SERMACS 2012
14-17 November 2012
Raleigh Convention Center, Raleigh, North Carolina

Catalyzing Sustainable Innovation

Meeting Program Book

64th Southeastern Regional Meeting of the American Chemical Society

Hosted by the North Carolina Section of the ACS
Welcome to the 2012 Southeastern Regional meeting of the American Chemical Society in Raleigh, North Carolina. With almost 1400 abstracts submitted, this 64th SERMACS continues a long tradition of strong participation that showcases both the innovative chemistry and the dynamic people associated with the Southeastern Region.

This is the first SERMACS to be held in downtown Raleigh at the state-of-the-art Raleigh Convention Center and the elegant Raleigh Marriott City Center hotel. We urge attendees to walk around Raleigh to enjoy traditional North Carolina hospitality at the vibrant downtown restaurants, museums, music venues, and other diverse cultural attractions. You can also explore the Research Triangle area, whose many companies and universities are leaders in catalyzing sustainable innovation.

The technical program covers a vast array of chemistry with 26 invited symposia and contributed papers together comprising over 100 oral sessions and over 40 poster sessions. SERMACS 2012 is fortunate to partner with three special conferences. The Energy Frontier Research Center (EFRC) and Solar Energy Research Center (SERC) will host a conference on “Photonic Assemblies, Materials, and Catalysts for Solar Fuels”. The North Carolina Local Section will have its 126th NC-ACS Local Section Conference Meeting featuring the NC Distinguished Speaker Award Lecture. Finally, The 41st Southeastern Magnetic Resonance Conference (SEMRC) will cover the latest developments in NMR, EPR, and MRI with presentations from established and emerging leaders. We look forward to a large contingent of students attending the Undergraduate Program, as well as the High School and Project SEED sessions. A Symposium on Project SEED Best Practices is the first of its kind at SERMACS.

Please visit the over 50 booths in the Exposition area to meet the vendors and organizations showcasing their products and services. Attend the special vendor seminars to learn the latest developments and applications. We welcome over 20 exhibitors in the Graduate School Fair, and the many undergraduate student presenters and attendees. Congratulations and thanks to the organizers of these activities.

Join us Wednesday evening for the Welcome Reception in conjunction with the NC-ACS Section Conference. On Thursday, we offer the Women Chemist Committee Luncheon, then science and socializing in the evening at Sci-Mix sponsored by Scynexis. On Friday, we celebrate Entrepreneurial Chemistry with a symposium and the Industrial Innovation Award Luncheon. Later Friday you can visit the fabulous North Carolina Museum of Natural Sciences while attending the SERMACS Awards Reception sponsored by Eastman Chemical. Finally on Saturday, two luncheons celebrate Undergraduate Award Winners and the ACS CHED High School Teacher Award winner.

We are pleased to have ACS courses on Leadership, Innovation, Supervising, PK/PD, and Water Analysis. Workshops on Chromatography, Negotiation for Women Chemists, Grant Writing, Lab Safety, and Chemistry Demonstrations offer important practical skills. Job seekers will enjoy ACS Career Workshops, Resume Review, Speed Networking, and Job Hunting Tips at the Career Connections office.

The SERMACS 2012 organizers thank all the generous sponsors whose support is critical to the meeting success. We are grateful for the warm welcome and cooperation from the Raleigh Convention Center, the Marriott City Center, the NC Museum of Natural Sciences, and visit Raleigh. We thank the ACS Regional Meetings staff for their constant guidance and organizational help. Finally, I extend my personal “THANK YOU!” to all the SERMACS 2012 Planning Committee members for their tremendous efforts.

Charlie Goss, SERMACS 2012 General Chair
Dear Friends and Colleagues:

On behalf of the North Carolina Section, it is my great pleasure to welcome you to the 64th Southeastern Regional Meeting of the American Chemical Society (SERMACS), November 14-17, 2012, at the downtown Raleigh Convention Center. While at the conference, we urge attendees to enjoy North Carolina hospitality at downtown restaurants, museums, and other cultural attractions, and to explore the vibrant Research Triangle area, which includes many companies and universities at the forefront of innovation. Opportunities abound for attendees to meet new people and to network with friends and colleagues.

The 64th SERMACS offers an outstanding technical program, with nearly 1,400 submitted and invited abstracts presented in over 100 oral and 40 poster sessions in diverse areas of chemistry. We would like to extend a ‘thank you’ to our sponsors and to our many symposia organizers who made this technical program possible. Conference attendees can also take advantage of the exhibition, which will offer an outstanding marketplace for cutting-edge technology and information from nearly 60 public and private sector booths.

SERMACS presents an opportunity to pay tribute to scientists who have distinguished themselves in their area of expertise or through their service to chemistry. This year, the North Carolina Section is proud to honor Drs. Jane S. and David C. Richardson with the North Carolina Distinguished Speaker Award for their significant contributions to understanding the 3D structures of proteins and nucleotides, and Dr. Laura Sremaniak with the Marcus E. Hobbs Service Award for her long-term contribution to the WCC and Project SEED. We would also like to recognize our special SERMACS award winners, including Dr. Christine S. Grant (ACS Stanley C. Israel Diversity Award), Dr. Christopher J. Bannochie (ACS E. Ann Nalley Award for Volunteer Service), Dr. Christian Melander (Industrial Innovation Award), and Ms. Susanne M. Dana (ACS Award for Excellence in High School Teaching).

Finally, on behalf of the North Carolina Section, I would like to express a heartfelt ‘thank you’ to the entire SERMACS 2012 Planning Committee and to Charlie Goss for his leadership in bringing this conference to Raleigh. I urge you to enjoy the conference and take advantage of all that it has to offer.

Sincerely,

Keith E. Levine, Ph.D.
2012 NC ACS Chair
RTI International
Welcome to Raleigh!

On behalf of the members of the Raleigh City Council and the more than 404,000 residents of our city, I would like to welcome the Southeast Regional Meeting of the American Chemical Society 2012 to Raleigh! We are glad to be your host city.

It will be an honor to have you here and we believe that Raleigh is the perfect location for SERMACS 2012. With your organization’s longstanding reputation of being on the forefront of chemical research and study, it is appropriate to meet in Raleigh where energy-related research, technology and education are definite mainstays of our local economy. We are proud of our reputation and that of nearby Research Triangle Park and know your attendees will feel at home while they are here.

You are also going to love our convention center! The Raleigh Convention Center is proudly Silver-LEED Certified and has a proven track record of being not only a state-of-the-art venue, but a strong, global partner with its sustainable practices. SERMACS attendees and exhibitors alike will enjoy 500,000 square-feet of meeting, event and exhibit space, complete with the latest in technology. The best of lighting and sound, fiber-optic data network, and high speed wireless and wired capabilities all contribute to a superb meeting environment. Even more, a great staff awaits your arrival!

While you are here we hope that you will explore and experience our great city. Raleigh is known for its hospitality and we invite you to see all that it has to offer. Great cultural attractions, fine restaurants and world class entertainment are just a few steps away from the Raleigh Convention Center. Our complimentary R-LINE connector service makes it easy to get around when you want to venture a little further away. The Official Visitor Information Center inside the Raleigh Marriott City Center, tourism ambassadors and downtown ambassadors are all close by and available to help you find your way.

Again, thank you for choosing Raleigh, welcome to the City and we wish you a successful conference!

Sincerely,

Nancy McFarlane
Mayor
SERMACS 2012 Organizing Committee

General Meeting Chair       Charles A. Goss, GlaxoSmithKline
Treasurer                   Sol Levine, NCSU, Retired & Nature's Images by Sol
General Program Chair       Marc ter Horst, UNC Chapel Hill
Symposia                    Kenneth B. Tomer (Chair), NIEHS
                            Richard A. Palmer, Duke University
                            Shri Kulkarni, KulTech Incorporated
SEMRC Conference            Alex Nevzorov (Chair), NCSU
                            Irina Nesmelova, UNC Charlotte
                            Tatyana Smirnova, NCSU
                            Alex Smirnov, NCSU
UNC SERC/EFRC Conference    Thomas J. Meyer, UNC-EFRC
                            Will Thauer, UNC-EFRC
Vendor Exposition           John W. Hines (Chair), RTI International
                            Reshan Fernando, RTI International
Sponsorships                RKM Jayanty, RTI International
                            Rachelle Bienstock, NIEHS, retired
                            Pauline Ondachi, RTI International
Workshops                   Catherine R. Brennan, UNC Chapel Hill
Poster Sessions             Yaroslava (Yara) Yingling, NCSU
Undergraduate Program       Dan Shin, Campbell University
                            Dan Barber, LORD Corporation
                            W. Lin Coker III, Campbell University
                            Jeremiah Feducia, NCSU
                            Phil Brown, NCSU
                            Kassy Mies, Meredith College
High School Program         Marc ter Horst, UNC Chapel Hill
Project SEED                Alan Tonelli, NCSU
Awards                      Jim Chao, IBM, retired
Graduate School Fair        Ana Muresan, USPTO
Program Book                Danna Mattocks, GlaxoSmithKline
Registration and Program Book Bill Gutknecht, RTI International, Scientist Emeritus
AV                          David Elam, Summa Consultants, Inc.
Signage, Internet and Social Media Anderson Cox, RTI International
Webmaster                   Dustin Wheeler, NCSU
Communications              William L. Switzer, NCSU
Chemistry Demos             Sol Levine, NCSU, Retired & Nature's Images by Sol
                            Kenneth S. Lyle, Duke University
                            Melinda Box, Wake Tech Community College
Site Planning               Sol Levine, NCSU, Retired & Nature's Images by Sol
                            Keith Dawes, NCSU
                            John Hines, RTI International
Communications             William L. Switzer, NCSU
ACS Office of Regional Meetings Michelle Stevenson, ACS
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General Meeting Information

On-site Registration
On-site registration is located on the 300 level in the Main Lobby.
Registration desk hours:
Wednesday: 10:00 a.m. – 7:00 p.m.
Thursday: 7:00 a.m. – 7:00 p.m.
Friday: 7:00 a.m. – 7:00 p.m.
Saturday: 7:00 a.m. – 5:00 p.m.

On-site Registration Fees
ACS Member $195
Nonmember $235
Undergraduate Student $70
Graduate Student $90
Post-Doctoral Fellow $100
Retired/Emeritus/Unemployed $50
K-12 Teacher $50
High School Student $10
One Day $50
Spouse/Guest* $35
Additional Exhibitors* $50
50 Year ACS Member No charge

Abstracts
Abstracts are available on-line at http://www.sermacs2012.org

Break Information
Times:
Morning Break: 9:40 – 10:40 a.m.
Afternoon Break: 2:40 – 3:40 p.m.
Location:
Wednesday, Nov. 14, Ballroom Lobby
Thursday, Nov. 15, Ballrooms B & C
Friday, Nov. 16, Ballrooms B & C
Saturday, Nov. 17, Ballroom C

The Greater Raleigh Convention and Visitors Bureau welcomes SERMACS 2012 to Downtown Raleigh!

Downtown Raleigh and Fayetteville Street epitomizes a cosmopolitan Southern city, setting the scene with distinctive restaurants and impressive skyscrapers mixed among restored historic buildings.

SERMACS delegates will find that Downtown has a distinct tourist vibe, with a view that stretches from the Progress Energy Center for the Performing Arts to the NC State Capitol.

To help you find "SERMACS" restaurants (close by the Raleigh Convention Center), learn about tours and how to ride the new complimentary R Line, or just to get answers to your questions, please stop by our welcome booth set up in the main lobby of the Raleigh Convention Center or our Visitor Information Center (VIC) http://www.visitraleigh.com/visitors/visitor-info-center/ located inside the Connector between the RCC and Raleigh Marriott City Center Hotel.

The welcome booth is stocked with visitor information and staffed with representatives of GRCVB staff and GRCVB Raleigh Tourism Ambassadors who will be happy to answer your questions. You'll also want to pick up your Greater Raleigh ZSpot SMART card. The card is provided complimentary by Zspotlight.com and visitRaleigh.com. When you use it, you'll save money at area restaurants and attractions! To preview the many businesses that accept our card, see http://www.zspotcard.com/
For more information about Raleigh, see http://www.visitraleigh.com/visitors/

Transportation: The R-LINE, FREE circulator service features hybrid electric buses that will connect you to restaurants, retail, entertainment venues, museums, hotels, and parking facilities in downtown Raleigh. Buses run every 10-15 minutes, it's a great new way to get around downtown.

Hours of Operation: Mon-Wed (7 am-11 pm); Thurs-Sat (7 am-2:15 am); Sun (1 pm-8 pm)

RCC Directions:
The Raleigh Convention Center is located adjacent to the Red Hat Amphitheater and the Marriot City Center. The address is: 500 South Salisbury Street, Raleigh, NC 27601
From Points West: I-40 east to exit 298B South Saunders Street.
From Points East: 64/264 to I-440 east; merge onto I-40 west and exit at 298B South Saunders Street.
From Points South: US-1 north to I-40 east; exit at 298B South Saunders Street.
From Points North: US-1 South into the city - left on Lenoir Street.

RCC Parking
Public Parking garages on Lenoir Street between Salisbury and McDowell Street; one on McDowell Street between Cabarrus and Davie Street; One on Salisbury Street between Cabarrus and Davie Street.
Charge: $7.00
Accessible Parking: 1st level of each garage
Meeting at a Glance
SERMACS 2012
Catalyzing Sustainable Innovation

Tuesday – 13 November 2012
8:30 a.m. – 5:00 p.m.
ACS Leadership Development Course: Extraordinary Leaders
Marriott University A

Wednesday – 14 November 2012

Events and Activities
5:00 p.m. – 6:45 p.m.
Welcome Reception and 126th NC-ACS Local Section Conference Posters
(Ticketed event sponsored by NC-ACS)
6:45 p.m. – 8:00 p.m.
NC-ACS Awards and NC Distinguished Speaker Presentation.
Jane and Dave Richardson, Duke University,
“Admiring, Analyzing, and Improving 3D Structures of Macromolecules”

Short Courses and Workshops
8:30 a.m. – 12:00 p.m.
COACh Workshop: Negotiations Workshop for Women Faculty & Professionals
Marriott Chancellor
8:00 a.m. – 5:00 p.m.
ACS Short Course: Pharmacokinetics and Pharmacodynamics in Drug Discovery for Chemists
ACS Short Course: The Essentials of Supervising Scientists & the Technical Staff
ACS Short Course: Electrochemical Measurement of pH and Ions: Troubleshooting and Correcting Error and Bias
Marriott University A
Marriott University B
Marriott University C
8:30 a.m. – 12:00 p.m.
TCDG Workshop: (1) Getting the Most Out of Your UHPLC Columns
(2) Fundamentals and Advancements in Analytical SFC/SFE
Glass Office
1:00 p.m. – 4:30 p.m.
COACh Workshop: Negotiations Workshop for Women Postdocs & Graduate Students
Marriott Chancellor

Center for Solar Fuels (UNC EFRC) Conference
1:00 p.m. – 5:00 p.m.
Photonic Assemblies for Solar Fuels (oral)
Ballroom A
3:00 p.m. – 3:40 p.m.
Photonic Assemblies for Solar Fuels (poster)
Wednesday – 14 November 2012 continued

Poster Presentations
2:00 p.m. – 4:30 p.m.  Ballroom Lobby
Computational, Inorganic, Nanochemistry, Physical
5:00 p.m. – 6:45 p.m.  Ballroom Lobby
126th NC-ACS Section Conference

Technical Sessions
1:20 p.m. – 5:20 p.m.  Marriott Congressional B
Electroanalytical Chemistry I
Inorganic Chemistry I 205
Innovations in Molecular Modeling 202
Physical Chemistry I 204
Polymer Chemistry I  Marriott Congressional A
Recent Advances in Micro- and Nano-Fabrication 203
The Exposome 206

Thursday - 15 November 2012

Vendor Exposition
8:30 a.m. – 8:00 p.m.  Ballrooms B/C

Events and Activities
12:00 p.m. – 1:30 p.m.  304
Women Chemists Committee Luncheon.
   Speaker: Dr. Barbara Ramsay Shaw, Duke University,
   “Challenges, Passions, and Opportunities Balancing Chemistry
   Careers and Our Lives” (Ticketed event)

Short Course and Workshops
8:30 a.m. – 10:30 a.m.  202
NIH Funding for Chemists: Grant Writing Tips for
New and Experienced Applicants
9:00 a.m. – 5:00 p.m.  Glass Office
Career Connections
1:00 p.m. – 5:00 p.m.  202
ACS Leadership Course: Fostering Innovation

Center for Solar Fuels (UNC EFRC) Conference
8:00 a.m. – 11:20 a.m.  Ballroom A
Catalysts for Solar Fuels (oral)
9:20 a.m. – 10:00 a.m.  Ballroom A
Catalysts for Solar Fuels (poster)
12:40 p.m. – 4:40 p.m.  Ballroom A
Materials for Solar Fuels (oral)
2:40 p.m. – 3:20 p.m.  Ballroom A
Materials for Solar Fuels (poster)
Thursday - 15 November 2012 continued

41st Southeastern Magnetic Resonance Conference (SEMRC)
1:15 p.m. – 5:15 p.m.
Edward O. Stejskal Memorial Symposium 306C

Poster Presentations
9:00 a.m. – 11:30 a.m.
  Bioinorganic, Organic, Organometallic Ballrooms B/C
2:00 p.m. – 4:30 p.m.
  Biochemistry, Chemical Biology Ballrooms B/C
6:00 p.m. – 8:00 p.m.
  Analytical, Biomaterials, Electroanalytical, Energy and Fuels, Polymer

Technical Sessions
8:00 a.m. – 12:00 p.m.
  Biochemistry I 205
  Chemistry and Applications of Smart Molecules and Materials I 206
  Chemistry and Bio-Nano Interfaces I 301A
  Clinical Diagnosis MS I 302A
  Computational Chemistry I 201
  Frontiers in Chemistry and Medicine I 303
  Inorganic Chemistry II 204
  Materials Chemistry I 304
  Medicinal Chemistry 302B
  Nanochemistry I 306A
  Organic Chemistry I 203
  Organometallic Chemistry I 305B
  Physical Chemistry II 302C
  Polymer Chemistry II 301B
  Scanning Force Microscopy in Biology 306B
  Separation Science in the Macro, Micro, and Nano World 306C
  Symposium honoring Royce W. Murray Session I 305A
  Vendor Seminars 307

1:00 p.m. – 5:00 p.m.
  Biochemistry II 205
  Bioinorganic Chemistry I 301A
  Biomaterials 306B
  Chemical Biology 302B
  Chemistry and Applications of Smart Molecules and Materials II 206
  Computational Chemistry II 201
  Frontiers in Chemistry and Medicine II 303
  Growing Impact of Public Domain Chemistry Resources 302C
  Inorganic Chemistry III 204
  Materials Chemistry II 304
  Nanochemistry II 306A
  New Applications, Ambient Ionization MS 302A
  Organic Chemistry II 203
  Organometallic Chemistry II 305B
  Polymer Chemistry III 301B
  Symposium honoring Royce W. Murray Session II 305A
  Vendor Seminar 307
Thursday - 15 November 2012 continued

SERMACS Plenary Lecture
5:20 p.m. – 6:20 p.m.
Royce W. Murray, Kenan Professor of Chemistry, UNC-Chapel Hill, Ballroom A
“Nanoparticle Science and its Analytical Chemistry”

Sci-Mix - Refreshments and Poster Session
6:00 p.m. – 8:00 p.m. (Sponsored by Scynexis) Ballrooms B/C

Friday - 16 November 2012

Vendor Exposition
8:30 a.m. – 5:00 p.m. Ballrooms B/C

Graduate School Fair
8:30 a.m. – 5:00 p.m. Ballroom Lobby

Events and Activities
12:00 p.m. – 1:30 p.m.
SERMACS Industrial Innovation Award Luncheon. 402
Speaker: Dr. Buck Goldstein, UNC Entrepreneur-in-Residence,
“Engines of Innovation: The Entrepreneurial University in the
Twenty First Century” (Ticketed event)

