awards
- Presentation of the 2006 Marcus E. Hobbs Award to **Kenneth Cutler** Director NC-ACS Project Seed

* **LUNCH will be served in the Lobby and Courtyard of the Mary M. Townes Science Center immediately after the General Session**

Questions about the program? Please contact:

Prof. Alan Tonelli, Program Chair
North Carolina State University
2401 Research Drive
Raleigh, NC 27695-8301
Phone: 919-4515-6588
E-mail: alan_tonelli@ncsu.edu

ANALYTICAL CHEMISTRY

Room 1221

9:00 am – 11:20 am

President: **Saundra F. DeLauder, NCCU.**

- 9:00** Methods for Distinguishing Isomeric Volatile Organic Compounds in a Quadrupole Ion Trap Mass Spectrometer, **Karen S. Wendling**, Gary L. Glish, Department of Chemistry, University of North Carolina, Chapel Hill
- 9:20** Determining Proton-Transfer Reaction Rate Constants of Volatile Organic Compounds Using Quadrupole Ion Trap Mass Spectrometry, **Jeremy A. Felton**, University of North Carolina, Chapel Hill
- 9:40** High Throughput Screening Applications of SUPREX, **Erin D.Hopper**, Petra L. Roulhac, Michael C. Fitzgerald, Department of Chemistry, Duke University
- 10:00** **BREAK and POSTER DISCUSSION – refreshments**
- 10:20** Application of SUPREX to Characterizing the Binding Affinity of Inhibitor Ligands for Non-two-state Folding Proteins, **Liangjie Tang**, Michael C. Fitzgerald, Duke University, Department of Chemistry
- 10:40** Method Comparison of Calcium Analysis: Flame AA vs. Ion-Selective Electrode, **Karen L. Parkes**, W. Lin Coker, Department of Chemistry, Campbell University
- 11:00** Applying Superfluid Helium Nanodroplets to the Study of Ions: New Possibilities, **Travis M. Falconer**, William K. Lewis III, Aaron M. Johnson, Raymond J. Bemish, Gary L. Glish, Roger E. Miller, Department of Chemistry, University of North Carolina, Chapel Hill
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ANALYTICAL CHEMISTRY POSTER SESSION

2nd Floor

Posted: 8:30 am – 12:00 pm

Discussion: 10:00 am – 10:20 am, 11:00 am – 11:40 am

- ANYL-1** Method Comparison of Calcium Analysis: Flame AA vs. Ion-Selective Electrode, **Karen L. Parkes**, W. Lin Coker, Department of Chemistry, Campbell University
- ANYL-2** Electrochemistry of Cytochrome c: A New Hypothesis for a Thermodynamic Anomaly, **Edward L. D'Antonio**, Edmond F. Bowden, North Carolina State University, Department of Chemistry
- ANYL-3** Development of a Pulsed, Multiplexed, nano-Electrospray Ionization Source, **Jared M. Bushey**, Gary L. Glish, Department of Chemistry, University of North Carolina, Chapel Hill
- ANYL-4** Bath gas pressure effects on protein charge state distribution and intensity, **Brittany L. Butler**, Gary L. Glish, Department of Chemistry, University of North Carolina, Chapel Hill
- ANYL-5** A Low Temperature Quadrupole Ion Trap for IRMPD and Laser Spectroscopy Experiments, **Philip M. Remes**, Alessandra L. Ferzoco, Gary L. Glish, University of North Carolina, Chapel Hill
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BIOCHEMISTRY

Room 1233

9:20 am – 11:00 am

President: **Pei Zhou, Department of Biochemistry, Duke University Medical Center**

- 9:20** Controlled Encapsidation of Nanoparticles by a Viral Protein Shell, **LiNa Loo**, Richard Guenther, Steven A. Lommel, Stefan Franzen, Department of Chemistry, North Carolina State University
- 9:40** Disulfide Bridges in Cry1Aa delta-endotoxin and its Relationship with Ion Channel Formation, **Oscar Alzate**, April Curtiss, Michel Claybon, Cristina Osorio, Alvaro M. Florez, Taek You, Donald H. Dean, Department of Neurobiology, Duke University Medical Center
- 10:00** **BREAK and POSTER DISCUSSION – refreshments**
- 10:20** Sequence Specific Effects on NMR Characterization of Platinated DNA Adducts, **Debadep Bhattacharyya**, Candice King, Yibing Wu, Sharon L. Campbell, Stephen G. Chaney, University of North Carolina, Chapel Hill, Departments of Biochemistry and Biophysics
- 10:40** Towards an Optimal Chemicogenomic Database, **ClarLynda R. Williams-DeVane**, Ann M. Richard, US EPA and North Carolina State University, Bioinformatics Program