2:30 p.m. – 3:30 p.m.
ACS District Director’s Ice Cream Social 304

6:00 p.m. – 9:00 p.m.
SERMACS Awards Reception and Plenary Lecture. NC Museum of
Natural Sciences
Speaker: Joseph M. DeSimone, UNC Chapel Hill and
North Carolina State University. "Research Alone is Not
Enough: Opportunities for Chemists in Uncertain Times"
(Ticketed event sponsored by Eastman Chemical)

Short Courses and Workshops
8:30 a.m. – 12:30 p.m., 1:30 p.m. – 5:00 p.m.
ACS Career Services Workshops: 201
Speed Networking (8:30 - 12:30)
Planning Your Job Search (8:30 - 9:30)
Preparing a Resume’ (9:30 - 11:00)
Effective Interviewing (11:00 - 12:30)
Resume’ Reviews (1:30 - 5:00)

8:40 a.m. – 12:00 p.m.
Government Relations and Science Policy 202

1:00 p.m. – 5:00 p.m.
Career Connections Glass Office

1:00 p.m. – 4:00 p.m.
SENCER Workshop: Backward Course Design 307
Friday - 16 November 2012 continued

41st Southeastern Magnetic Resonance Conference (SEMRC)

8:35 a.m. – 12:20 p.m.
Structure and Dynamics by NMR/EPR I 306B

8:20 a.m. – 12:20 p.m.
Membrane Proteins and Peptides 306C

1:30 p.m. – 3:00 p.m.
SEMRC Poster Session 306 B/C Lobby

3:00 p.m. – 5:10 p.m.
NMR/EPR Methods/Materials 306B

3:00 p.m. – 5:15 p.m.
Contrast Methods/MRI 306C

Poster Presentations

9:00 a.m. – 11:30 a.m.
Medicinal Chemistry Ballrooms B/C
Undergraduate: Inorganic, Organic, Organometallic

2:00 p.m. – 4:30 p.m.
Chemical Education Ballrooms B/C
Undergraduate: Computational, Environmental, Materials, Physical, Polymer

Technical Sessions

8:00 a.m. – 12:20 p.m.
Advanced Materials – Surface and Interfacial Chemistry 204
Analytical Chemistry I 305B
Atmospheric Chemistry: Gas-Particle Interactions and Climate Change I 301B
Chemical Biology: Chemical Answers to Biological Questions I 306A
Chemical Education I 206
Chemistry of Bio-Nano Interfaces II 301A
Energy and Fuels 205
Entrepreneurial Chemistry: Academia/Industry Interactions I 402
Frontiers in Chemistry and Medicine III 303
Frontiers in Nucleic Acid Chemistry I 302C
Instrumentation and Applications for Future MS III 302A
Microorganisms: Organic Chemists Culture I 305A
MS Information: Static Knowledge or Driving New Scientific Innovations 302B
Organic Chemistry III 203
Photochemistry 304
Vendor Seminars 307
Friday - 16 November 2012 continued

Technical Sessions
1:00 p.m. – 5:20 p.m.
Atmospheric Chemistry: Gas-Particle Interactions and Climate Change II 301B
Chemical Biology: Chemical Answers to Biological Questions II 306A
Chemical Education II 206
Chemistry of Bio-Nano Interfaces III 301A
Dye-sensitized Solar Cells I 302B
Emerging Environmental Contaminants MS IV 302A
Energy and Fuels II 205
Entrepreneurial Chemistry: Academia/Industry Interactions II 402
Frontiers in Chemistry and Medicine IV 303
Frontiers in Nucleic Acid Chemistry 302C
Microorganisms: Organic Chemists Culture II 305A
PAT and Chemometrics 305B
Undergraduate I: Analytical, Bioanalytical 202
Undergraduate II: Biochemistry, Biomedical 203
Undergraduate III: Organic, Organometallic 204

Saturday - 17 November 2012

Events and Activities
8:00 a.m. – 11:00 a.m.
SERMACS Regional Board Meeting 402

12:00 p.m. – 1:30 p.m.
Undergraduate Awards and Scholarships Luncheon 402
Speaker: Marty St. Clair, GlaxoSmithKline
“Thirty Years of HIV Drug Development: A Message of Hope”
(Ticketed event)

12:00 p.m. – 1:30 p.m.
ACS CHED Regional Award for Excellence in High School Teaching Luncheon 304
Speaker: Dr. Brian Thomas, RTI International,
“Detection of Designer Drugs and Formulations”
(Ticketed event)

Short Course and Workshops
9:00 a.m. – 12:00 p.m.
Career Connections Glass Office

11:00 a.m. – 12:00 p.m.
Chemistry Demonstration 301A/B

2:00 p.m. – 4:00 p.m.
Chemistry Demonstration Workshop 301A/B

Graduate School Fair Ballroom Lobby
8:30 a.m. – 5:00 p.m.
Saturday - 17 November 2012 continued

41st Southeastern Magnetic Resonance Conference (SEMRC)

8:20 a.m. – 12:25 p.m.
  Structure and Dynamics by NMR/EPR II
  306C
1:30 p.m. – 3:00 p.m.
  SEMRC Poster Session
  306 B/C Lobby
3:00 p.m. – 5:55 p.m.
  NMR/EPR New Methods
  306C

Poster Presentations

9:00 a.m. – 11:00 a.m.
  Project SEED and High School
  Ballroom C
  Undergraduate: Analytical, Bioanalytical, Biochemical, Biomedical
2:00 p.m. – 4:30 p.m.
  Agricultural and Food Chemistry, Bioanalytical,
  Ballroom C
  Chemical Toxicity, Environmental, Materials, Nucleic Acid,

High School Programs

8:00 a.m. – 11:00 a.m.
  High School and ACS Project SEED Oral Presentations
  305A
  High School Teacher Program Orientation with LEARN NC (invitation only)
  304
9:00 a.m. – 11:00 a.m.
  High School and ACS Project SEED Poster Presentations
  Ballroom C
  Panel Discussion: Preparing Students for College Chemistry
  305B
12:00 p.m. – 1:30 p.m.
  ACS CHED Regional Award for Excellence in High School Teaching Luncheon
  304
  Speaker: Dr. Brian Thomas, RTI International,
  “Detection of Designer Drugs and Formulations”
  (Ticketed event)
1:20 p.m. – 5:00 p.m.
  ACS Project SEED Best Practices: What Works?
  305A
3:00 p.m. – 6:00 p.m.
  High School Teacher Program Continued
  304

Technical Sessions

8:00 a.m. – 12:30 p.m.
  Analytical Chemistry II
  306B
  Chemistry of Bio-Nano Interfaces IV
  306A
  Dye-sensitized Solar Cells II
  302B
  Environmental, Agricultural, and Food Chemistry
  302A
  Frontiers in Nucleic Acid Chemistry III
  302C
  Undergraduate IV: Computational/Environmental
  203
  Undergraduate V: Inorganic/Physical Chemistry
  204
  Undergraduate VI: Materials/Polymer Chemistry
  205
1:00 p.m. – 5:00 p.m.
  Bioanalytical Chemistry I
  306B
  Chemistry and Applications of Colorants in the 21st Century
  306A
  Chirality in Agrochemicals
  302C
Symposium to be held at Southeast Regional Meeting of the American Chemical Society
Wednesday Nov 14 – Thursday Nov 15, 2012
Raleigh Convention Center
Raleigh, North Carolina

Wednesday Afternoon, November 14
PHOTONIC ASSEMBLIES FOR SOLAR FUELS (Ballroom A)
1:00 p.m. Welcome – Thomas Meyer, UNC Chapel Hill
1:05 p.m. Marcey Waters, UNC Chapel Hill
1:40 p.m. Niels Damrauer, University of Colorado
2:20 p.m. Greg Scholes, University of Toronto
          Break and Poster Session
3:40 p.m. Sharon Hammes-Schiffer, University of Illinois
4:20 p.m. George Schatz, Northwestern University

Thursday Morning, November 15
CATALYSTS FOR SOLAR FUELS (Ballroom A)
8:00 a.m. Karen Brewer, Virginia Tech
8:40 a.m. Etsuko Fujita, Brookhaven National Laboratory
          Break and Poster Session
10:00 a.m. Craig Hill, Emory University
10:40 a.m. Cynthia Schauer, UNC Chapel Hill

Thursday Afternoon, November 15
MATERIALS FOR SOLAR FUELS (Ballroom A)
12:40 p.m. Frank Osterloh, University of California at Davis
1:20 p.m. Bruce Parkinson, University of Wyoming
2:00 p.m. Paul Hoertz, RTI, International
          Break and Poster Session
3:20 p.m. Heinz Frei, Lawrence Berkeley National Laboratory
4:00 p.m. Anders Hagfeldt, Uppsala University

MORE INFORMATION at http://serc.unc.edu/conf/
Southeastern Magnetic Resonance Conference (SEMRC) is the largest annual conference on nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR), and magnetic resonance imaging (MRI) in the Southeast. Its participants represent over 50 research groups in the Southeast and beyond. Renowned speakers from all over US are invited as plenary or keynote speakers. The location of the Conference varies throughout the Southeastern US, but in its 41-year history this is the first time the Conference will be held in Raleigh as Joint Symposia with 2012 SERMACS. Moreover, this time it will be dedicated to the memory of our esteemed NCSU colleague, Prof. Edward Stejskal. His work has resulted in numerous breakthroughs in solution and solid-state NMR and diffusion-based MRI, and a special half-day symposium will be dedicated to his outstanding contributions to the field.

Cutting-edge results on structure determination of biological macromolecules by the NMR and EPR methods will be presented, including protein structure and dynamics, biochemical reaction mechanisms, and molecular recognition processes. Other topics will include novel applications in MRI, magnetic resonance of materials, and sensitivity enhancement by Dynamic Nuclear Polarization (DNP) method. Furthermore, SEMRC has always been a forum for graduate students and postdoctoral scholars to present the results of their work. In accord with these traditions, the SEMRC program features numerous talks by young investigators.

JOINT 2012 SEMRC/SERMACS SYMPOSIA PROGRAM

Thursday, Nov. 15 1:15 PM-5:30 PM Room 306C

Special Symposium dedicated to the memory of NCSU Professor Edward O. Stejskal (1932-2011)

Speakers:
Jacob Schaefer (Washington University – St. Louis)
Charles Johnson (UNC – Chapel Hill)
James Prestegard (University of Georgia)
Robert Tycko (National Institutes of Health)
Matthew Merritt (UT Southwestern – Dallas)

Friday, Nov. 16 8:20 AM-12:30 PM
Membrane Proteins/Peptides – Structure and Dynamics by NMR and EPR (Parallel Sessions in Rooms 306B and 306C)

Friday, Nov 16 1:30-3:00 PM SEMRC Poster Session (Hallway next to Rooms 306B and 306C)

Friday, Nov 16 3:30-5:15 PM
Contrast Methods/MRI – NMR/EPR Methods and Materials (Parallel Sessions in Rooms 306B and 306C)

Saturday, Nov 17 8:20 AM-12:30 PM
Structure and Dynamics by NMR and EPR (Room 306C)

Saturday, Nov 17 1:30-3:00 PM SEMRC Poster Session (Hallway next to Rooms 306B and 306C)

Saturday, Nov 17 3:30-5:15 PM
New NMR/EPR Methods (Room 306C)

For more information please refer to the Joint 2012 SEMRC/SERMACS Conference website: www.sermacs2012.org/semrc
126th NC ACS Local Section Awards

At the SERMACS Welcome Reception on
Wed., Nov. 14th, Raleigh Convention Center, 5-8 pm
http://ncacs.sites.acs.org/

2012 NC ACS Distinguished Speaker Lecture

Jane and Dave Richardson
Duke University
“Admiring, Analyzing, and Improving the 3D Structures of Macromolecules”

The Richardsons have jointly headed a research group at Duke University since 1970, focusing on analysis, understanding, and representation of protein and RNA 3D structures. They solved two of the first few protein crystal structures and were among the first groups to do protein \textit{de novo} design. They have developed free, cross-platform software that displays molecular graphics optimized for the communication of specific ideas in 3D, called kinemages. A long-term vision is to enable the determination of accurate models even from low-resolution data. Jane is best known for developing the ribbon diagram to show protein structures, first published in 1981 and initially hand-drawn, but later computer generated. These now-ubiquitous renditions help to simplify and organize the visualization of these complex molecules and to convey their elegance. Dave is the author of the kinemage graphics concept and the Mage display program, and has made substantial contributions in methods development for crystallography, multi-dimensional data analysis, and molecular graphics.

Dave and Jane met in the physics library at Swarthmore College, have been married for 50 years, and have two children. Jane was awarded a MacArthur Fellowship for her work in structural biology. She is a member of the National Academy of Sciences, the American Academy of Arts and Sciences, and the Institute of Medicine, and was elected president of the Biophysical Society for 2012-2013.

2012 NC ACS Marcus Hobbs Award

Dr. Laura Sremaniak received her BS degree in Chemistry from the University of South Carolina in 1991, and a PhD in theoretical chemistry from the University of North Carolina at Chapel Hill in 1996. She joined the chemistry faculty at North Carolina State University in 1996 and is now a Teaching Associate Professor and Associate Chair of the department. In addition to teaching physical chemistry, she has developed and implemented two Computational Chemistry Laboratory courses in the BS curriculum. Her research interests include electronic structure calculations of adsorbates on metal, oxide and zeolite surfaces. Laura has been an ACS member since 1990 and is currently a Councillor for the NC-ACS Local Section. At the national level, she is a member of the Women Chemists Committee (WCC), chairing the Awards Subcommittee and Task Force on non-tenure track faculty. She also chairs the local WCC and the advisory subcommittee for Project SEED.
Barbara Ramsay Shaw is the first William T. Miller Distinguished Professor of Chemistry at Duke University. Shaw’s research focuses on boranophosphates, their interactions with DNA and RNA, and their clinical and therapeutic uses. During her career she has published over 130 scientific articles, been issued eight patents, and presented 160 invited lectures. She received the American Cancer Society Faculty Research Career Development Award and the Camille and Henry Dreyfus Foundation Teacher-Scholar Award. Shaw received her Bachelor’s degree in Chemistry from Bryn Mawr College and her doctorate from the University of Washington at Seattle with Dr. J. Michael Schurr. She also was a visiting graduate student in the laboratory of Dr. Walter Kauzmann at Princeton University. Shaw completed a postdoctoral fellowship at Oregon State University working with Dr. K.E. van Holde and immediately following this became a faculty member at Duke in 1975. During her 37 years at Duke, she has mentored 26 postdoctoral fellows, 25 doctoral students and 6 masters’ students. They have presented over 300 papers at scientific conferences.
Royce W. Murray is Kenan Professor of Chemistry at the University of North Carolina, Chapel Hill. He joined the UNC faculty in 1960 and became Kenan Professor of Chemistry in 1980. Murray has been colleague to nearly 160 graduate and post-graduate students, with whom he has published over 450 papers. His contributions have been recognized by a number of awards including the ACS Award in Analytical Chemistry, and by his election to the National Academy of Sciences. He served for 1991-2011 as Editor-in-Chief of the journal Analytical Chemistry. His research interests are broad, currently focusing on the molecular design and analysis of electroactive nanoparticles.
Christian Melander received a B.S. in Chemistry with departmental honors from UC Davis in 1994 where he worked under the direction of Professor Mark Kurth developing combinatorial approaches to small molecule libraries. He subsequently received a Ph.D. in organic chemistry, supported by an NIH chemistry and biology-training grant, studying with Professor David Horne at Columbia University where he investigated the catalytic potential of nucleic acid bases. From 1998-2001 Christian was an NIH postdoctoral scholar at Caltech under the direction of Professor Peter Dervan studying the sequence-specific recognition of DNA with pyrrole/imidazole polyamides. Christian then directed the organic synthesis department at Xencor, Inc. in Monrovia, CA as a Lead Scientist from February of 2001 until September of 2002. He returned to academic research as a Research Associate at The Scripps Research Institute in the laboratory of Professor Joel Gottesfeld in the Department of Molecular Biology from 2002-2004. At Scripps, Christian utilized pyrrole/imidazole polyamides to explore potential therapeutics for both colon cancer and Friedrich’s ataxia. In July of 2004, Christian accepted a position as an Assistant Professor at North Carolina State University in the Department of Chemistry and in August, 2010 was promoted to Associate Professor with tenure. At NCSU, Christian’s research is focused on 1) defining small molecules that control bacterial behavior and 2) small molecule-coated nanoparticles that have antibacterial and antiviral properties. During his independent career, Christian has received the Sigma Xi faculty research award as well as the Industrial Innovation Award from the Southeastern ACS.

"Bacteria in biofilms present significant challenges in healthcare and many other industries, as they are upwards of 1000 times more resistant to antimicrobial agents than free-floating bacteria. Dr. Melander discovered the first class of small molecule that will both inhibit and disperse bacterial biofilms across order, class, and phylum. This discovery was based on pioneering research using nitrogen-dense alkaloids from sea sponges as a source of structural inspiration for the development of anti-biofilm molecules. Dr. Melander’s discovery has resulted in 41 primary publications, 17 filed provisional patents, 7 US patent applications, 10 PCT applications, 2 awarded US patents, and one assigned trademark since 2007. Given this broad range of applications, this technology has been referred to as “NC State’s Gatorade” to truly capture (and) articulate the potential this technology possesses.

To commercialize the anti-biofilm and antibiotic reactivation technology, Dr. Melander co-founded Agile Sciences in 2007. This company has received 9 SBIR/STTR grants, that with private investment has totaled more than $6M in operating expenses, currently has 6 full time employees, and has served as the poster child for the North Carolina Biotechnology Center for the commercialization of academic-based technology.”—excerpt from award nomination packet
Buck Goldstein is the University Entrepreneur in Residence and a Professor of the Practice in the Department of Economics. Prior to returning to the University, Goldstein co-founded Information America, an online information company which was publicly traded and subsequently acquired by the Thomson Corporation. Subsequently, he was a partner in Mellon Ventures, the venture capital arm of Mellon Bank. He is a Phi Beta Kappa graduate of UNC and an honors graduate of the UNC Law School.

Buck Goldstein has been involved in entrepreneurship most of his professional life. After six years as a practicing attorney, in 1982 he co-founded Information America, an online information company that developed hundreds of products from databases of public records collected and compiled from courthouses throughout the United States. Over the next sixteen years he led the company from start-up through several stages of venture capital financing to an initial public offering. In 1994, West Publishing, the largest legal publisher in the United States, acquired Information America. Goldstein served on the Executive Committee of West before and after its subsequent acquisition by Thomson, a multinational information and publishing company. Goldstein has been recognized as Entrepreneur of the Year by the Information Industry Association and Information America appeared numerous times in the Inc 500 list of rapidly growing businesses. In 1998, Goldstein founded NetWorth Partners, a venture capital fund focusing on information based enterprises with Mellon Ventures as its largest investor. NetWorth combined with Mellon Ventures in 2000 and Goldstein became a Mellon Ventures Partner. He served on the Board of Directors of both private and public companies during his tenure at Mellon Ventures.

In the spring of 2004, Goldstein was appointed University Entrepreneur in Residence at the University of North Carolina at Chapel Hill. Subsequently he was named Professor of the Practice in the Department of Economics. In these positions Goldstein is intimately involved in numerous activities aimed at making UNC a more entrepreneurial university including teaching and development work. He also serves as Chairman of Medfusion, a Raleigh based medical information technology company, a Board observer for I-Contact, an RTP based email marketing company, and an advisor to Liquidia, a nano-technology company that was founded in the UNC chemistry department.

Goldstein received his A.B. from the University of North Carolina in 1970 where he was elected to Phi Beta Kappa and the Order of the Golden Fleece, the University’s Highest Honorary Society. He received a M.Ed. from the University of Massachusetts in 1973, and a J.D. with Honors from the University of North Carolina in 1976 where he served on the Editorial Board of the UNC Law Review. In the spring semesters of 1997 and 1998, he served as an Adjunct Professor at the Goizueta School of Business at Emory University teaching an MBA course entitled Entrepreneurship on the Internet.

Goldstein has been active in numerous civic and charitable organizations over his career. He is married to Kay Goldstein and has two children, Katherine and Max. He and his wife live in Chapel Hill, North Carolina.
Dr. Christine Grant has been devoted for over 30 years to promoting and fostering inclusiveness at all levels of the STEM pipeline for underrepresented minorities and females in the chemical sciences and engineering.

She is currently a Professor of Chemical Engineering at North Carolina State University, only one of 5 African American women in the U.S. at that rank. She also serves as Associate Dean of Faculty Development and Special Initiatives in the College of Engineering.

Dr. Grant is an accomplished researcher in the chemical sciences and engineering, thus serving as an excellent role model for underrepresented minorities and females in STEM. Her dedication to promoting and fostering inclusion extends nationally and internationally with over 40 invitations to speak across the globe on mentoring and professional development. She has mentored over 150 students and postdoctoral fellows, the majority of whom are female and/or from underrepresented groups, and almost all of whom have continued onto careers in the chemical sciences and engineering. Dr. Grant has also mentored over 200 junior science and engineering faculty at NC State and beyond.

The “Promoting Underrepresented Presence on Science and Engineering Faculties (PURPOSE) Institute” founded by Grant is celebrating over seven years of promoting careers of minority and women faculty while providing role models for students at all stages in the pipeline. Her K-12 mentoring includes innovative programs that mentor the parents along with each student.

Her awards and service include: Council for Chemical Research Diversity Award; NSF Presidential Award for Excellence in Science, Math and Engineering Mentoring (PAESMEM); American Institute of Chemical Engineers Board of Directors; and Boeing Senior Fellow of the National Academy of Engineering’s Center for the Advancement of Scholarship on Engineering Education.
The E. Ann Nalley Award

Volunteer Service to the Southeast Region of the ACS

Dr. Chris Bannochie

6:00 p.m., Friday, 16 November 2012
NC Museum of Natural Sciences

Chris Bannochie is currently a Fellow at the Savannah River National Laboratory. From 1998 – 2001 he was a Visiting Scientist at Lawrence Livermore National Laboratory. Dr. Bannochie received a B.A. degree in Chemistry with a minor in Mathematics from St. John’s University and a Ph.D. in Inorganic Chemistry from Texas A&M University under Art Martell. He completed a postdoctoral fellowship under Michael Welch at the Mallinckrodt Institute of Radiology of the Washington University School of Medicine in St. Louis. Dr. Bannochie is a graduate of Leadership Augusta.


At the region level Dr. Bannochie served in the Chair succession for SERMACS, Inc., the Southeastern Regional Meeting from 2008 – 2010 where he helped create a regional meeting identity for SERMACS including the commissioning of its first logo and a redesigned website to capture the contributions of and recognize past regional award winners. He worked with the ten regional meeting steering committees to finance the creation of the E. Ann Nalley Volunteer Service Award in order to provide ongoing recognition of member service to the Society.

At the Division level as Member-At-Large (2002), Treasurer (2003 – 2008), Program Chair (2007 – 2008), Secretary (2009), and Chair succession (2010-2012) for the Division of Professional Relations. He led the first strategic planning efforts for the division in 2006 which resulted in the formation of diversity oriented subdivisions serving younger chemists, women chemists, chemist with disabilities, underrepresented racial and ethnic minority chemists, and gay & transgender chemists. Division membership has grown 40% in the five years since the subdivision structure became active.

At the National level Dr. Bannochie chaired the Council Committee on Economic and Professional Affairs (CEPA) Subcommittees on Professional Services & Programs (1998 – 1999) and Public Policy (2003 – 2006). His efforts in public policy lead to ACS policy statements covering Income Security for Retirees, Nondiscrimination, and L1 Visas. He was a Consultant to the ACS Committee on Meetings and Expositions (2008 - 2010). He is a member of the ACS Committee on Science (ComSci) (2007 – 2013) and chairs the ComSci Subcommittee on Public Policy. Dr. Bannochie served as an ACS Topic Reviewer for the 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem), and he is serving again in this role for the 2015 Pacifichem conference.
Research Alone is Not Enough: Opportunities for Chemists in Uncertain Times

Dr. Joseph M. DeSimone

6:00 p.m., Friday, 16 November 2012
NC Museum of Natural Sciences

Joseph DeSimone is the Director of the Frank Hawkins Kenan Institute of Private Enterprise and is the Chancellor’s Eminent Professor of Chemistry at the University of North Carolina at Chapel Hill and William R. Kenan Jr. Professor of Chemical Engineering at North Carolina State University and of Chemistry at UNC. DeSimone is also an Adjunct Member at Memorial Sloan-Kettering Cancer Center in New York. DeSimone has published over 280 scientific articles and has 120 issued patents in his name with over 120 patents pending. DeSimone is an elected member of both the National Academy of Sciences and the National Academy of Engineering as well as the American Academy of Arts and Sciences. DeSimone has received over 40 major awards and recognitions including the 2012 Walston Chubb Award for Innovation by Sigma Xi, 2011 Mendel Medal from Villanova, 2010 AAAS Mentor Award, the 2009 NIH Director’s Pioneer Award, the 2009 North Carolina Award, and the 2008 Lemelson-MIT Prize for Invention and Innovation.

DeSimone, an innovative polymer chemist, has made breakthrough contributions in green chemistry, fluoropolymer synthesis, colloid science and nano-biomaterials. He pioneered supercritical CO2-based polymerization reactions and the self-assembly of molecules in compressible media. He has shown the benefit of novel fluoro-elastomers for soft lithographic applications, including the synthesis of shape-controlled nano-biomaterials. DeSimone received his BS in Chemistry in 1986 from Ursinus College in Collegeville, PA and his Ph.D. in Chemistry in 1990 from Virginia
Marty St. Clair was born in Oregon. She attended Oregon State University, majoring in Biochemistry, before attending graduate school at Duke University. Marty started working in the new virology laboratory at Burroughs Wellcome in 1976. She spent the next four years working with herpes viruses and was instrumental in determining the mechanism of action of acyclovir.

In 1984, Marty switched to HIV in order to discover and develop an antiviral against this new, devastating disease. Marty is an inventor of the first drug to be used against HIV/AIDS, AZT. Marty has worked in HIV ever since as the company morphed into Glaxo Wellcome and now GlaxoSmithKline. She is presently working on an integrase inhibitor which will be submitted for approval before the end of the year.
Susanne M. Dana from Blacksburg High School is the recipient of the 2012 SERMACS Award for Excellence in HS Teaching. Ms. Dana earned both her B.S. and M.S. from Virginia Tech and has been teaching in Virginia public schools for 17 years. She taught at New Horizons Governor's School for Science and Technology and the Roanoke Valley Governor's School before moving to Montgomery County in 1999. Ms. Dana has taught math, physics, and STEM courses in addition to both introductory and advanced chemistry courses. Her colleagues have noted that she has a deep and broad expertise in chemistry content knowledge as well as an exceptional understanding of how to design classroom instruction.

For the past 10 years, she has designed an annual science safety workshop for student teachers using several teaching methods (inquiry-based learning, case-based teaching approach, hands-on activities) to model best teaching practices and help future teachers deal with safety, ethical, and classroom management issues. She has served on numerous state committees concerning curriculum and assessment. At BHS, she has supported her fellow teachers by serving as the teacher representative on the new building committee as well as serving as the chair on school leadership and governance committees.

Ms. Dana was the first teacher in Montgomery County to attain National Board Certification through the National Board for Professional Teaching Standards. She is an active member of the Virginia Blue Ridge American Chemical Society and was chosen by the society as the Outstanding High School Chemistry Teacher of the Year in 2002. She has been teacher of the year for BHS, Montgomery County Public Schools, and received the Virginia Region VI Teacher of the Year award in 2008.
Detection of Designer Drugs and Formulations

Dr. Brian F. Thomas

12:00 p.m., Saturday, 17 November 2012

Dr. Brian F. Thomas received his Ph.D. from the Department of Pharmacology and Toxicology at the Medical College of Virginia/Virginia Commonwealth University, where he was awarded the Lauren A. Woods Award for Research Excellence. After receiving his degree, Dr. Thomas began his career at RTI International, and is currently serving at RTI as the Senior Director of the Center for Analytical Chemistry and Pharmaceutics. This management role involves overseeing the activities of over 50 scientists involved in the development and application of quantitative and qualitative analytical methods, and the interpretation and dissemination of their results. In addition to his management activities, Brian has continuously served as Principal Investigator on two contracts funded through the National Institute on Drug Abuse (NIDA) for over 20 years. He has also held two R01-funded research grants through NIDA, and has served as key personnel on additional contracts or grants funded by the National Cancer Institute, the National Institute on Neurological Diseases and Stroke, the National Institute on Environmental Health Sciences, and other Institutes within the National Institutes of Health. His publication record includes over 60 peer reviewed manuscripts, 6 book chapters or research monographs, and he has been awarded 2 US Patents. In recognition of his research contributions, Dr. Thomas has been awarded RTI’s President’s Award three times, in 2005, 2006, and again in 2012. He is an active member in the College on Problems of Drug Dependence and the International Cannabinoid Research Society, where he has served on numerous organizational committees, and is currently serving as the Society’s Newsletter Editor. He also serves on the Editorial Board of ISRN Pharmacology, is an occasional reviewer for a wide variety of scientific publications, and has provided continuous service on NIDA contract and grant review committees for the last 20 years.
## SERMACS 2012 Short Courses and Workshops

### Tuesday, Nov 13th

| Marriot University A | 8:30AM-5:00PM | *Extraordinary Leaders (ACS Leadership Development Course)*  
In a volunteer organization like ACS and in the workplace, great leaders can significantly impact the productivity of a team, the effectiveness of a local section, and the performance of a committee. Being a competent leader starts with knowing what it takes to be a great leader and gaining an understanding of your own strengths. The ACS Extraordinary Leader course provides a model for effective leadership that will help you achieve exceptional results. As part of the program you will participate in a 360° feedback process that gives you personal feedback on your leadership competencies. You will then use this feedback to create a personal plan for developing your leadership strengths to become an extraordinary leader. |

### Wednesday, Nov 14th

| Marriot University A | 8:00AM-5:00PM | *Pharmacokinetics and Pharmacodynamics in Drug Discovery for Chemists*  
This one-day, Special Topics course is designed to increase understanding of the fundamental concepts governing drug pharmacokinetics (ADME studies) as they are utilized in new drug discovery. The course consists of lectures on the biological concepts and assays used for the pharmacokinetics description of in vivo drug action (ADME estimation of the concentration of the drug at the target). Emphasis is placed on the use of ADME principles to chemically optimize favorable druglike activity and reduce unfavorable side effects. Additionally, in course exercises are used to illustrate principles. |

| Marriot University B | 8:00AM-5:00PM | *The Essentials of Supervising Scientists & the Technical Staff*  
In just one day, learn the essential techniques for successfully leading scientists, engineers and other members of the technical staff. Perfect for supervisors and team leaders who want immediate and practical help in managing in a high-performance lab environment. |

| Marriot University C | 8:00AM-5:00PM | *Electrochemical Measurement of pH and Ions: Troubleshooting and Correcting Error and Bias*  
Use of and interpretation of the data obtained from pH and ion selective electrode will be covered in this hands-on course designed for scientists and engineers engaged in regulatory compliance in the chemical, petroleum, coatings, food, electronics, pharmaceutical, cosmetics, water, and wastewater industries. |

| Marriot Chancellor | 8:30AM-12:00PM | *Negotiations Workshop for Women Faculty & Professionals (COACH)*  
In this workshop participants learn  
• The importance of negotiation  
• The necessary elements of a successful negotiation  
• The importance of developing alternatives to an agreement  
• Techniques for handling difficult people and conversations  
• The importance of listening and appreciating different viewpoints  
• Follow-up techniques.  
This interactive workshop involves self-examination of negotiation styles, role playing of case studies and personal coaching.  
1:00PM-4:30PM | *Negotiations Workshop for Women Postdocs & Graduate Students (COACH)*  
The ability to negotiate effectively can play a key role in your career advancement, from determining time on shared equipment, to authorship on papers, to when a thesis will be completed.  
This workshop teaches the fundamentals of negotiation including identifying why negotiation is important, what issues are and aren’t negotiable, the steps towards reaching a final agreement, tactics useful for difficult negotiations and identifying when to end the negotiation.  
The session consists of a presentation on these issues with plenty of time for role playing and practicing the techniques learned. |
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| 8:30AM-12:00PM | Glass Office | **Getting the Most Out of Your UPLC™/UHPLC Columns** (TCDG)  
Every day, more and more chromatographers are recognizing the power of UHPLC for improved resolution, speed, and sensitivity. As this ultra-performance technique gains broader popularity, the need for basic column care and use recommendations has increased. In this workshop, we will present a number of practical tips for achieving optimum column performance and lifetime with a focus on:  
- mobile phase preparation  
- sample preparation  
- column installation, use, and storage  
- troubleshooting common column issues  
While the focus of the workshop will be on UPLC/UHPLC column use, the troubleshooting principals and recommendations will have broader applicability to HPLC work as well. |
| 8:30AM-12:00PM | Glass Office | **Fundamentals and Advancements in Analytical SFC/SFE** (TCDG)  
This workshop will cover the basics of supercritical fluid chromatography and supercritical fluid extraction. SFC utilizes supercritical CO2 as the main mobile phase component and the solvating properties can be manipulated using temperature and pressure. The technique greatly reduces the use of organic solvents. It's also the perfect complement to MS due to its low solvent load and high resolution, narrow peaks and faster separation than liquid chromatography.  
SFC is a normal phase technique providing orthogonal separations to reversed phase chromatography, and better separation of isomers without the disadvantages of traditional normal phase separations. It is also the technique of choice for chiral separations.  
Supercritical fluid extraction takes advantage of all of the same benefits of supercritical CO2 for chromatography (high diffusivity and low viscosity) but applies them to a tunable extraction technique.  
We will cover the basics and applications of both techniques. |
| 8:00AM-12:00PM | Room 203 | **NIH Funding for Chemists: Grant Writing Tips for New and Experienced Applicants**  
This workshop is intended to give both new and experienced grant writers valuable information on how to find grant opportunities at NIH, how to prepare their applications, and what to expect from the review process. It is broken into two parts. The first session will provide an overview of NIH, describe opportunities relevant to chemists, and give tips on preparing a competitive application at a level appropriate for experience researchers. The second session will build on the overview and delve more deeply into reading a solicitation, writing the specific aims and research plan, and what happens during an NIH review meeting. While it's intended that new grant writers attend both sessions, experienced grant writers are welcome to stay for the second session as well. |
| 1:00PM-5:00PM |         | **Fostering Innovation** (ACS Leadership Development Course)  
We are constantly challenged to come up with new ideas, approaches, and solutions, yet most of us feel ill-equipped to do this effectively. With a systematic and proven process to generate ideas you can lead your team to develop new ideas. Gain the understanding and tools to tap into your own innovation style and stimulate innovative thinking among your committee members. |
### Friday, Nov 16th

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<th>Room 201</th>
<th>Time</th>
<th>Event Description</th>
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<tr>
<td></td>
<td>8:30-9:30AM</td>
<td>Planning Your Job Search (ACS Career Services Workshop)</td>
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<td>9:30-11:00AM</td>
<td>Preparing a Resume (ACS Career Services Workshop)</td>
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<td>11:00-12:30PM</td>
<td>Effective Interviewing (ACS Career Services Workshop)</td>
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<td>1:30PM-5PM</td>
<td>Resume Reviews (ACS Career Services Workshop)</td>
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<th>Room 201</th>
<th>Time</th>
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<tr>
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<td>Speed Networking 8:30AM -12:30PM</td>
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<th>Room 307</th>
<th>Time</th>
<th>Event Description</th>
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<tr>
<td></td>
<td>1:00PM-4:00PM</td>
<td>Backward Course Design (IC-bG)</td>
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<td>This workshop will provide participants with a roadmap for transforming their teaching through effective course design. Effectively designed courses can lead to increased student engagement, reinvigorate academic programs and make teaching more enjoyable. After a brief introduction, workshop participants will explore and share strategies for designing innovative courses using the principles of backward course design. Our goal is that they will leave this workshop with a concrete plan for their own new or modified course. In addition, we will offer examples of active learning strategies that incorporate civic issues, technology, and problem solving, based on the needs of the participants. The majority of the session will be participants sharing ideas in small groups while we act as facilitators.</td>
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### Saturday, Nov 17th

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<tr>
<th>Room 301 A/B</th>
<th>Time</th>
<th>Event Description</th>
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<tbody>
<tr>
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<td>2:00PM-4:00PM</td>
<td>Chemistry Demonstration</td>
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<td>The demonstration workshop is planned for high school teachers and other educators with somewhat limited facilities and laboratories. This will be a hand’s on workshop with some 10 15 different stations where the attendees can learn and try a series of demonstrations in various areas of chemistry……..and all will use readily available and inexpensive materials with a bare minimum of hazards involved. Included will be such demonstrations as the electrolysis of water and of potassium iodide, the Daniel Cell, the chemistry of money, chemical “magic”, chromatography, luminescence, distilling alcohol from Listerine, chemistry and your health, elasticity, time-related properties of polymers using slime and others. Demonstration “instructors” will be from North Carolina State University, University of North Carolina at Chapel Hill and Duke University. Write-ups of the details of the various experiments will be available on line prior to start of the workshop.</td>
</tr>
</tbody>
</table>
The Undergraduate Program will run from **Friday, November 16 through Saturday, November 17** with **Technical Sessions, Career Offerings and Special Events** for students. Undergraduate programming is open to all SERMACS attendees.

**Friday, November 16**

**8:30 a.m. – 12:30 p.m.**
ACS Job Search/Resume/Interviewing Workshop/Speed Networking 201

**8:30 a.m. – 5:00 p.m.**
Graduate School Fair Ballroom Lobby

**9:00 a.m. – 11:00 a.m.**
Poster Session I Organic/Organometallic/Inorganic Ballroom C

**1:00 p.m. – 4:40 p.m.**
Undergraduate Oral Presentation I Analytical/Bioanalytical 202
Undergraduate Oral Presentation II Biochemistry/Biomedical 203
Undergraduate Oral Presentation III Organic/Organometallic 204

**1:00 p.m. – 5:00 p.m.**
Career Connection Glass Office
ACS Resume Review 201

**2:00 p.m. – 4:00 p.m.**
Poster session II Computational/Environmental/Material/Physical/Polymer Ballroom C

**Saturday, November 17**

**8:00 a.m. – 11:00 a.m.**
Undergraduate Oral Presentation VI Material/Polymer 205

**8:30 a.m. – 5:00 p.m.**
Graduate School Fair Ballroom Lobby

**8:40 a.m. – 11:00 a.m.**
Undergraduate Oral Presentation IV Computational/Environmental 203
Undergraduate Oral Presentation V Inorganic/Physical 204

**9:00 a.m. – 11:00 a.m.**
Panel Discussion – Preparing students for college chemistry 306

**9:00 a.m. – 12:00 p.m.**
Career Connection Glass Office

**11:00 a.m. – 12:00 p.m.**
Chemistry Demo- see Special events below 301
Saturday, November 17 continued

12:00 p.m. – 2:00 p.m.
Undergraduate Awards Luncheon
Keynote Address: Thirty Years of HIV Drug Development: a Message of Hope
by Marty St. Clair, GlaxoSmithKline

2:00 p.m. – 4:00 p.m.
Chemistry Demo Workshop-see Special Events below

Undergraduate Special Events

Panel Discussion: “Preparing Students for College Chemistry” 9:00 a.m.– 11:00 a.m., Room 306

What are the common traits seen in students that succeed in College Chemistry? What are the common
difficulties that students experience in College Chemistry? That is the starting point for this panel discussion. Our
panelists represent a wide variety in the education spectrum. When thinking of College Chemistry, usually public
and private institutions are thought about as well as large and small institutions. We have panelists representing
all of these. There are some other areas that might not immediately come to mind where people take College
Chemistry: to represent them, we have AP Chemistry as well as Community College represented. Come and
join the discussion about preparing students for college chemistry.