BIOCHEMISTRY POSTER SESSION*2nd Floor***Posted: 8:30 am – 12:00 pm****Discussion: 10:00 am – 10:20 am, 11:00 am – 11:40 am**

- BIO-1** Conformation Coupled Enzyme Catalysis: Single Molecule and Transient Kinetics Investigation of Dihydrofolate Reductase, **Ronald D. Smiley** (1), Nina M. Antikainen (2), Stephen J. Benkovic (2), Gordon G. Hammes (1), (1) Department of Biochemistry, Duke University Medical Center, (2) Department of Chemistry, Pennsylvania State University

INORGANIC and ENVIRONMENTAL CHEMISTRY*Room 1225***9:00 am – 11:00 am****Presider: Shawn Sendlinger, NCCU.**

- 9:00** The Environment, The Public, and Education, **L. Jacqueline Arroyo**, John J. Bang, Yolanda Banks-Anderson, Sandra DeLauder, North Carolina Central University-Environmental Science Program, Chemistry Department
- 9:20** Nano-material Synthesis for Photocatalytic Water Decontamination, **John Bang**, : Sandra DeLauder, Yolanda B. Anderson, Geoffrey B. Saupe, North Carolina Central University, Department of Chemistry and Environmental Science Program, and University of Texas, El Paso, Department of Chemistry
- 9:40** Solid State NMR, X-ray, and Neutron Diffraction Study of Structural Phase Transitions involved in Crystal Melting of CuAlCl₄, **Stan S. Toporek**, Amanda Josey, James D. Martin, Department of Chemistry, North Carolina State University
- 10:00** **BREAK and POSTER DISCUSSION – refreshments**
- 10:20** Temperature and Loading Rate Dependence Single Molecule Force Spectroscopy of alpha-synuclein 12-mer, **Chad J. Ray**, Boris B. Akhremitchev, Department of Chemistry, Duke University
- 10:40** Dependence of Ligand Recombination as a Function of Temperature and Glycerol Content in Dehaloperoxidase, **Jennifer L Belyea** (1), Scott Brewer (1), Robin Casey (1), Robert Stanley (2), Martin Vos (3), Audrus Jasaitis (3), Stefan Franzen (1), (1) Department of Chemistry, North Carolina State University, (2) Temple University, (3) Ecole Polytechnique

NUCLEAR MAGNETIC RESONANCE*Room 2221***9:20 am – 11:00 am****Presider: Jeff MacDonald, Department of Biomedical Engineering, University of North Carolina, Chapel Hill**

- 9:20** Fast J-Resolved Experiment for Metabolomics Analysis. **Thomas M. O'Connell**, Ronald Crouch, Metabolomics Laboratory, University of North Carolina, Chapel Hill and Varian NMR Instruments
- 9:40** A 2-Iminohydantoin from the Oxidation of Guanine, **Karl M. Koshlap**, Wenjie Ye, R. Sangaiah, Diana E. Degen, Avram Gold, K. Jayaraj, Gunnar Boysen, Jason Williams, Kenneth B. Tomer, and Louise M. Ball, School of Pharmacy and Department of Environmental Science & Engineering, University of North Carolina, Chapel Hill and NIEHS, NIH
- 10:00** **BREAK and POSTER DISCUSSION – refreshments**
- 10:20** H-1 NMR Hyperfine Resonance Assignments in Cyanide-Ligated Dehaloperoxidase, **Michael F. Davis**, Jennifer Belyea, Hanna Gracz, Stefan Franzen, Sean M. Decatur, North Carolina State University, Chemistry Department and Mount Holyoke College, Chemistry Department
- 10:40** H-1 NMR Hyperfine Resonance Assignments in Cyanide-Ligated Dehaloperoxidase, **Michael F. Davis**, Jennifer Belyea, Hanna Gracz, Stefan Franzen, Sean M. Decatur, North Carolina State University, Chemistry Department and Mount Holyoke College, Chemistry Department

ORGANIC and PHYSICAL CHEMISTRY*Room 1233***9:00 am – 11:20 pm****Presiders: Robert A. Izydore and Darlene Taylor, NCCU.**

- 9:00** First Total Synthesis of Rottlerin, **Marc J. Adler**, Steven W. Baldwin, Department of Chemistry, Duke University
- 9:20** Raman, EPR and Electrochemical Studies of the Active Site of Dehaloperoxidase from *Amphitrite ornata* as a Function of pH, **Jennifer L. Belyea**, Michael Davis, Lauren Gilvey, Reginaldo Rocha, Andrew P. Shreve, Stefan Franzen, North Carolina State University, Department of Chemistry and Los Alamos National Laboratory
- 9:40** Targeted Drug Delivery for Neuroblastoma using MIBG, **James B. Springer**, Gamcsik MP, Driscoll TA, Vaidyanathan G, Colvin OM, Ludeman SM, Duke University, Department of Chemistry, Comprehensive Cancer Center
- 10:00** **BREAK and POSTER DISCUSSION – refreshments**