Chemistry Demo: 11:00 a.m. – 12:00 p.m., Room 301

Class demonstrations make the whole class fun and engaging. The students learn and absorb the subject better
and it stays in their memory longer, if not forever. Come see some experienced presenters perform some
educational and crowd tested chemistry demonstrations.

Chemistry Demo Workshop: 2:00 p.m.– 4:00 p.m., Room 301

Enhance your class with these eye-catching Demos. The demonstration workshop is planned for high school
teachers, other educators and anyone presenting chemistry with somewhat limited facilities and laboratories.
This will be a hands-on workshop with different stations where the attendees can learn and try a series of
demonstrations in various areas of chemistry……..and all will use readily available and inexpensive materials with
a bare minimum of hazards involved.

Included will be such demonstrations as the electrolysis of water and of potassium iodide, the Daniel Cell, the
chemistry of money, chemical “magic”, chromatography, luminescence, distilling alcohol from Listerine, chemistry
and your health, elasticity, time-related properties of polymers using slime and others.

Demonstration “instructors” will be from North Carolina State University, University of North Carolina at Chapel
Hill and Duke University. Write-ups of the details of the various experiments will be available on line prior to start
of the workshop.
SERMACS 2012 Career Program

Career Workshops - Friday, 16 November, Room 201

**Speed Networking (8:30 AM – 12:30 PM)**
It works just like the ‘Speed Dating.’ This fun activity gives the participants multiple, non-threatening opportunities to put into practice important interviewing skills. Find out if you can effectively present yourself to prospective employers.

**Planning Your Job Search (8:30 AM – 9:30 AM)**
Your success in conducting an effective job search depends on the ability to organize your search and target the job market segment that’s right for you. This session will help you plan and execute an effective job search. You’ll learn about the changing trends in the employment marketplace for chemical professionals, and carry out a personal assessment to help you identify which jobs will be best suited to your values, skills and motivations. You’ll also discover how to find hidden job markets through networking, how to make effective cold calls to employers, and how to find useful information about potential employer organizations.

**Preparing a Résumé (9:30 AM – 11:00 AM)**
There is only one purpose of a résumé: to get an interview for the job you want. In this workshop you'll learn what content to include and not include in your résumé and how you should think about organizing that content. We'll also focus on the visual appeal - the length and layout that invites the recruiter to review it. We will also discuss how to send your résumé electronically.

**Effective Interviewing (11:00 AM – 12:30 PM)**
Performing well in a job interview and acing an exam in school have one thing in common: the more prepared you are, the more successful you will be. This workshop provides practical steps to help you prepare for an interview with specific focus on 3 key aspects: 1) becoming familiar with the questioning format used by many interviewers, 2) preparing your responses to some “tough” interview questions, and 3) conducting “due diligence” research on the organization. You will also learn to highlight your unique strengths and the special ways you can contribute to the hiring Organization without appearing to be boastful.

**ACS Résumé Review (1:30 PM – 5:00 PM)**
Have your résumé evaluated by an experienced professional.

Career Connections – 9-5 Thursday, 1-5 Friday, 9-12 Saturday, Glass Office

Attention Job Seekers! We will be dedicating a powerful resource throughout the conference just for you. The Career Connections room will be a busy place throughout the conference. Approximately every two hours throughout the event you will be able to see a short talk on a variety of job hunting topics like Networking Do’s and Don'ts, Navigating Applicant Tracking Systems, LinkedIn Profiles, Professional Dress and more. There will be a position bulletin board where you will be able to find current openings from great companies. You can drop by to print off your résumé, get it critiqued by a professional recruiter or network with other fellow job seekers. We would also like to offer you a great opportunity to get your résumé in front of many of the organizations attending the conference. As a special offering for employers, we will be creating a résumé CD filled with great candidates. If you would like your résumé to be included, all you will need to do is simply forward your résumé to SERMACS2012Career@gmail.com in either a MS Word or PDF format only and answer the following questions in the body of your email.

1. Available to relocate (yes or no), and list any geographical restrictions if applicable
2. Shift or hours requirements/limitations
3. List highest Education Obtained
4. List Areas of Expertise (no more than three please)
5. Name, Phone Number, and email address

Space will be limited, so please make sure to limit the size of your attachment. Excessively large files may be excluded. This is a great opportunity to be seen by some of the best employers in the country. We will do our best to include all those that are submitted by 17-Nov-2012.
High School and ACS Project SEED Program

The High School Program at SERMACS 2012 Meeting in Raleigh, NC, that is scheduled on **Saturday, November 17th**, 8:00 a.m. – 6:00 p.m. will have four exciting special events for the students and all attendees.

**High School and Project SEED oral presentations**: Room 305A, 8:00 a.m. – 11:00 a.m.

**High School and Project SEED poster presentations**: Room 305A, 9:00 a.m. – 11:00 a.m.

**High School Teacher program orientation by Learn NC**: Room 304, 8:00 a.m. – 11:00 a.m.  
Invitation only

**Panel Discussion: Preparing Students for College Chemistry**: Room 305B, 9:00 a.m. – 11:00 a.m.

What are the common traits seen in students that succeed in College Chemistry? What are the common difficulties that students experience in College Chemistry? That is the starting point for this panel discussion. Our panelists represent a wide variety in the education spectrum. When thinking of College Chemistry, usually public and private institutions are thought about as well as large and small institutions. We have panelists representing all of these. There are some other areas that might not immediately come to mind where people take College Chemistry: to represent them, we have AP Chemistry as well as Community College represented. Come and join the discussion about preparing students for college chemistry.

**Chemistry Demo & Workshop**: Room 301  
11:00 a.m. – 12:00 p.m. Demo and 2:00 – 4:00 p.m. Demo Workshop, Room 301

Class demonstrations make the whole class fun and engaging. The students learn and absorb the subject better and it stays long time in their memory if not forever. Enhance your class with these eye-catching Demos in the Workshop. You can register for the workshop while you register for the meeting.

**High School Teacher Award Luncheon – Ticketed event**: Room 304, 12:00-1:30 p.m.

**Keynote Address**: Thirty Years of AIDS Research: A Message of Hope, Marty St. Clair, GlaxoSmithKline

**Project SEED Best Practices Symposium**: Room 305A, 1:20-5:00 p.m.  
In the morning a SEED student Poster session will be held and judged to select the best posters, with awards presented at the end of this afternoon Workshop session. In the SEED Workshop, SEED coordinators from the Southeast ACS region will share experiences in their SEED programs, these will be discussed, and an attempt will be made by all participants to arrive at “What works best in Project SEED”. Anyone interested in outreach programs to increase the number of economically disadvantaged and minority students attending College, majoring in a STEM curriculum, and preparing for a STEM career should find this symposium of great interest and value.

**High School Teacher program orientation by Learn NC- Invitation only**: Room 304, 3:00 p.m. – 5:00 p.m.
ACS District Director’s Ice Cream Social

Friday, November 16, 2:30 p.m. – 3:30 p.m.
Room 304

During the Ice Cream Social, we will feature, Let’s Talk Strategy!

This time will be designed to engage the Society’s stakeholders in the goals of the Society and how their ideas contribute to fulfilling these goals. The conversations are short, informative, and fun. Come share your strategy with us – let’s talk!

Sponsored by the ACS Council Policy Committee

The Board of Directors composed of the President, President-Elect, the most recent Past President, six district directors, one elected from each of six geographical Districts, and six Directors-at-Large, is chartered to “have, hold, and administer all the property, funds, and affairs of the Society.

ACS Directors:

- William F. Carroll, Jr., Director at Large, Chair
- Valerie J. Kuck, Director at Large
- Kathleen M. Schulz, Director at Large
- Neil D Jespersen, Director District I
- Pat N. Confalone, Director District III
- Peter K. Dorhout, Director District V
- Dennis Chamot, Director at Large
- Barbara A. Sawrey, Director at Large
- Kent J. Voorhees, Director at Large
- George M Bodner, Director District II
- Larry K. Krannich, Director District IV
- Bonnie Charpentier, Director District VI

The American Chemical Society Southeastern Regional Meeting Board (SERMACS, Inc.) selects the location of the Southeastern Regional Meetings, administers regional ACS awards, and provides guidance to meeting planners.

Officers
- Past Chair: Stuart Burris, Nashville Section
- Chair: Keith Hollis, Ole Miss Section
- Chair-Elect: Ann Sullivan, Virginia Section
- Treasurer: Sol Levine, North Carolina Section
- Secretary: Angela Peters, South Carolina Section

General Chairs
- Most Recent Completed – Richmond 2011: Joe Pompano, Virginia Section
- Current – Raleigh 2012: Charlie Goss, North Carolina Section
- Next Future – Atlanta 2013: Deborah Sauder & Terry Say, Georgia Section
  - Nashville 2014: Stuart Burris, Nashville Section

Learn more about the Southeastern Regional Board and SERMACS meetings at www.sermacs.org
# SERMACS 2012 Vendor Exposition

**Ballrooms B & C**

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<thead>
<tr>
<th>Thursday, November 15</th>
<th>Friday, November 16</th>
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<tr>
<td>Vendor Exposition: 8:30 a.m. – 6:00 p.m.</td>
<td>Vendor Exposition: 8:30 a.m. – 5:00 p.m.</td>
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<td>Sci-Mix: 6:00 p.m. – 8:00 p.m.</td>
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<td>Airgas National Welders</td>
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<td>Alfa Aesar, A Johnson Matthey Company</td>
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<td>Anasazi Instruments</td>
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<td>Anton Paar USA</td>
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<td>SERMACS 2013 &amp; 2014</td>
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<td>Tosoh Bioscience</td>
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<td>Triangle Chromatography Discussion Group</td>
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<td>Vernier Software &amp; Technology</td>
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<td>Wasatch Photonics &amp; Spectrecology</td>
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<td>Waters Corporation</td>
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<td>Wilmad-LabGlass</td>
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<td>44</td>
<td>World Wide Medical Products</td>
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SERMACS 2012 EXHIBITS

Commercial Exhibit
November 15-16, 2012
Thursday-Friday

Raleigh Convention Center
Ballrooms B-C, 3rd Floor

Thursday: 8:30 a.m. - 8:00 p.m.
(includes 6-8pm Sci-Mix reception in Exhibit Area)

Friday: 8:30 a.m. - 5:00 p.m.

COMMERCIAL EXHIBITOR SEMINARS

RCC Room 307

<table>
<thead>
<tr>
<th>DAY</th>
<th>TIME</th>
<th>EXHIBITOR SEMINAR TITLE, PRESENTER</th>
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<tbody>
<tr>
<td>Thursday, Nov. 15</td>
<td>10:00 - 11:00 a.m.</td>
<td><strong>Waters Corporation</strong> “UPC2 : An Alternative Technology for LC Applications and Extractions”</td>
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<td>Friday, Nov. 16</td>
<td>9:00 - 10:00 a.m.</td>
<td><strong>Gamry Instruments</strong>, Dr. Chris Beasley, &quot;Electrochemical Simulation of Non-conventional Experiments&quot; &amp; &quot;Gaining Insight to Interface Processes Using EQCM&quot;</td>
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<td>10:00 - 11:00 a.m.</td>
<td><strong>NETZSCH Instruments</strong> &quot;Thermal Analysis &amp; Thermal Properties Measurement of Polymers&quot;</td>
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<td>Booth Number</td>
<td>Company Name and Contacts</td>
<td>Company Description</td>
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| 56 | **Advion, Inc.**  
Garry Williams  
607-280-0865  
gwilliams@advion.com | Advion is a leader in MS & synthesis solutions. The expression CMS is a high performance, compact, affordable single quad mass spectrometer. Its compact size allows it to fit in space-limited labs for direct access and immediate results for chemists requiring mass confirmation, reaction monitoring, QC and purity analysis.  
[www.expressioncms.com](http://www.expressioncms.com) |
| 33 | **Airgas National Welders**  
Steve Baldwin  
800-943-0333  
Steve.Baldwin@airgas.com | Airgas, Inc. (NYSE: ARG), through its subsidiaries, is the largest U.S. distributor of industrial, medical and specialty gases, and hard goods, such as welding equipment and supplies. Airgas is also a leading U.S. producer of atmospheric gases, carbon dioxide, dry ice, and nitrous oxide, one of the largest U.S. distributors of safety products, and a leading U.S. distributor of refrigerants, ammonia products, and process chemicals.  
[www.airgas.com](http://www.airgas.com) |
| 43 | **Alfa Aesar, A Johnson Matthey Company**  
Goerge Wachter  
800-343-0660  
goerge.wachter@alfa.com | Alfa Aesar, a Johnson Matthey Company, is a leading global manufacturer and supplier of chemicals, materials and life science products for research. Our products are utilized by pharmaceutical, biotechnology and other advanced technology companies in applications such as drug discovery, genomic and proteomic research, and high technology product development.  
[www.AlfAesar.com](http://www.AlfAesar.com) |
| 25 | **Anasazi Instruments, Inc.**  
William H. Bearden  
whbeard@attglobal.net | No cryogen NMR! Anasazi Instruments, Inc. makes cryogen-free 60 and 90 MHz NMR instruments. These high resolution; permanent magnet NMR instruments are robust and have applications in R&D, quality control, and teaching. These instruments are available in three configurations, \(^1\)H, \(^1\)H/\(^13\)C, and \(^1\)H/multinuclear. The Eft spectrometer can measure simple 1D spectra as well as 2D COSY and 2D HETCOR spectra. Anasazi Instruments provides strong support and a strong warranty.  
[www.AINMR.com](http://www.AINMR.com) |
| 23 | **Anton Paar USA**  
Mark Coombs  
804-550-1051  
704-491-4880  
mark.coombs@anton-paar.com | Anton Paar produces high-quality measuring and analysis instruments for laboratory, research, and industrial applications. In the fields of density and concentration measurement we are the established world leader. Our product portfolio also includes viscometers, rheometers, polarimeters, refractometers, instruments for X-Ray structure analysis, microwave synthesis and microwave decomposition.  
[www.Anton-Paar.com](http://www.Anton-Paar.com) |
| 30 | **Asylum Research**  
Terry Mehr  
805-696-6444  
terry@asylumresearch.com | The AFM/SPM technology leader offers Cypher™, the world’s fastest and highest resolution AFM, for the most accurate images and precise measurements possible today. With a larger sample size and numerous environmental and advanced options, Asylum also offers the MFP-3D™ family of AFMs, including the MFP-3D-BIO, Stand Alone and Nanolindenter. Ask us about our new Electrochemical Strain Microscopy technique for energy storage research and our new tools for quantitative viscoelastic mapping-AM-FM and Loss Tangent imaging.  
[www.AsylumResearch.com](http://www.AsylumResearch.com) |
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<td>Matt Barnard</td>
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<td>Scott Klayner</td>
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<td>Bruker Daltonic</td>
<td>Ben Owens</td>
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<td>26</td>
<td>CEM Corporation</td>
<td>Michael Howe</td>
<td>800-726-3331</td>
<td><a href="mailto:mike.howe@cem.com">mike.howe@cem.com</a></td>
<td><a href="http://www.cem.com">http://www.cem.com</a></td>
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<td>Doty Scientific, Inc.</td>
<td>Laura Holte, Ph.D.</td>
<td>803-788-6497</td>
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<td><a href="http://www.dotynmr.com">www.dotynmr.com</a></td>
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<td>57</td>
<td>Environmental Express</td>
<td>Berna Mazon</td>
<td>843-576-1124</td>
<td><a href="mailto:bernam@envexp.com">bernam@envexp.com</a></td>
<td><a href="http://www.envexp.com/">http://www.envexp.com/</a></td>
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<td>14</td>
<td>Extrel CMS</td>
<td>Brian Begel</td>
<td>412-963-7530</td>
<td><a href="mailto:brian.begel@extrel.com">brian.begel@extrel.com</a></td>
<td><a href="http://www.extrel.com">www.extrel.com</a></td>
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| 51 | **Fun Science**  
    funscience@mindspring.com | The Fun Science was established in 1991 and its mission is to interject energy and enthusiasm about science into the teaching experience. At Fun Science we make the learning process fun and productive for kids at all ages. We have helped training thousands of teachers every year and clearly understand the time and resource limitations today’s teachers are facing. Over the years Fun Science has improved its products based on direct teacher feedback and evolved into much more than a provider of “science accessories”. Our focus is to create ready to use experiments – complete scientific kits that are fun, engaging and teach valuable scientific principles that will promote a lifetime love of learning. Each of our one-of-a-kind Fun Science Kits offer a variety of experiments with easy-to-follow instructions: scientific skills, outcomes, observation and results – A COMPLETE lesson plan!  
    http://www.funsciencekits.com  
    http://fivedollarfunscience.com/ |
| 47 | **Gamry Instruments**  
    Chris Beasley  
    215-682-9330 x115  
    cbeasley@gamry.com | Gamry Instruments offers a full-line of potentiostats/galvanostats/impedance analyzers, and other electrochemical instrumentation and accessories. We will also be demonstrating our electrochemical simulation software used to simulate adsorption, electrocatalysis, PCET, SWV, and FT voltammetry. Stop by to learn how Gamry can assist you with your research.  
    www.Gamry.com |
| 9-12  
17-20 | **IKA Works Inc.**  
    Matthew Ginos  
    910-452-7059  
    matthew.ginos@ika.net | IKA celebrates over 100 years as a global market leader in laboratory and analytical equipment. IKA technology offers a vast spectrum of innovative devices for mixing, tempering, distilling and crushing applications. Magnetic stirrers, overhead stirrers, dispensers, shakers, mills, rotary evaporators, calorimeters, laboratory reactors and incubation shakers make up the laboratory and analytical equipment portfolio. The company is headquartered in Staufen, Germany. Today, IKA employs over 800 people worldwide at six different locations on four continents.  
    www.IKA.com |
| 24 | **Innovative Technology, Inc.**  
    Ryan Bentley  
    978-462-4415  
    ryan.bentley@gloveboxes.com | Innovative Technology, Inc. is a leading worldwide manufacturer of inert atmosphere glovebox systems and solvent purification systems. We offer both standard and custom gloveboxes tailored to the individual customer requirements. Our PureSolv solvent purification systems deliver dry solvent at the turn of a valve eliminating hazardous & time-consuming thermal distillation processes.  
    www.gloveboxes.com |
| 15 | **Interchim, Inc.**  
    Cathy Dyer  
    913-349-6426  
    cdyer@intercheminc.com | Interchim is a global company which manufactures chromatography products for purification, analytical and sample preparation. The column product range is comprised of Flash, Prep, SPE, UPLC, and HPLC. Instruments for purification include the first Flash system to withstand pressures of 435 psi / 30 bar. The company has introduced high efficiency Flash Cartridges which run three times faster than conventional columns. Flash columns are available in 30 different bonded phases for normal and reverse phase, ion-exchange and chiral chromatography. The company continues to introduce innovative products to support the demands of speed and efficiency for discovery and analytical chemists.  
    www.interchiminc.com |
| 50 | **LEAP Technologies**  
    Tamara Navarro  
    919-929-8814  
    tnavarro@leaptec.com | LEAP Technologies offers customized automation applications including NMR sample handling, Bubble free automated NMR microtube filling station, mixing, reconstituting for comprehensive sample preparation, sample isolation, SPE. Transfer integrates HLPC purification with SPE functionality. LEAP eVol NMR, electronic syringe for NMR capillaries to improve results, save time and money.  
    www.leaptec.com |
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<td>13</td>
<td>MeasureNet Technology</td>
<td>Glenn Davis</td>
<td>866-396-6765</td>
<td><a href="mailto:davis@measurenet-tech.com">davis@measurenet-tech.com</a></td>
<td>MeasureNet brings Laboratory Information Management System (LIMS) functionality to teaching laboratories. MeasureNet's network design provides high-quality data acquisition and unparalleled classroom management without the cost and maintenance of bench-cluttering, stand-alone PCs. MeasureNet's patented network technology enables live data monitoring via the internet and remote storage for collaborative exercises between multiple labs and multiple institutions. Each network supports up to 15 work stations for experiments that include temperature, pressure, pH, voltage, and mass measurements. A shared UV-vis spectrometer delivers 1-nm resolution spectroscopy to student workstations. Additional acquisition tools include a dual-beam colorimeter, ion-selective electrodes, and electrochemistry probeware. MeasureNet users can integrate GCs, HPLCs, and calorimeters for advanced laboratory applications. <a href="http://www.measurenet-tech.com">www.measurenet-tech.com</a></td>
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<td>Metrohm USA</td>
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<td>866-METROHM</td>
<td><a href="mailto:info@metrohmusa.com">info@metrohmusa.com</a></td>
<td>Metrohm USA is your go-to source for precision, user-friendly titrators, ion chromatography systems, pH/ion meters, voltammetric analyzers, oxidative stability instrumentation and more. All feature 3 year warranties, and our IC suppressor features an unprecedented 10-yr warranty! All backed by expert application support and services—we’re there when you need us. <a href="http://www.metrohmusa.com">www.metrohmusa.com</a></td>
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<td>62</td>
<td>Mettler Toledo</td>
<td>Jeff Horsman</td>
<td>410-910-8118</td>
<td><a href="mailto:jeff.horsman@mt.com">jeff.horsman@mt.com</a></td>
<td>METTLER TOLEDO enabling technologies help companies bring products to market faster, at lower costs and with higher quality. Our PAT tools ensure processes are within boundary conditions, eliminating the risk of batch failures, delivering higher yields at lower cost and allow users to realize the benefits of QbD through the transfer of more robust, lower cost commercial processes to manufacturing. <a href="http://www.mt.com/reactir">www.mt.com/reactir</a></td>
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<td>39</td>
<td>Netzsch Instruments N.A. LLC</td>
<td>Bob Fidler</td>
<td>704-948-9534</td>
<td><a href="mailto:bob.fidler@netzsch.com">bob.fidler@netzsch.com</a></td>
<td>Thermal Analysis and Thermal Properties Instruments, Adiabatic Calorimetry, and contract testing services; DSC, DTA, TGA, STA (Simultaneous DSC/DTA-TGA), Dilatometers and TMA for thermal expansion specific heat, thermal conductivity and thermal diffusivity by laser flash method, coupling to MS, GC/MS, and FTIR for evolved gas analysis, Dynamic Mechanical Analysis (DMA), and DEA for dielectric analysis. <a href="http://www.Netzsch.com">www.Netzsch.com</a></td>
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<td>Parker Hannifin</td>
<td>Bruce Lasche</td>
<td>803-810-2931</td>
<td><a href="mailto:blasche@parker.com">blasche@parker.com</a></td>
<td>Parker Balston Gas Generators for analytical instruments eliminate the expense, inconvenience and danger associated with high pressure compressed gas cylinders. Parker Balston offers Gas Generators for a variety of analytical applications including LCMS, GC, FTIR, and NMR. Parker offers global distribution and support. <a href="http://www.labgasgenerators.com">www.labgasgenerators.com</a></td>
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<td>PCI</td>
<td>Nick Jones</td>
<td>317-557-3314</td>
<td></td>
<td>A premium service at a fair price, PCI is committed to providing you with fast turnaround, increased equipment availability, and compliant documentation. These attributes help us meet the demand of all our valued clients whose diversified products must comply with stringent quality standards in today's highly competitive marketplace. <a href="http://www.pci-llc.com">www.pci-llc.com</a></td>
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<td>Pine Research Instrumentation</td>
<td>Marion Jones</td>
<td>919-782-8320</td>
<td><a href="mailto:mjones@pineinst.com">mjones@pineinst.com</a></td>
<td>If you need to introduce your students to modern electroanalytical chemistry in an easy and inexpensive way, then Pine’s WaveNow potentiostat and instructional Three-Electrode Cell are exactly what you need! This potentiostat is a lightweight instrument with a USB interface. The instructional cell contains disposable, screen-printed electrodes. <a href="http://www.pineinst.com/echem">www.pineinst.com/echem</a></td>
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|   | **Prism Research Glass, Inc.**  
Steven J. Foscato, VP  
919-571-0078  
sfoscato@prismresearchglass.com | Prism Research Glass, a manufacturer of Scientific Glassware, provides high quality Borosilicate and Quarts glass products for use in Environmental, Chemical, and Pharmaceutical laboratories as well as for Fiber Optic and Semi-Conductor applications. We produce everything from small Bench Top to Large Scale systems and offer custom glassblowing services.  
[www.prismresearchglass.com](http://www.prismresearchglass.com) |
|---|---|
| 52 | **Proteovations**  
Benjamin Cargile  
919-806-2158  
benjamin.cargile@proteovations.com | Proteovations is dedicated to protein and peptide mass spectrometry analytics in support of academic, pharmaceutical, and biotechnology applications. Our specialized services include fit-for-purpose qualitative and quantitative analytical method development for peptide and protein biomarkers and therapeutics, detailed characterization of biological therapeutic molecules, drug target deconvolution, proteomic profiling, and custom informatics.  
[www.proteovations.com](http://www.proteovations.com) |
| 45 | **Quark Glass**  
Charles Hasseman  
919-522-2808  
quarkglass@pobox.com | Since 1983 Quark Glass has been serving the needs of the scientific and academic research communities for high quality specialty glassware and offer a repair service. We are known for very quick delivery of custom as well as standard products.  
[www.quarkglass.com](http://www.quarkglass.com) |
| 16 | **Sarstedt, Inc.**  
Peter Rumswinkel  
800-257-5101  
customerservice@sarstedt.us | Established in 1961, the Sarstedt Group develops, manufactures, and markets equipment and consumables in the fields of medicine and research. Laboratory and research products include specialty cell culture devices; consumables for molecular biology and PCR; liquid handling items; test, centrifuge, and cryotubes; and benchtop instrumentation.  
[www.sarstedt.com](http://www.sarstedt.com) |
| 58 | **SERMACS 2013**  
**SERMACS 2014**  
SERMACS 2013 will be hosted by the ACS Georgia Local Section.  
The meeting will be held at Loews Hotel Atlanta on November 12 through 17.  
SERMACS 2014 will be hosted by the ACS Nashville Local Section.  
The meeting will be held in Nashville Tennessee.  
[http://nashville.sites.acs.org/aboutus.htm](http://nashville.sites.acs.org/aboutus.htm) |  |
| 36 | **Shimadzu Scientific Instruments Inc.**  
Antoinette Swan  
Tom Hayes  
Jeff Ratliff  
919-425-1010 | Shimadzu Scientific Instruments is the American subsidiary of Shimadzu Corporation, headquarters in Kyoto, Japan. We are a leading manufacturer of scientific instrumentation, including gas and liquid chromatographs, mass spectrophotometers, environmental/TOC analyzers, balances, and physical measurement equipment.  
[www.shimadzu.com](http://www.shimadzu.com) |
| 34 | **Sigma Aldrich**  
Dawn Redington  
dawn.redington@sial.com | Sigma-Aldrich is a leading Life Science and High Technology company. Our chemical and biochemical products and kits are used in scientific research, including genomic and proteomic research, biotechnology, pharmaceutical development, the diagnosis of disease and as key components in pharmaceutical, diagnostic and other high technology manufacturing.  
[http://www.sigmaaldrich.com](http://www.sigmaaldrich.com) |
| 46 | **SP Scientific**  
Eric Goldman  
267-229-8018  
eric.goldman@spscientific.com | SP Scientific, is a leading manufacturer of specialty equipment for pharmaceutical, biotechnology, industrial, academic, and OEM applications. Products are sold under marketing leading brands that include Genevac solvent evaporators and mIVac sample concentrators, FTS precision thermal control systems and LyoStar freeze dryers with SMART control for freeze drying cycle development, Virtis laboratory, pilot-plant, and production scale freeze dryers, and Hotpack glassware washers.  
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| 8    | Spectrum Chemicals & Laboratory Products, Inc. | Laura Sluss  
843-343-6672  
lssluss@spectrumchemical.com | Spectrum manufacturers and distributes fine chemicals and laboratory products with quality and delivery you can count on every time; serving chemists in all industries with analytical reagents, solvents, solutions and fine chemicals, including >22,000 TCI organic chemicals and >400 chromatography/spectroscopy consumables from PerkinElmer.  
A one-stop lab shop: chemicals, equipment, supplies.  
[www.SpectrumChemical.com](http://www.SpectrumChemical.com) |
| 42   | Synthonix                            | Nick White  
919-875-9277  
nwhite@synthonix.com | Synthonix specializes in the synthesis of building blocks and synthons that allows for chemical diversification for hit-to-lead, fragment based design, focused library synthesis, and lead optimization. Please do not hesitate to call to speak with one of our researchers. We are here to help you in your efforts.  
[www.synthonix.com](http://www.synthonix.com) |
| 32   | TA Instruments                      | Neil Demarse  
302-562-4196  
ndemarse@tainstruments.com | Visit TA Instruments for innovative technology in thermal analysis, rheology and microcalorimetry. We provide the highest accuracy and sensitivity measurements for polymers, organic and inorganic materials, and biological and life science characterization. Our new Discovery DSC and TGA deliver unparalleled accuracy for the most challenging measurements.  
[www.tainstruments.com](http://www.tainstruments.com) |
| 49   | ThruPore Technologies LLC            | Martin Bakker  
205-348-9116  
bakker@bama.ua.edu | ThruPore Technologies LLC, is proud to announce the availability of trail quantities of our new HePoreCat™ palladium on carbon catalyst. Developed under NSF funding, this patent pending material provides higher activity, longer lifetime and greater ease of use. Drop by and tell us about your catalyst needs and ask for a free sample. |
| 53   | Tosoh Bioscience LLC                 | Kevin Thomas  
856-562-9899  
kevin.thomas@tosoh.com | Tosoh Bioscience is a global leader in the manufacturing and sales of high quality, innovative pre-packed HPLC columns and bulk resins with the TSKgel, TOYOPEARL and ToyoScreen brand names. We now offer a dedicated system for GPC analysis, the EcoSEC GPC System.  
[www.tosohbioscience.com](http://www.tosohbioscience.com) |
| 59   | Triangle Chromatography Discussion Group, NC-ACS (TCDG) | | The purpose of the Triangle Chromatography Discussion Group (TCDG) is to maintain and promote an interest in and to provide an opportunity for discussion and exchange of information with respect to all fields of chromatography. The membership is open to anyone interested in the field of chromatography. The group sponsors various seminars and workshops in the triangle area throughout the year and our signature event includes the annual “Triangle Chromatography Symposium and Instrument Exhibit”.  
| 22   | Vernier Software & Technology        | Vernier Software & Technology  
888-837-6437  
info@vernier.com | Stop by the Vernier Software & Technology booth to see our exciting products for college chemistry such as our new Organic Chemistry with Vernier lab book. Our new Polarimeter graphs light intensity versus angle so students don’t have to determine optical maximum with their eye.  
[www.vernier.com](http://www.vernier.com) |
| 31   | Wasatch Photonics & Spectrecology    | Cindy Gong  
765-413-4022  
cgong@wasatchphotonics.com | Wasatch Photonics, Inc. is the leader in high performance Volume Phase Holographic Gratings (VPHGs) and Volume Phase Holographic Optical Elements (VHOEs). Products developed by our world class design team include; Raman sensors and instrumentation, advanced holographic components for spectroscopy, hyperspectral imaging, astronomy and OCT.  
[www.wasatchphotonics.com](http://www.wasatchphotonics.com)  
Spectrecology is your source for the best solutions to your spectroscopy measurement problems. We can design the perfect system that meets your needs and your budget. We carry the best products – Wasatch Photonics Raman, Ocean Optics UV VIS spectrometers, Starna cuvettes, Spectrecology optical O₂ sensors and TSI LIBS.  
[www.spectrecology.com](http://www.spectrecology.com) |
| 27 | **Waters Corporation**  
Mike Keilholz  
800-252-4752 Ext. 6371 | Waters Corporation creates business advantages for laboratory-dependent pharmaceutical organizations by delivering scientific innovation to enable customers to make significant advancements. Waters helps customers make profound discoveries, optimize laboratory operations, deliver product performance, and ensure regulatory compliance with a connected portfolio of separations and analytical science, laboratory informatics, mass spectrometry, as well as thermal analysis.  
[www.waters.com](http://www.waters.com) |
|---|---|---|
| 29 | **Wilmad-LabGlass**  
Doug Grady/Dir. Of Sales & Marketing  
856-691-3200 X3758; doug.grady@wilmad-labglass.com | Wilmad-LabGlass, an ISO9001:2008 Certified Company, has been manufacturing and distributing laboratory and scientific glassware. Wilmad is a leading manufacturer of high precision engineered glass components. Wilmad is also the market leader in NMR and EPR. LabGlass manufactures and distributes a wide variety of specialty laboratory glassware products and equipment.  
| 44 | **World Wide Medical Products, Inc.**  
Megan Trivette  
919-407-9032  
mtrivette@wwmponline.com | WORLDWIDE is a technologically advanced, quality-driven provider of essential laboratory products and services to the scientific community. Our mission is to utilize our unique comprehension and understanding of the research and development market while remaining dedicated to exceeding the wants and needs of our clients.  
[www.wwmponline.com](http://www.wwmponline.com) |
Graduate Fair

Jackson State University, Department of Chemistry & Biochemistry
*Booth 1, Friday and Saturday*
Jackson State University Department of Chemistry & Biochemistry ranks 3rd in Bachelor’s, 2nd in Master’s, and 4th in Doctoral degrees in Physical Sciences (mainly chemistry) awarded to African Americans in the country (Diverse Issues in Higher Education, 2011). The Department consists of 20 outstanding and diverse faculty members aimed at providing a quality education to a diverse undergraduate and graduate student body in fundamental, applied, and interdisciplinary areas of the chemical sciences.

Website: [http://chem.jsums.edu/](http://chem.jsums.edu/)

Clemson University
*Booth 2, Friday and Saturday*
Clemson University is a public research institution located in the foothills of the Blue Ridge Mountains in a rapidly developing upstate region of South Carolina. It is a comprehensive research university with a traditional emphasis on science and engineering. The Department of Chemistry at Clemson University is a mid-size graduate program offering both MS and PhD degree programs, with 24 research faculty and approximately 100 graduate students. The department has faculty members with research efforts in all of the traditional areas of chemistry, with strengths in advanced materials, chemical biology, computational chemistry, nanoscale materials, solid-state chemistry, and chemical education.

Website: [http://www.clemson.edu/chemistry](http://www.clemson.edu/chemistry)

Kennesaw State University
*Booth 3, Friday*
Kennesaw State University in metropolitan Atlanta is proud to offer a new thesis-based M.S. in Chemical Sciences. Tracks in Chemistry and Biochemistry will offer students a flexible graduate curriculum and highly individualized attention. Research opportunities abound in areas ranging from synthetic organic chemistry to enzymology with research mentors funded by agencies including the NIH and the NSF. A recent addition to our campus is a new 74,000 ft$^2$, $21$ million science laboratory building that houses state-of-the-art instrumentation including a recently-acquired SPR biosensor and confocal microscope. Students accepted into the new program will be awarded a highly competitive stipend and a tuition waiver.

Website: [http://science.kennesaw.edu/chem/](http://science.kennesaw.edu/chem/)
North Carolina Central University, Department of Chemistry  
**Booth 3, Saturday**  
The Department of Chemistry at North Carolina Central University, a public HBCU in Durham NC offers a thesis based Master’s degree in Chemistry. Graduate assistantships and tuition remission are available on a first-come, first serve basis. Faculty research interests range from biochemistry to polymer chemistry to inorganic chemistry and electrochemistry. Faculty have research support from agencies including NIH and NSF. Industrial internships are also available to exceptionally qualified students. Interested students can complete an online application at the website below. NCCU also now offers an Integrated Biosciences PhD program which includes faculty from the Departments of Biology and Pharmaceutical Sciences as well.

Website: [http://web-shared.nccu.edu/cfusion-site001/wip2011/sgs/sgs-apply-now.cfm](http://web-shared.nccu.edu/cfusion-site001/wip2011/sgs/sgs-apply-now.cfm)

Vanderbilt University  
**Booth 4, Friday**  
Vanderbilt University, located in Nashville, Tennessee, is renowned for its medical school and scientific research programs. The Graduate Program in Chemistry offers dedicated students a faculty that is active in research and deeply committed to the development of scholars, combining solid research, intensive training, and exceptional education. We have state-of-the-art facilities and instrumentation, exceptional resources and excel at interdisciplinary research. Commitment to our students’ success is our highest priority.

Website: [http://www.vanderbilt.edu/chemistry](http://www.vanderbilt.edu/chemistry)

University of South Florida, Department of Chemistry  
**Booth 4, Saturday**  
USF’s Chemistry Department offers a variety of interdisciplinary research programs focusing on various areas of chemistry including: analytical, chemistry education, inorganic, organic/biochemistry, physical/computational, and polymer. We also have strengths in materials and drug discovery. The recently adopted, restructured Ph.D. program features minimal, flexible course requirements with an emphasis on research. We are looking for academically strong students (GPA of 3.0 or greater), especially those with an interest in interdisciplinary, cutting-edge projects who are motivated to start research early in their graduate school career.

Website: [http://chemistry.usf.edu](http://chemistry.usf.edu)
University of Rochester

**Booth 5, Friday and Saturday**

Outstanding scholarly and professional achievement: These are the goals of graduate study at the University. Admission is selective, the environment intimate and challenging. Here, promising candidates work closely with faculty to develop in-depth knowledge of their chosen fields as they establish themselves as independent, innovative scholars. The University of Rochester offers graduate students the chance to pursue research at the highest level in an environment scaled to the individual. Graduate education is central to the mission of all schools and is an important vehicle for the missions of both research and professional preparation. At one of the nation’s leading universities, graduate students at Rochester work closely with faculty who are at the forefront of their fields. Students have exceptional opportunities for interdisciplinary study that few universities can match.

Website: [http://www.chem.rochester.edu](http://www.chem.rochester.edu)

UNC Charlotte

**Booth 6, Friday and Saturday**

The Master of Science (M.S.) degree in Chemistry is a research-based program which provides the background necessary for further graduate or professional studies in the physical, life or medical sciences or a career in science. The M.S. degree requires a minimum of 30 credit hours and a thesis based on original research carried out under the direction of a member of the graduate faculty. Student participation in research activities is through a selection of a faculty adviser and enrollment in the special research courses offered. Major emphasis is placed upon the research project and required thesis. The Ph.D. in Nanoscale Science is an interdisciplinary program that addresses the development, manipulation, and the use of materials and devices on the scale of roughly 1-100 nanometers in length, and the study of phenomena that occur on this size scale.

Website: [http://chemistry.uncc.edu](http://chemistry.uncc.edu)

The University of Mississippi

**Booth 7, Friday and Saturday**

The Ole Miss Department of Chemistry and Biochemistry program combines southern hospitality and academic rigor yielding an exciting environment to seek the technological solutions of tomorrow for the world's challenges today.