- 10:20** Generalized Mulliken-Hush Analysis of Electronic Coupling Interactions in Compressed pi-Stacked Porphyrin-Bridge-Quinone Systems, **Jieru Zheng**, David N. Beratan, Department of Chemistry, Duke University
- 10:40** A Facile and Efficient Direct Aldol Addition of Simple Thioesters, **Julianne M. Yost**, Guoqiang Zhou, Don M. Coltart, Duke University, Department of Chemistry
- 11:00** Single-molecule Force Spectroscopy Measurements of "Hydrophobic Bond" between Tethered Hexadecane Molecules, **Chad Ray**, Jason R. Brown, Boris B. Akhremitchev, Duke University, Department of Chemistry

ORGANIC, PHYSICAL, & POLYMER CHEMISTRY POSTER SESSION

2nd Floor

Posted: 8:30 am – 12:00 pm

Discussion: 10:00 am – 10:20 am, 11:00 am – 11:40 am

- ORG-1** Recent Advances on Nicotine Chemistry at NC State University, **Florence C. Fevrier**, Daniel L. Comins, Department of Chemistry, North Carolina State University
- ORG-2** Sulfonylhydrazone Syn-dianion Effect in the Development of a Novel Approach to Polyol Synthesis, **Fang Fang**, Don M. Coltart, Duke University, Chemistry and Biochemistry Departments
- ORG-3** A Novel Approach to the Development of Small Molecule Inhibitors of Cdc25 Phosphatase, **Anna V. Gromova**, Julianne M. Yost, Johannes Rudolph, Don M. Coltart, Duke University, Chemistry and Biochemistry Departments
- PHYS-1** Polymeric Linker Length Dependence of Intermolecular Rupture Forces in Single Molecule Force Spectroscopy, **Jason R. Brown**, Chad Ray, Boris B Akhremitchev, Duke University Department of Chemistry
- ORG-4** Contemporary Applications of Sulfonyl Hydrazones to Carbon-Carbon Bond Formation, **Fang Fang**, Daniel Lim, Don M. Coltart, Duke University, Chemistry Department
- ORG-5** A Facile and Efficient Three Component Direct Aldol Addition Involving Simple Thioester Enolates - A Rapid and Versatile Entry to Polyketide Motifs, **Guoqiang Zhou**, Julianne M. Yost, Don M. Coltart, Duke University Chemistry Department
- PHYS-2** Development and Reactivity of Ru(II) Hydroarylation Catalysts, **Karl A. Pittard**, T. Brent Gunnoe, Jeffrey L. Petersen, Cynthia S. Day, Department of Chemistry, North Carolina State University
- POLY-1** Interfacial Behavior of Heteropolymers with Adjustable Monomer Sequences (HAMS), **Young Kuk Jhon**, Jan Genzer, North Carolina State University, Department of Chemistry & Biomolecular Engineering

POLYMER CHEMISTRY

Room 1111

8:40 am – 11:00 am

Presider: C. Maury Balik, NC-State.

- 8:40** Scalable Fabrication of Organic Nanoparticles using Particle Replication in Non-wetting Templates (PRINT), **Benjamin W. Maynor**, Joseph M. DeSimone, Department of chemistry, University of North Carolina, Chapel Hill
- 9:00** Solid-State Complexation of Polymer-Cyclodextrin Inclusions, **Marcus A. Hunt**, Alan E. Tonelli, C. Maurice Balik, Department of Material Sciences and Textiles, North Carolina State University
- 9:20** Functionalized Liquid Precursors for New Fluorinated Elastomers, **Jennifer Y. Kelly**, Joseph M. DeSimone, Department of Chemistry, University of North Carolina, Chapel Hill
- 9:40** High Surface Area, Highly Conductive Proton Exchange Membranes from Liquid Precursors, **Zhilian Zhou**, Joseph M. DeSimone, Department of Chemistry, University of North Carolina, Chapel Hill
- 10:00** **BREAK and POSTER DISCUSSION – refreshments in Dabney Hall Room 210**
- 10:20** Alternative Fluoropolymers to Avoid the Challenges Associated with PFOA, **Ji Guo**, Paul Resnick, Joseph M. DeSimone, Department of Chemistry University of North Carolina, Chapel Hill
- 10:40** Polymerization of Nitroaromatics using Inorganic Lewis Acids, **Robert J. Wilcox**, Jacob Folmer, James Martin, Department of Chemistry, North Carolina State University