Website: [http://www.olemiss.edu/depts/chemistry](http://www.olemiss.edu/depts/chemistry)
University of South Carolina  
_Booth 8, Friday and Saturday_
USC’s highly rated Department of Chemistry and Biochemistry contains 30 faculty and 130 graduate students working in all areas of chemistry as well as nanoscale, marine, forensic and environmental chemical sciences. The highly collaborative learning environment fostered by the department trains students to think independently using advanced research tools and insights. Our award-winning faculty, nationally competitive stipends, research facilities, support staff and nationally ranked funding base provides students with all the elements required for their advanced study. The sunny and vibrant Columbia region also provides the richly fulfilling lifestyle desired by candidates who value breadth as well as depth in their careers.

Website: [http://www.chem.sc.edu](http://www.chem.sc.edu)

The University of Georgia  
_Booth 9, Friday and Saturday_
Modern, multidisciplinary chemical research integrates diverse fields of knowledge and technologies. The Department of Chemistry at the University of Georgia is committed to excellence in multidisciplinary education and training of professional chemists for entry into industry, academia and government. The graduate program emphasizes strong interdisciplinary and specialized research areas, including computational chemistry, materials science/nanochemistry, gas phase chemistry, biomolecular structure/spectroscopy, environmental and atmospheric chemistry, photochemistry, synthetic organometallic/organic chemistry, biophysics, chemical education, and many others, that complement the traditional areas. High stipends, world-class facilities, a low cost of living, and a unique cultural and intellectual environment augment this exceptional graduate opportunity.

Website: [http://www.chem.uga.edu](http://www.chem.uga.edu)

The University of Miami  
_Booth 10, Friday and Saturday_
The University of Miami is a private research university with three campuses in Miami and Coral Gables. The Department of Chemistry, with 15 faculty and 61 graduate students, is consistently highly ranked. Our research is at the cutting edge of modern chemical sciences for both traditional areas and multidisciplinary fields. UM chemistry offers a unique opportunity for graduate students with an internationally recognized program and strong support for student travel, all in a vibrant and livable metropolitan locale. Our alumni have accepted positions in high profile careers in academia, industry, and government.

Website: [http://www.as.miami.edu/chemistry](http://www.as.miami.edu/chemistry)
The University of Alabama

Booth 11, Friday

The Department of Chemistry at The University of Alabama offers a rigorous graduate program granting M.S. and Ph.D. degrees. Students acquire competence in their chosen area through coursework, followed by a focus on research under the direction of their chosen advisor. Financial support is provided through teaching and research assistantships, as well as through merit based fellowships. The Department is made up of 26 faculty members and approximately 85 graduate students. It is housed in Shelby Hall (completed in 2004) on the University of Alabama campus, where state-of-the-art facilities provide students with hands-on access to a wide variety of modern instrumentation.

Website: http://www.bama.ua.edu/~chem/

University of Arizona, Department of Chemistry & Biochemistry

Booth 12, Friday and Saturday

The Department of Chemistry and Biochemistry at the University of Arizona is dedicated to expanding the boundaries of the chemical and biochemical services and to educating the next generation of professionals. Some of our greatest assets include our State-of-the-art research facilities which are among the very best in chemistry and biochemistry. Each facility is staffed by full-time Ph.D.’s focused on providing expert technical assistance and hands-on-training to students. We invite you to become an integral member of an exciting community of scholars. Our internationally renowned faculty members attract more than $23,000,000 each year in extramural grants to support research.

Website: http://www.biochem.arizona.edu

Georgia Tech

Booth 13, Friday and Saturday

Applications are being accepted for positions in the Ph.D. program at Georgia Tech. Teaching assistantships starting at $25,000 (plus waiver of tuition and health insurance) for Fall 2013 are available. In addition, there are a number of supplemental scholarships ($1,500-$5,500) available to highly qualified candidates. Research areas include: organic and inorganic materials, biomolecular structure, biophysics, computational chemistry, environmental chemistry, drug design, nanochemistry.

Website and FREE application: http://www.chemistry.gatech.edu
Emory University  
**Booth 14, Friday and Saturday**  
The Department of Chemistry at Emory University supports a vibrant and world-class research program integrated with outstanding graduate education. We are a top-35 ranked department with a wide range of cutting edge research, from novel drugs for fighting disease to the latest environmentally friendly catalysts for energy production, from exploring the origin of life to paradigm shifts in computational chemistry. While the department is formally organized into four divisions (organic, inorganic, physical, and biomolecular chemistry) our highly collaborative environment encourages students to tackle problems that cross the traditional disciplines. Come learn more about your future graduate education at Emory University!

Website: [http://www.chemistry.emory.edu](http://www.chemistry.emory.edu)

Duke University  
**Booth 15, Friday**  
The doctoral program in chemistry at Duke features research programs that span the "traditional" sub-disciplines of chemistry, including analytical, biological, inorganic, organic, physical and theoretical chemistry. However, many, if not most of the research programs are interdisciplinary, either overlapping the traditional boundaries of chemistry or the boundaries between chemistry and the other sciences, for example biological, materials, and environmental sciences. Many chemistry faculty and students participate in university-wide interdisciplinary training programs and centers, including those in biological chemistry, toxicology, pharmacology, molecular biophysics, biologically inspired materials, and cellular and biosurface engineering. Research in all fields is supported by state-of-the-art equipment and facilities.

Website: [http://www.chem.duke.edu](http://www.chem.duke.edu)

North Carolina State University, Department of Chemistry  
**Booth 16, Friday and Saturday**  
The Department of Chemistry at North Carolina State University houses award-winning researchers and teachers who guide students through a broad, rigorous curriculum. Our graduates succeed in both academia and industry. Our research programs cover a diverse spectrum including analytical, inorganic, organic, physical, biological, polymers, materials, nanoscience, theoretical, and magnetic resonance.

Website: [http://www.ncsu.edu/chemistry](http://www.ncsu.edu/chemistry)
University of Kentucky College of Pharmacy

Booth 17, Friday and Saturday
The Department of Pharmaceutical Sciences at the UK College of Pharmacy offers exciting opportunities for students seeking Ph.D. training in diverse areas of Drug Discovery, Drug Development, Clinical and Experimental Therapeutics, and Pharmaceutical Outcomes and Policy. Our program is housed within a new 286,000 sq. ft., state-of-the-art academic and research facility. Graduates of our program are highly valued by the pharmaceutical industry, government agencies and academia. All accepted students receive a competitive stipend, full tuition waiver and paid health insurance. For more information contact Jim Pauly, Ph.D. (jpauly@uky.edu).

Website:  [http://pharmacy.mc.uky.edu](http://pharmacy.mc.uky.edu)

Joint School of Nanoscience and Nanoengineering

Booth 18, Friday and Saturday
The Joint School of Nanoscience and Nanoengineering (JSNN) offers four graduate degree programs: a Professional Science Master's (PSM) in Nanoscience, a Ph.D. in Nanoscience, a M.S. in Nanoengineering and a Ph.D. in Nanoengineering. Distance learning options are also under development. JSNN has six research focus areas: Nanobiology, Nanometrology, Nanoenergy, Nanobioelectronics, Computational Nanotechnology and Nanomaterials (with a special emphasis on Nanocomposite materials).

Website:  [http://jsnn.ncat.uncg.edu/](http://jsnn.ncat.uncg.edu/)

University of Memphis

Booth 19, Friday
The Department of Chemistry at the University of Memphis confers degrees at both the undergraduate (B.S.) and graduate levels (M.S. and Ph.D.). Current research conducted by the twenty-two faculty within the department is focused in the areas of computational, medicinal and environmental chemistry and nanomaterials. These projects are facilitated through two university initiatives, the Computational Research on Materials Institute (CROMIUM) and the Institute for Nanomaterials Development and Innovation (INDIUM). Departmental research is supported, in part, through investigator-initiated grants from the NIH, NSF, PRF, NASA, AHA, and private foundations. Additional information about chemistry at UM can be found at the website below.

Website:  [http://www.chem.memphis.edu](http://www.chem.memphis.edu)
University of Tennessee (Knoxville) Department of Chemistry

*Booth 20, Friday and Saturday*

The Department of Chemistry at the University of Tennessee offers a long-standing tradition of excellence in chemical research and education, stretching from 1947, when the department granted the University's first Ph.D. degree, to the present. Our 30 faculty members have research interests that both span the traditional areas of chemistry and encompass new interdisciplinary fields such as materials, environmental chemistry, and life sciences. We offer Ph.D. and M.S. degrees in analytical, inorganic, organic, physical, and polymer chemistry. Ph.D. students may also specialize in theoretical chemistry or may, in cooperation with the Department of Physics, pursue a degree in chemical physics.

Website: [http://www.chem.utk.edu](http://www.chem.utk.edu)

The University of North Carolina at Greensboro

*Booth 21, Friday and Saturday*

At the University of North Carolina at Greensboro we offer M.S. degrees in Chemistry, M.S. degrees in Biochemistry include a Ph.D. in medicinal bio-chemistry.

Website: [http://www.uncg.edu/che/](http://www.uncg.edu/che/)

The Florida State University

*Booth 22, Friday and Saturday*

The Florida State University Department of Chemistry and Biochemistry offers M.S. and Ph.D. degrees in Chemistry and Biochemistry, as well as undergraduate B.S. and B.A. degrees. We prepare students for a variety of career choices—from chemical, biochemical, environmental, pharmaceutical, medicinal, and related industries to positions in national labs and academia. The FSU Department of Chemistry and Biochemistry is proud of its highly interdisciplinary research and educational programs. We boast of state-of-the-art research facilities, with the NMR and X-ray facilities being among the best in the Southeast region. Our faculty are actively involved in other University-supported centers, such as the National High Magnetic Field Laboratory, High-Performance Computing Cluster, and Institute for Molecular Biophysics.

Website: [http://www.chem.fsu.edu](http://www.chem.fsu.edu)

Dr. Patricia Hagan Von Dreele

*Literature Table*

Successful Women in Chemistry Series; Professional Relations Division information; Women Chemists Committee information; Preparing for Your ACS Examination in General Chemistry; Local section women chemists committee contact information.
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FALL APPLICATION DEADLINES

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APPLICATION REQUIREMENTS

• Fee ($65 domestic waived when paying by check; $75 international, no waiver available)
• Transcripts
• Personal Statement
• Three letters of Recommendation
• GRE General Test scores
• TOEFL or IELTS scores (international)

CONTACT US
Department of Chemistry Graduate Office
North Carolina State University
2620 Yarbrough Drive
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Wednesday Summary – 14 November 2012

Events and Activities
5:00 p.m. – 6:45 p.m.
Welcome Reception and 126th NC-ACS Local Section Conference Posters
(Ticketed event sponsored by NC-ACS)
6:45 p.m. – 8:00 p.m.
NC-ACS Awards and NC Distinguished Speaker Presentation.
Jane and Dave Richardson, Duke University,
“Admiring, Analyzing, and Improving 3D Structures of Macromolecules”

Short Courses and Workshops
8:30 a.m. – 12:00 p.m.
COACCh Workshop: Negotiations Workshop for Women Faculty & Professionals
Marriott Chancellor
8:00 a.m. – 5:00 p.m.
ACS Short Course: Pharmacokinetics and Pharmacodynamics in Drug Discovery for Chemists
Marriott University A
ACS Short Course: The Essentials of Supervising Scientists & the Technical Staff
Marriott University B
ACS Short Course: Electrochemical Measurement of pH and Ions: Troubleshooting and Correcting Error and Bias
Marriott University C
8:30 a.m. – 12:00 p.m.
TCDG Workshop: (1) Getting the Most Out of Your UHPLC Columns
(2) Fundamentals and Advancements in Analytical SFC/SFE
Glass Office
1:00 p.m. – 4:30 p.m.
COACCh Workshop: Negotiations Workshop for Women Postdocs & Graduate Students
Marriott Chancellor

Center for Solar Fuels (UNC EFRC) Conference
1:00 p.m. – 5:00 p.m.
Photonic Assemblies for Solar Fuels (oral)
Ballroom A
3:00 p.m. – 3:40 p.m.
Photonic Assemblies for Solar Fuels (poster)

Poster Presentations
2:00 p.m. – 4:30 p.m.
Computational, Inorganic, Nanochemistry, Physical
Ballroom Lobby
5:00 p.m. – 6:45 p.m.
126th NC-ACS Section Conference

Technical Sessions
1:20 p.m. – 5:20 p.m.
Electroanalytical Chemistry I
Inorganic Chemistry I
Innovations in Molecular Modeling
Physical Chemistry I
Polymer Chemistry I
Recent Advances in Micro- and Nano-Fabrication
The Exposome
Marriot Congressional B
205
202
204
Marriot Congressional A
203
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SERMACS 2012

Technical Program

C. Goss, M. ter Horst, and K. Tomer, *Program Chairs*

**BUSINESS MEETING:**

**SERMACS Regional Board Meeting**
Saturday, 17 November 2012
8:00 AM – 11:00AM
Raleigh Convention Center
Room 402

**WEDNESDAY AFTERNOON**

**Center for Solar Fuels (UNC EFRC)**
**Photonic Assemblies for Solar Fuels**

Raleigh Convention Center
Ballroom A

T. Meyer, *Organizer*
D. Beratan, J. Papanikolas, *Presiding*

1:00 1. Peptide-Based Scaffolds for Light Harvesting and Energy Transfer. **M. Waters**, D. Ma, D. Wilger, S. Bettis, M. Mlnakova, J. Papanikolas, G. Papoian

1:40 2. Manipulating nuclear motions to control excited state energy conversion. **N. H. Damrauer**


3:00 Coffee Break, Posters, and Exhibition.

3:40 4. Proton-coupled electron transfer in catalysis and energy conversion. **S. Hammes-Schiffer**

4:20 5. Theories of plasmon enhanced optical processes important in solar energy. **G. C. Schatz**
Recent Advances in Micro and Nano-Fabrication
Raleigh Convention Center
203
Supported by Liquidia and RTI International
G. Rothrock, D. Schorzman, Organizers, Presiding


2:00 7. Continuous and high-throughput patterning techniques and their applications in photonics and transparent conductors. L. J. Guo


3:00 Coffee Break, Posters and Exposition.

3:40 9. Leveraging advanced nanofiber technologies to achieve energy efficiency. J. Davis

4:20 10. Electric field-induced nanolithography: Recent advances to manipulate soft matter on surfaces. S. Zauscher, R. Ferris


Electroanalytical Chemistry I
Marriot Hotel
Congressional B
M. ter Horst, Organizer
P. Flowers, Presiding


2:00 13. Electrochemical studies in the detection of a GSTP-1 DNA sequence. S. Patterson, A. Saheb, M. Josowicz


3:00 Coffee Break, Posters, and Exhibition.
3:40 16. Single-molecule spectroelectrochemistry (SMS-EC) of (4, 4′-difluoro-4-bora-3a, 4a-diaza-s-indacene) BODIPY dyes. J. Liu, S. Pan

4:00 17. Sub-microliter electrochemistry and spectroelectrochemistry using standard electrodes and a polymer electrolyte salt bridge. P. A. Flowers, D. A. Blake


Innovations in Molecular Modeling: New Tools and Applications

Raleigh Convention Center
202
D. Brenner, Organizer, Presiding


3:00 Coffee Break, Posters and Exposition.


Inorganic Chemistry I

Raleigh Convention Center
205
M. ter Horst, Organizer

Octadentate europium complexes as sensors for aromatic dicarboxylates: pH dependent sensing of phthalic acid by formation of ternary complexes. A. S. de Sousa, D. Sannasy, H. M. Marques

Development of Ru(II) catalysts for the hydroarylation of olefins: Comparison of TpRu(L)(NCMe)Ph catalysts (Tp = hydridotris(pyrazolyl)borate: L = CO, P(OCH₂)₃CEt, PMe₃, P(N-pyrrolyl)₃ or 4-methyl-2,6,7-trioxa-1-phosphabicyclo[2,2,1] heptane. E. E. Joslin, T. Gunnoe, M. Sabat, W. H. Myers

Coffee Break, Posters and Exposition.

Synthesis and reactivity of a new (mercaptoimidazolyl)quinoline mixed-donor ligand. P. J. Quinlivan, D. Rabinovich

Synthesis and reactivity of a new bis(picolyl)selone ligand. B. L. Gray, D. Rabinovich

Bis(pyridyl)selone complexes of zinc, cadmium, mercury and tin. L. Hernandez, D. Rabinovich

Mixed-donor pyridine/thione and pyridine/selone complexes of indium(III). N. K. Spencer, D. Rabinovich

Physical Chemistry I

Raleigh Convention Center
204

M. ter Horst, Organizer
T. Whiteside, Presiding

Diffusion of squalene in squalane. B. A. Kowert, M. B. Watson

Mass effect on the thermal decomposition of calcium oxalate monohydrate. T. DeVore, A. C. Bagley, J. Hill

A non-radiative method for measuring energy transfer efficiencies using photoacoustic calorimetry: PAC-FRET. W. A. Maza, R. W. Larsen

Coffee Break, Posters and Exposition.

Regulation of the tyrosyl radical redox chemistry in ribonucleotide reductase. A. R. Offenbacher, L. A. Burns, C. Sherrill, B. A. Barry

Reaction Kinetics and Mechanism of Nitrate Radicals with Unsaturated Organic Surfaces. Y. Zhang, J. R. Morris, J. Lu
4:20 36. Model donor-bridge-acceptor systems to study charge transfer kinetics in ionic liquids. 
R. Abdel Malak Rached

4:40 37. An extensive hydrogen-bonding network plays a catalytic role in photosynthetic water 
oxidation. B. C. Polander, B. A. Barry

The Exposome

Raleigh Convention Center
206

J. Swenberg, Organizer, Presiding

1:40 38. The Exposome Paradigm. M. T. Smith


3:00 Coffee Break, Posters and Exposition.

3:40 40. The Exposome and Biomonitoring – The CDC National Exposure Report on Human 
Exposure to Environmental Chemicals. J. D. Thomas, A. M. Calafat

4:20 41. Relationships of endogenous DNA damage to exogenous DNA damage, mutations and 
risk assessment. J. A. Swenberg, B. C. Moeller, K. Lu, V. Sharma, L. B. Collins, J. Nakamura, 
E. Mutlu, L. Gao

Computational Chemistry Poster Session

Posters are presented from 2:30 to 4:00

Raleigh Convention Center
Ballroom Foyer

Y. Yingling, Organizer

2:00 - 4:30

42. Reproducing solvatochromic behavior in cyano-containing chromophores: Explicit solvent 
vs. implicit model. D. N. Bowman, R. C. Rocha, E. Jakubikova

Nivedha

44. Orbital analysis and excited state calculations in the energy-based fragment method. T. 
Tsuchiya, K. Shrestha, E. Jakubikova

46. Simulations of carbon nanotube welding under Ar bombardment. M. U. Kucukkal, S. J. Stuart

47. High accuracy simulations of liquid water using Fragment Molecular Orbital method. J. H. Blew

48. The effect of novel ligands on the HIV-1 protease. K. E. Pugh

49. Molecular dynamics simulation of the interaction between cholates and cholesterol. M. Reed


51. Simulations of temperature-dependent conformational transitions of the elastin-like peptide (VPGVG)n. N. Li, Y. Yingling

Inorganic Chemistry Poster Session
Posters are presented from 2:30 to 4:00

Raleigh Convention Center
Ballroom Foyer

Y. Yingling, Organizer

2:00 - 4:30


53. Metal to metal charge transfer in Cr-O-Ti oxygen bridge complex: synthesis of u-Oxo Chromium (III)-Titanium (IV) complex. T. Huang, W. W. Weare

54. Metal complexes containing aryl-phenylene-vinylene bipyridine ligands for reverse saturable absorbers. G. K. Kosgei, R. H. Schmehl

55. Synthesis, characterization and metal-metal charge transfer study of Ti-O-Fe system. X. Wu, W. W. Weare

56. Magnesium-Based 2D Metal-Organic Frameworks. G. J. McManus


64. Selective Separation of Actinoids from Lanthanoids by Polypridyl Ligands Diphen and TPTZ. **G. C. Littmann**, R. D. Hancock


68. Aggregation of platinum(II) diimine complexes in solution and condensed phases. **M. H. Hudson**, R. E. Bachman

69. Toward liquid crystalline supramolecular squares based on platinum(II) diimine complexes. **E. N. Brahni**, R. E. Bachman

70. Spectral and structural study of a molecular metal oxide supported metal carbonyl cluster. **C. Zhao**, W. Rodríguez-Córdoba, A. L. Kaledin, Y. Yang, Y. V. Geletii, T. Lian, D. G. Musaev, C. L. Hill


72. Exploration of Excited State Dynamics in Metal Complexes with Photogenerated Semiquinone-NitronylNitroxide Biradicals. **C. Tichnell**, D. A. Shultz
73. Nature of the lowest-energy visible excitations in \textit{trans}\-Re$_2$(O$_2$C-$n$-C$_3$H$_4$N)$_2$X$_2$(Ph$_2$PCH$_2$PPh$_2$)$_2$ ($n = 4$ or $3$; X = Cl or Br). \textbf{D. R. Derringer}

74. Separation effects in donor-bridge-acceptor semiquinone-nitronylnitroxide biradical compounds. \textbf{G. Wang}, D. Shultz

\textbf{Nanochemistry Poster Session}
\textbf{Posters are presented from 2:30 to 4:00}

Raleigh Convention Center
Ballroom Foyer
Y. Yingling, \textit{Organizer}

\textbf{2:00 - 4:30}

75. Delivery and controlled release of anticancer drugs containing alcohol OH group using nanoparticles. \textbf{O. Klep}


78. Photodegradation study of Copper (I) Oxide nanoparticles synthesized with different geometries. \textbf{E. L. Jewell}, E. Hernandez-Pagan, J. E. Macdonald

79. New ligands for the synthesis of water soluble nanoparticles of the copper sulfides. \textbf{M. J. Turo}, J. E. Macdonald

80. Increased efficiency of gold conversion via a re-seeding approach. \textbf{S. Canonico-May}, \textbf{J. Wagenaar}, J. Stone

81. Activation of hydrazone-based molecular switches through coordination coupled proton transfer. \textbf{X. Su}, \textbf{J. T. Foy}, I. Aprahamian

82. Withdrawn


86. Selective Oxidation of Target Contaminants on Engineered Porous TiO₂ Photocatalysts: Size Exclusion of NOM. **A. Zakersalehi, W. Lawal, H. Choi**


88. Single walled carbon nanotubes inhibit biofilm formation by Bacillus anthracis spores. **U. E. Abaessien, X. Dong, E. Addae, L. Yang**


90. Enhancing surface plasmon resonance imaging (SPRi) signal to detect a wide range of biomarkers in serum. **S. Vance, M. Sandros**

91. Palladium-Coated Gold Nanorods: A Highly Active Catalyst for Photo-Reduction of Resazurin to Resorufin. **P. Cobb, L. Zhao, G. Wang**


93. The cobalt oxide nanowall array film prepared by pulsed laser deposition for supercapacitors with superb-rate capability. **Y. Wang, H. Wang, X. Wang**

94. Fabrication of patterned -ITO for localized surface Plasmon resonance sensing. **M. Kang, S. Franzen, J. Maria, M. Losego**

95. Nanoparticulate aerosol formulation of salmeterol xinafoate and fluticasone propionate combination. **F. Nalbantoglu, O. Karban, M. Ozbek, E. Er, M. Karabulut, G. Kaynar, T. Onkol, T. Ozden**

Physical Chemistry Poster Session
Posters are presented from 2:30 to 4:00

Raleigh Convention Center
Ballroom Foyer
Y. Yingling, Organizer

2:00 - 4:30


98. Photoelectron Imaging of CH-. C. M. Pruitt, K. C. Kamena, B. Bandyopadhyay, D. J. Goebbert


100. Size exclusion chromatography studies of silver clusters conjugated with DNA. I. Miller, D. Nicholson, B. Giri, O. Sergev, J. Petty


103. Radical-Triplet Pair Interactions as Probes of Long-range polymer motion in solution. S. SIM, M. D. Forbes

104. Static and time-resolved X-ray crystallography study of dehaloperoxidase-hemoglobin A-carbon monoxide complex. j. zhao, V. Srajer, V. de Serrano, S. Franzen

Polymer Chemistry I

Marriot Hotel
Congressional A
M. ter Horst, Organizer
A. Tonelli, Presiding

2:00 105. Restructuring Polymers via Nano-Confinement and Subsequent Release. A. E. Tonelli

2:20 106. Investigation of growth and degradation behaviors of biodegradable polymer brushes and their bio-applications. X. HU, C. Gorman

3:00 Coffee Break, Posters and Exposition.

3:40 108. Toward thermoplastic lignin polymers; thermal & polymer characteristics of kraft lignin & its derivatives. H. Sadeghifar, C. Cui, S. Sen, D. Argyropoulos


4:40 111. Synthesis and characterization of UV cross-linkable aromatic polyimides for gas separation membranes. K. E. Gaines, C. Fuller, K. Stevens, R. Guo, B. D. Freeman, J. E. McGrath

Center for Solar Fuels (UNC EFRC) Poster Session I

Photonic Assemblies for Solar Fuels (Posters on display Wednesday through 5 pm on Thursday)

Ballroom A

T. Meyer, Organizer

3:00 - 3:40


119. Using peptide scaffolds to control chromophore placement both in solution and on the surface. S. Bettis, D. Ma, M. Minakova, D. Wilger, G. Papoian, M. Waters, J. Papanikolas

120. Flexibility matters: The role of scaffold tethers in Ru(II) and Os(II) chromophore separation. W. E. Fondrie, S. Bettis, D. Ma, M. Minakova, D. Wilger, G. Papoian, M. Waters, J. Papanikolas


123. Photoactive metal-organic frameworks for sensing and solar energy applications. S. M. Barrett, C. Wang, W. Lin


126. Cobalt Oxide Core–Silica Shell Units for Artificial Photosynthesis. H. Frei


133. Physical constraints on exciton harvesting in molecular systems. **N. Polizzi**, D. N. Beratan

**WEDNESDAY EVENING**

**Welcome Reception and NC Local Section Poster Session**

Raleigh Convention Center
Ballroom Foyer
M. Pasquinelli, Organizer, Presiding

5:00 - 6:45

42, 44, 45, 53, 65, 76, 77, 87, 92, 104, 106. See previous listings.

134. A new 1:1 complex between the aromatic molecules thiophene and perfluorobenzene. **A. Forest**, L. M. Heist, E. T. Samulski

135. The effect of calculation of solvation free energy on FKBP proteins. **L. S. Smith**

136. Coexistence of two dewetting mechanisms in homopolymer/diblock copolymer bilayered nano-laminate. **X. Cai**


139. The Role of SP-C in the Inhibition and Recovery of LPS-Induced Pulmonary Inflammation. **E. L. Bao**, M. D. Maxfield, K. Page, J. E. Baatz, S. W. Glasser
140. Molecular Dynamics Simulations of Surface-Modified Polypropylene Nonwovens for Clean Water Technologies. S. M. Jasper, L. Liu, J. A. Willoughby, M. A. Pasquinelli

141. Characterization of polymers with the Kerr Effect. R. Gurarslan, A. E. Tonelli


NC Distinguished Speaker Presentation
NC ACS Local Section awards

Raleigh Convention Center
Ballroom A

M. Pasquinelli, Organizer, Presiding
K. Levine, Presiding

7:00 142. Admiring, Analyzing, and Improving the 3D Structures of Macromolecules. J. Richardson/D. Richardson
Thursday Summary – 15 November 2012

Vendor Exposition
8:30 a.m. – 8:00 p.m. Ballrooms B/C

Events and Activities
12:00 p.m. – 1:30 p.m.
Women Chemists Committee Luncheon.
Speaker: Dr. Barbara Ramsay Shaw, Duke University,
“Challenges, Passions, and Opportunities Balancing Chemistry
Careers and Our Lives” (Ticketed event)

Short Course and Workshops
8:30 a.m. – 10:30 a.m.
NIH Funding for Chemists: Grant Writing Tips for
New and Experienced Applicants
9:00 a.m. – 5:00 p.m.
Career Connections Glass Office
1:00 p.m. – 5:00 p.m.
ACS Leadership Course: Fostering Innovation

Center for Solar Fuels (UNC EFRC) Conference
8:00 a.m. – 11:20 a.m.
Catalysts for Solar Fuels (oral) Ballroom A
9:20 a.m. – 10:00 a.m.
Catalysts for Solar Fuels (poster) Ballroom A
12:40 p.m. – 4:40 p.m.
Materials for Solar Fuels (oral) Ballroom A
2:40 p.m. – 3:20 p.m.
Materials for Solar Fuels (poster) Ballroom A

41st Southeastern Magnetic Resonance Conference (SEMRC)
1:15 p.m. – 5:15 p.m.
Edward O. Stejskal Memorial Symposium 306C

Poster Presentations
9:00 a.m. – 11:30 a.m.
Bioinorganic, Organic, Organometallic Ballrooms B/C
2:00 p.m. – 4:30 p.m.
Biochemistry, Chemical Biology Ballrooms B/C
6:00 p.m. – 8:00 p.m.
Analytical, Biomaterials, Electroanalytical, Energy and Fuels, Polymer Ballrooms B/C
Technical Sessions
8:00 a.m. – 12:00 p.m.

- Biochemistry I
- Chemistry and Applications of Smart Molecules and Materials I
- Chemistry and Bio-Nano Interfaces I
- Clinical Diagnosis MS I
- Computational Chemistry I
- Frontiers in Chemistry and Medicine I
- Inorganic Chemistry II
- Materials Chemistry I
- Medicinal Chemistry
- Nanochemistry I
- Organic Chemistry I
- Organometallic Chemistry I
- Physical Chemistry II
- Polymer Chemistry II
- Scanning Force Microscopy in Biology
- Separation Science in the Macro, Micro, and Nano World
- Symposium Honoring Royce W. Murray Session I
- Vendor Seminars

1:00 p.m. – 5:00 p.m.

- Biochemistry II
- Biominerical Chemistry I
- Biomaterials
- Chemical Biology
- Chemistry and Applications of Smart Molecules and Materials II
- Computational Chemistry II
- Frontiers in Chemistry and Medicine II
- Growing Impact of Public Domain Chemistry Resources
- Inorganic Chemistry III
- Materials Chemistry II
- Nanochemistry II
- New Applications, Ambient Ionization MS
- Organic Chemistry II
- Organometallic Chemistry II
- Polymer Chemistry III
- Symposium honoring Royce W. Murray Session II
- Vendor Seminar

SERTMACS Plenary Lecture
5:20 p.m. – 6:20 p.m.

- Royce W. Murray, Kenan Professor of Chemistry, UNC-Chapel Hill, "Nanoparticle Science and its Analytical Chemistry"

Sci-Mix - Refreshments and Poster Session
6:00 p.m. – 8:00 p.m. (Sponsored by Scynexis)
THURSDAY MORNING

Center for Solar Fuels (UNC EFRC) II
Catalysts for Solar Fuels

Raleigh Convention Center
Ballroom A

T. Meyer, Organizer, Presiding
M. Brookhart, Presiding


8:40 144. Is thermal CO₂ hydrogenation better than direct photochemical CO₂ reduction? E. Fujita

9:20 Coffee Break, Posters and Exposition.


10:40 146. Metallocarboxylic acids and metallocarboxylates on the pathway to CO₂ reduction. C. K. Schauer, A. J. Toman, M. A. Mendez, T. J. Meyer

Chemistry and Applications of Smart Molecules and Materials I

Raleigh Convention Center
206

S. Craig, K. Franz, Organizers, Presiding

8:00 147. Applications of PRINT technology for the production of monodisperse, shape specific particles. B. W. Maynor

8:40 148. Polyester biomaterials: Variation and study of functionality, shape memory effects, topography and processing. V. S. Ashby

9:20 149. Smart Plastics Via Stimuli-Induced Depolymerization. S. T. Phillips

10:00 Coffee Break, Posters and Exposition.

10:40 150. Dye-doped conjugated polymer nanoparticles for metal ion sensing. E. J. Harbron

Materials Chemistry I

Raleigh Convention Center
304

M. ter Horst, Organizer
R. Larsen, Presiding

8:00 152. Gallium nitride surface functionalization towards clinical diagnostic sensors. M. S. Makowski, A. Ivanisevic


9:00 155. Synthesis and UV curing of multi-functional monomers with degradable property. M. Shirai


9:40 Coffee Break, Posters and Exposition.

10:20 157. Engineering the yield properties of a nanoscale semiconducting membrane ($\text{Ga}_2\text{O}_3$) on a liquid metal alloy. M. R. Khan, J. So, M. D. Dickey

10:40 158. Novel Ruthenium(II)tris(2,2'-bipyridine) templated Zinc(II)1,3,5,-tris(4-carboxyphenyl)benzene metal organic frameworks: Photophysical properties. C. L. Whittington, L. Wojtas, R. W. Larsen
8:00 159. Boronic acid functionalized squarylium cyanine dye for detection of sugar-based analytes by fluorescence and polymer-enhanced capillary transient isotachophoresis. S. Saito, T. L. Massie, T. Maeda, H. Nakazumi, C. L. Colyer


9:00 161. Virus nanoparticles: chemistry, self-assembly and biomedical applications. Q. Wang

9:40 Coffee Break, Posters and Exposition.


11:00 163. Reservoir-based Dielectrophoresis (rDEP) for Microfluidic Particle Manipulation. X. Xuan

11:20 164. Microfluidic Systems for Rapid Forensic DNA Analysis. J. P. Landers

Symposium Honoring Royce W. Murray - I

8:00 165. Iridium oxide (IrOₓ) nanoparticles as catalysts for water oxidation. A. A. Gambardella, R. W. Murray

8:20 166. Electrochemical Modification of J. J. Roberts, R. W. Murray

9:00 168. EDL Structure and Dynamics at Nanoscale Interfaces: A Case When Ion Flux Is NOT Normal to the Surface. G. Wang, D. Wang, J. Liu, W. Brown, Y. Li, M. Kvetny

9:20 169. GOLD NANOMOLECULES: Gold Nanoparticles of Molecular Definition. A. Dass

9:40 Coffee Break, Posters and Exposition.

10:20 170. Subsecond detection of hydrogen peroxide using fast-scan cyclic voltammetry at carbon-fiber microelectrodes. L. A. Sombers, J. G. Roberts


11:00 172. Imaging flow cytometry of fission yeast: cell morphology and effects of toxins. R. Pyati


**Frontiers in Chemistry and Medicine I: Impact of Medicinal Chemistry on Infectious Diseases**

Raleigh Convention Center
303

Sponsored by GlaxoSmithKline
V. Srivastava, K. Widdowson, *Organizers*
B. Johns, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 174. Discovery of HCV NS5A inhibitor GSK2336805: From early lead to clinical POC. C. D. Roberts


9:40 Coffee Break, Posters and Exposition.

10:15 Introductory Remarks.

11:00 177. Identification of the first potent inhibitors of tRNA (m’G37) methyltransferase (TrmD) via an integrated screening approach. A. T. Price

11:40 Concluding Remarks.

Organic Chemistry I
Raleigh Convention Center
203
M. ter Horst, Organizer
T. Hollis, Presiding

8:20 178. Addition reactions catalyzed by Re(V)oxo complexes. K. A. Nolin


9:00 180. Taking advantage of the chemistry of heterocycles in advanced catalyst ligand supports. A. E. Gorden, Y. Li, K. Weerasiri, E. Buss, A. V. Gamble


9:40 Coffee Break, Posters and Exposition.

10:20 182. Small molecule encapsulation in PAMAM dendrimers. A. Jolly, M. Bonizzoni


Polymer Chemistry II
Raleigh Convention Center
301B
M. ter Horst, Organizer
S. Tallury, Presiding


8:40 187. Moisture Vapor Transport through Surface-Modified Films. R. Grewal, J. A. Willoughby


9:20 189. Synthesis And Characterization Of Poly(Ethylene Oxide)-Poly(Arylene Ether Sulfone) Based Segmented Polyurethanes For Water Or Gas Separation Membranes. A. Nebipasagil, J. E. McGrath

9:40 Coffee Break, Posters and Exposition.

10:20 190. Thermosetting networks derived from disulfonated poly(arylene ethers) for water purification reverse osmosis and pressure retarded osmosis (PRO) membranes. B. J. Sundell, C. H. Lee, J. Cook, B. D. Freeman, J. E. McGrath


11:00 192. Formation and Characterization of UV Crosslinkable Reverse Osmosis Membranes from Hydrophobic Poly(Tetra Methyl BisA Ether Ketone) and Hydrophilic Sulfonated Poly(Arylene Ether Sulfone) Block Co-Polymers. A. Shaver, Y. Chen, J. Cook, B. Freeman, J. McGrath

Chemistry of Bio-Nano Interfaces
Modeling and simulations

Raleigh Convention Center
301A

A. Smirnov, Organizer
Y. Yingling, Organizer, Presiding
D. Brenner, Presiding

8:40 194. Mechanisms of Molecular Recognition and Assembly at the Nanoscale: Computation Meets Experiment. **H. Heinz**


10:00 Coffee Break, Posters and Exposition.

10:40 196. Nano-Pipette Directed Motion of Bio-Inspired Transmembrane Channel. **M. Dutt**

11:20 197. Understanding interactions of gold nanoparticles with DNA by tuning ligand chemistry. **A. Singh, N. Li, Y. G. Yingling**

Inorganic Chemistry II

Raleigh Convention Center
204

M. ter Horst, Organizer
S. Jones, Presiding


9:00 199. Effect of methylene spacers on the molecular structures of pyridine-thione complexes of the group 12 metals. **K. Tokmic, E. A. Amenson, D. Rabinovich**


9:40 201. Kinetic studies of highly preorganized pyridyl based ligands with d8 metal ions. **R. H. Tillman, R. D. Hancock, S. B. Jones**

10:00 Coffee Break, Posters and Exposition.

11:00 203. Determination of formation constants of highly pre-organized low solubility ligands with metals using long path length UV-vis spectroscopy. S. B. Jones, R. D. Hancock, F. L. Vázquez Rivera


11:40 205. Actinide selective ligands for extractions and sensing applications. A. E. Gorden, M. A. DeVore, B. A. Maynard

Mass Spectrometry I: Clinical Diagnosis

Raleigh Convention Center
302A
G. Glish, Organizer
R. Grant, Organizer, Presiding

8:40 206. Applications of tandem mass spectrometry and microfluidics in newborn screening. D. S. Millington, R. Sista, V. Pamula

9:20 209. Designer drug phenomenon: Chemists chasing chemists. M. McMullin

10:00 Coffee Break, Posters and Exposition.

10:40 207. Endogenous Small Molecule Biomarker Analysis in the Clinic: Sensitivity, Selectivity and Speed. R. P. Grant

11:20 208. Quantifying proteins in mixtures is complex. A. N. Hoofnagle

Nanochemistry I

Raleigh Convention Center
306A
M. ter Horst, Organizer
J. Macdonald, Presiding


9:00 211. Ammonium ion-coated magnetic iron oxide nanoparticles for drug delivery. M. H. Nantz, S. J. Mattingly, G. J. Clark, S. Biswas, J. Jasinski

9:40 213. Surface properties of ionic liquid adsorbate layer are influenced by the dipole of the underneath substrate. **x. zhang**, L. Lu, Y. Cai

10:00 Coffee Break, Posters and Exposition.


**Organometallic Chemistry I**

Raleigh Convention Center
305B

M. ter Horst, *Organizer*
B. Quillian, *Presiding*

8:40 218. Carbonylation reactions with oxorhenium complexes. **C. P. Lilly**, E. A. Ison


9:20 220. Sequential reactions of boron and silicon substituted 1,3-dienes. **M. E. Welker**, C. Junker, L. Wang

9:40 Coffee Break, Posters and Exposition.


11:00 223. Synthesis of cis and trans bis-alkynyl complexes of Cr(III) and Rh(III) supported by a tetradeutate macrocyclic amine: Building blocks for molecular magnets and/or molecular wires. **C. Sun**, P. S. Wagenknecht
Physical Chemistry II
Raleigh Convention Center
302C

M. ter Horst, Organizer
J. Lyon, Presiding

8:40 224. Computational Studies of Ion-Molecule Reactions Important to Interstellar Chemistry. S. A. Abrash, L. Wright, A. Weaver, L. Gallagher, S. Roscoe, M. S. El Shall

9:00 225. Silver cluster based sensors for DNA. B. Giri, D. Nicholson, I. Miller, O. Sergev, J. T. Petty


9:40 227. Heterogeneity in fast folding β-proteins. C. Davis, B. Dyer

10:00 Coffee Break, Posters, and Exhibition.

10:40 228. Effects of Ligand Binding on Exciton Recombination Dynamics in Colloidal Quantum Dot Nanocrystals. M. Jones, E. S. Williams, K. J. Major

11:00 229. Measurement of the optical properties of polystyrene spheres using cavity ring-down spectroscopy and nephelometry. S. Singh, G. Tedla, M. N. Fiddler, S. Bililign


11:40 231. Excitonic states in a (Ti6O12)3 nanotube. B. N. Papas, J. L. Whitten

Scanning Force Microscopy in Biology: New Tricks and New Insights
Raleigh Convention Center
306B

Supported by Asylum Research
D. Erie, Organizer, Presiding

8:40 232. Nanoscale Dynamics of Protein-DNA Complexes. Y. L. Lyuchenko

9:20 233. Topology that divides DNA. D. Dunlap

10:00 Coffee Break, Posters and Exposition.

11:20 235. Tuning the biomechanics of cell-cell adhesion. S. Sivasankar

12:00 236. Visualizing the Path of DNA through Proteins using DREEM Imaging. D. Wu, D. Erie

Biochemistry I

Raleigh Convention Center
205

M. ter Horst, Organizer
M. F. Santiago, Presiding

9:00 237. NMR-based metabolomic study of Neuropeptide Y and Corticotropin-releasing factor treatment in an immortalized rat hypothalamic cell line. S. Pati, S. Sheriff, M. Watanabe, L. Wilson, A. Balasubramaniam, A. Boroujerdi


9:40 239. Biochemical studies on HipB binding to the TATCC motif of the hipBA operator. M. Depani

10:00 Coffee Break, Posters and Exposition.

11:00 240. Modulation of the Kv4.3-KChIP3 interactions by Ca^{2+} and NS5806. W. G. Gonzalez, J. G. Miksovska

11:20 241. Role of Tyr 44 in transmitting structural information between the CD-loop and heme binding site in neuroglobin. J. Miksovska

Bioinorganic Chemistry Poster Session
Posters are presented from 9:30 to 11:00

Raleigh Convention Center
Ballroom B/C

Y. Yingling, Organizer

9:00 – 11:30

243. EPR-based metrologies for nanofabrication and energy applications. V. A. Szalai, C. D. Bohn, R. Kinney

244. Myoglobin Binds Phenol in Proximal Cavity. C. Wang, X. Huang, L. R. Celeste, L. L. Leslie, S. Sun, J. H. Dawson, L. Lebioda

245. Ruthenium(II)-arene complexes with naphthalimide-tagged chelating schiff base ligands: synthesis and DNA-binding studies. A. Peralta, K. Ghebreyessus

246. Substrate-directed peroxygenase reactivity of dehaloperoxidase from Amphitrite ornata via nitrophenol hydroxylation. D. A. Barrios, J. D'Antonio, R. A. Ghiladi

247. Volume and enthalpy profile for CO photo-dissociation of chloramine-T modified horse heart cytochrome-c. T. A. Word, R. Larsen

Computational Chemistry I

Raleigh Convention Center
201

M. ter Horst, Organizer
D. Clabo, Presiding

9:00 248. Theoretical and conformational studies of decalin-1,4-dione derivatives. J. Bowen

9:20 249. Why does Sulfuric Acid have a much stronger gas phase acidity than Methanol? A Density Functional Theory study to determine the contributions by Polarizability, Resonance and Inductive effects. K. Lynch, J. Karty

9:40 250. Molecular dynamics simulations of nAChR transmembrane domain: Exploring the effects of single point mutations. T. G. Kucukkal, S. J. Stuart

10:00 Coffee Break, Posters and Exposition.


11:00 252. Effect of calculation of solvation free energy on FKBP proteins. L. S. Smith
11:20 253. Studies of $\pi$-$\pi$ interactions of fullerene fragments using density functional methods.
A. N. Karunarathna, S. Saebo


Medicinal Chemistry
Raleigh Convention Center
302B

M. ter Horst, Organizer
J. Klenc, Presiding

9:00 255. A wolf in sheep's clothing: Sophisticated software and ease of use are not mutually exclusive. C. Detering


10:00 Coffee Break, Posters and Exposition.


11:00 259. Novel conjugation chemistries for the functionalization and cellular imaging of potent platinum-acridine anticancer agents. S. Ding, X. Qiao, G. L. Kucera, U. Bierbach

Organic Chemistry Poster Session
Posters are presented from 9:30 to 11:00

Raleigh Convention Center
Ballroom B/C

Y. Yingling, Organizer

9:00 - 11:30


266. One-pot enol silane formation-Mannich-type addition of ketones, thioesters, and amides to nitrones. C. M. Dombrowski, E. N. Maxwell, C. L. Safran, O. A. Akomah, C. W. Downey


270. Synthetic investigations toward the angucycline antitumor antibiotic galtamycin. A. Shrestha, J. L. Davenport, R. Pontege

271. Photochemical release of metal ions: A modified caging design Development of a photocleavable chelator for the light-directed release of metal ions. M. A. McKinley, V. V. Popik
272. Flash chromatographic isolation and characterization of organic molecules using advanced λ-All detection with full range photo-diode array analysis. B. Bickler

273. Lewis acid-catalyzed Csp³-H functionalization of 2-methyl-azaarenes with α-Trifluoromethyl Carbonyl Compounds. J. Heimberger, K. Bowe, A. Shaikh


275. Catalyst- and solvent-free high yielding Ullmann's coupling reactions. A. N. Morris, C. A. Brown, G. R. Mandouma


277. Green chemistry: oxidation reactions under high pressures of oxygen. E. E. Buss, Y. Li, A. E. Gorden


280. Exploring the reactivity of 1,5-sulfonyl-triazoles; thermolysis and Rh(II) catalyzed reactions. M. Meza Avina, M. K. Patel, M. P. Croatt


286. Regioselective nucleophilic addition of alcohols and thiols to 3-alkoxy/aryloxypyrazinium salts: Facile synthesis of 2-alkoxy/aryloxy-3-oxo-3,4-dihydropyrazines. S. R. Dandepally, A. L. Williams
287. Applications of phenyl isothiocyanates in one-pot elimination reactions. T. C. Irvin, G. F. Majetich


289. Synthesis of novel 4-oxazolidinones as antimicrobial agents. N. V. Shymanska, J. G. Pierce

290. Thiourea-catalyzed aminolysis of N-acyl homoserine lactones. M. A. Bertucci, M. R. Gagne

291. Progress towards the pentacyclic guanidine core of the monanchocidin family of apoptosis-inducing natural products. Y. Moazami, J. G. Pierce

292. Thiohydroxamic acids as versatile reagents for synthesis. B. C. Lemercier, J. G. Pierce

293. Progress towards the unprecedented morpholine fragment of the monanchocidin family of guanidine natural products. Y. Shi, J. G. Pierce


296. Structural Characterization of Natural Products from a Medicinal Plant. R. de Guzman, C. Smith, K. Knight

297. Regioselective Lithiation of N-Boc-3-Bromo-4-Methylpyrrole --- A New Synthesis of SU-5402. D. Dai, B. Venepalli, V. Chittineni


299. Investigation into the importance of the diphenylpropynone structure against melanoma and prostate cancer. A. J. Petree, P. B. Honeycutt, K. S. Petersen


301. Reactions of Hypervalent Iodonium Alkynyl Triflates with Azides: Generation of Cyanocarbenes. I. D. Hyatt, M. P. Croatt

302. Synthesis and spectroscopy of silicon Corrole derivatives for use in solar cells and photodynamic therapy. Z. Lyles, N. Pham, K. Fessler, M. G. Walter


305. Synthesis and reactivity of a cyclic six-membered oxocarbenium ion containing an electron-withdrawing beta-esther. C. P. Merryman


310. Design and synthesis of heterocyclic combretastatin analogues: 2-Aroyl indoles and 2-(aryl-1,2,3-triazolyl) indoles via indole aldehydes and ethynyl indoles. B. J. Shields, H. L. Holt


312. Synthesis of (+)-malbrancheamide B utilizing a stereoselective Diels-Alder cycloaddition to establish the [2.2.2]-diazaoctane bicyclic core. S. W. Laws, J. R. Scheerer

313. Direct reductive amination of aldehydes and ketones with sodium borohydride and polyethylene glycol 200 under solvent-free conditions. R. Lee, S. Lee, J. Lee

314. One-pot oxidation of aldehyde, B-cyclodextrin in water, and in mild conditions. S. Jeong, J. Lee

315. Kinetic resolution of α-hydroxy lactones via silylation. M. Moore, S. Wiskur, R. Clark, Y. Zhang

316. Structural and Functional Characterization of Short Helical Peptides as Catalysts for Acyl Transfer. S. Bezer, M. waters, m. gagne


320. Application of 4-pyridinylmethyl esters of glutamic and aspartic acids in solid-phase peptide synthesis. **S. Garapati**, C. S. Burns


323. Ortho-a minochlorination of arynes via an insertion reaction of N-chloramines. **C. E. Hendrick**, S. L. McDonald, Q. Wang


325. Abiotic Adenine and Purine Synthesis in Formamide. **J. Hudson**, G. Springsteen


**Organometallic Chemistry Poster Session**

**Posters are presented from 9:30 to 11:00**

Raleigh Convention Center
Ballroom B/C

Y. Yingling, **Organizer**

9:00 - 11:30

327. Design of novel metallosupramolecular helicates containing 2,4-(bis-1-ferrocenyl-prop-3-enol-1-one)pyridyl. **D. Myers**, S. Atim, M. Raja

328. Room temperature Au(I)-catalyzed enantioselective intramolecular hydroamination of unactivated alkenes. **S. Lee**, R. A. Widenhoefer

329. Transition metal based catalysis at Eastman: Why it matters. **D. W. Norman**


332. Synthesis and structure of cationic Au(I) enamine complexes. **M. Sriram, A. C. Jones**

333. Two approaches to metal-catalyzed C-glycoside synthesis. **L. L. Adduci, R. S. Andrews, C. Munro-Leighton, M. R. Gagne**


335. Synthesis of 2-siloxacyclopentene containing 1,3 dienes and their Diels-Alder/cross-coupling reactions. **P. P. Choudhury, M. E. Welker**


338. Investigations into the ruthenium catalyzed formation of methanol from Syngas. **V. M. Ibe, J. Lee, T. A. Nile, D. Wass, R. L. Wingad**


341. The synthesis of three-fold symmetric 1,3,5-tris-phenylbenzene cyclopentadienyl ligands. **J. T. Foy, I. Aprahamian**


343. Mercury(II) catalyzed cis-trans isomerization of transition metal complexes. **S. D. Hastings, G. M. Gray**

344. Preparation, characterization, and a theoretical study of the novel imidazolylferrocene-based ligand, 4,5-dipyridyl-1H-imidazol-2-yl ferrocene, Fc$^{di}$. **K. J. Brown, T. L. Davis**


Center for Solar Fuels (UNC EFRC) Poster Session II
Catalysts for Solar Fuels (Posters on display Wednesday through 5 pm on Thursday)

Raleigh Convention Center
Ballroom A

T. Meyer, Organizer

9:20 - 10:00


349. Water oxidation electrocatalysis via electroflocculated films of iridium oxide nanoparticles (IrOx NPs). K. E. Michaux, R. W. Murray


353. Electrocatalysis of water oxidation by simple Cu(II) salts. Z. Chen, T. J. Meyer

354. Impact of bridging ligand variation on photoinduced charge separation in Ru(II),Pt(II) supramolecular complexes. J. D. Knoll, M. K. Brennaman, T. J. Meyer, K. J. Brewer

355. Predicting redox potentials for catalysts with density functional reactivity theory. S. Liu


358. CO2 reduction using anionic cyclopentadienone ruthenium hydrides. B. C. Landers, C. K. Schauer
359. Component variation in Ru(II),Rh(III) bimetallic supramolecules capable of photocatalytically reducing water to hydrogen fuel. **H. E. Mallalieu**, T. A. White, G. F. Manbeck, B. N. Stone, K. J. Brewer


366. Ultrafast studies of electron and energy transfer in polynuclear Ru-based complexes. **S. Yamazaki**, A. Cadranel, J. Tate, L. M. Baraldo, V. D. Kleiman
THURSDAY AFTERNOON

Center for Solar Fuels (UNC EFRC) III
Materials for Solar Fuels

Raleigh Convention Center
Ballroom A

T. Meyer, Organizer
K. Schanze, W. You, Presiding

12:40 367. Solar energy conversion with nanostructured photocatalysts: Importance of entropy.
F. E. Osterloh

1:20 368. Combinatorial and Distributed Search for Semiconducting Oxides that Photoelectrolyze Water. B. A. Parkinson

2:00 369. Conducting and Semiconducting Oxide Nanoparticles for Solar Fuel Generation. P. G. Hoertz, A. Rieth, J. Bittle, A. Miller

2:40 Coffee Break, Posters and Exposition.

3:20 370. Cobalt oxide core–silica shell units for artificial photosynthesis. H. M. Frei

4:00 371. Recent Development of Solar Cells and Solar Fuels at the Center for Molecular Devices. A. Hagfeldt

Growing Impact of Public Domain Chemical Resources

Raleigh Convention Center
302C

A. J. Williams, S. Ekins, Organizers, Presiding

1:00 372. DSSTox ToxCast and Tox21 Chemical Inventories: Laying the Foundation for the U.S. EPA's Computational Toxicology Research Programs. A. M. Richard

1:20 373. FDA/USP Substance Registration System (SRS) and its UNII identifier codes. F. L. Switzer, L. N. Callahan, Y. Borodina


2:00 375. Connecting chemistry across the internet using ChemSpider. A. J. Williams, V. Tkachenko
2:20 376. Mobile apps for chemistry: real world workflows using next generation platforms. A. M. Clark


3:00 Coffee Break, Posters and Exposition.

3:40 378. PubChem has lots of data, but what about data quality? E. Bolton

4:00 379. Creating one of the pillars of the semantic web for chemistry by curating public chemistry databases. V. Tkachenko, A. Williams, A. Pshenichnov, D. Ivanov

4:20 380. On the correctness of chemical structures found on the internet and the need of curated datasets for any molecular modeling studies. A. D. Fant, E. Muratov, D. Fourches, D. Sharpe, A. Williams, A. Tropsha

4:40 381. The Royal Society of Chemistry chemical validation and standardization platform. K. Karapetyan, A. Williams, V. Tkachenko, C. Batchelor

Symposium Honoring Royce W. Murray - II
Raleigh Convention Center
305A

Supported by Pine Research Instrumentation, Gamry Instruments, CH Instruments, ACS Division of Analytical Chemistry
R. Wightman, Organizer
L. Horne, Organizer, Presiding

1:00 382. Gold Nanoparticles: Size-Dependent Electrochemical Oxidation and Thiol Place-Exchange Reactions for Controlled Assembly. F. Zamborini, R. Masitas, L. Bao, A. Fang


2:20 Coffee Break, Posters, and Exposition.


Frontiers in Chemistry and Medicine II: Advances in Catalysis and Sustainable Process Chemistry
Raleigh Convention Center
303
Sponsored by GlaxoSmithKline
M. McClure, V. Srivastava, Organizers
V. Elitzin, Organizer, Presiding

1:15 Introductory Remarks.


2:00 388. Necessity is the mother of greener chemical inventions: Two case studies. W. F. Kiesman

2:40 Coffee Break, Posters and Exposition.

3:15 Introductory Remarks.


4:40 Concluding Remarks.

SEMRC - Edward O. Stejskal Memorial Symposium
Raleigh Convention Center
306C
Sponsored by NCSU Dept. of Chemistry, Doty Scientific, Bruker Biospin
A. Nevzorov, I. Nesmelova, Organizers

1:15 Introductory Remarks.

1:30 391. Development of CPMAS at Monsanto with Ed Stejskal. J. Schaefer


2:40 Coffee Break, Posters and Exposition.

3:20 393. Structural diversity of amyloid fibrils: Insights from solid state NMR. R. Tycko
4:05 394. Long range NMR constraints in the assembly of protein-carbohydrate complexes. J. Prestegard

4:50 395. Dynamic nuclear polarization at 4.6 T and 1.15 K using a homebuilt prepolarizer. L. Lumata, Z. Kovacs, M. E. Merritt

Bioinorganic Chemistry I

Raleigh Convention Center
301A

M. ter Horst, Organizer
A. Spuches, Presiding


1:40 397. Peroxide shunt reaction of cytochrome P450cam with substituted perbenzoic acids: Evidence for an Fe(III) acylperoxo intermediate and the kinetics of its formation and conversion to compound I. D. P. Collins, J. H. Dawson, D. P. Ballou, E. Johnson, E. D. Coulter, Z. Beharry


2:20 Coffee Break, Posters and Exposition.


3:40 400. Development of bioinspired catalysts for efficient peptide hydrolysis. R. Prabhakar

4:00 401. Mixed-donor ligands and the preparation of synthetic analogues of methanobactin. D. Rabinovich

4:20 402. Side by side comparison: Cerium(IV)-assisted hydrolysis of sphingomyelin and phosphatidylcholine at lysosomal pH. D. E. Williams, S. S. Cepeda, K. B. Grant
Biomaterials I
Raleigh Convention Center
306B

M. ter Horst, Organizer
J. Stone, Presiding

1:20 403. Chromatography-free purification and site-specific modification of tag-free recombinant proteins enabled by Sortase A and elastin-like polypeptides. J. Bellucci, M. Amiram, J. Bhattacharyya, D. McCafferty, A. Chilkoti

1:40 404. Modification of a gallium nitride surface for manipulating cell-substrate interactions. L. Bain, A. Ivanisevic

2:00 405. Position-specific chemical modification and quantitative proteomics disclose adsorbed protein orientation on silica nanoparticles. J. H. Nuffer, S. Shrivastava, R. W. Siegel, J. S. Dordick


2:40 Coffee Break, Posters and Exposition.


3:40 408. Fabrication of Chitosan-Cyclodextrin Electrospun Nanofiber Blends. N. A. Burns, S. Khan

4:00 409. Principal Component Analysis to mine metabolomics data. A. A. Harley, A. Mondal, P. Timalsina

4:20 410. Encapsulation of pancreatic islet cells to protect from immune injury during transplantation. V. Kozlovskaya, H. M. Tse, J. A. Thompson, E. Kharlampieva

Chemical Biology I
Raleigh Convention Center
302B

M. ter Horst, Organizer
C. McInnes, Presiding

1:20 411. Small molecules targeting sub-cellular localization through the Polo-Box Domain of PLK1. C. McInnes, S. Craig, M. Baxter, M. D. Wyatt
1:40 412. Isolation and structure elucidation of new hamigerans from the New Zealand marine sponge *Hamigera tarangaensis*. J. Dattelbaum, P. Northcote

2:00 413. Bioanalytical and cellular imaging studies of the DNA damage produced by platinum-acridine anticancer agents. X. Qiao, S. Ding, A. S. Essader, K. E. Levine, G. L. Kucera, U. Bierbach


2:40 Coffee Break, Posters and Exposition.


3:40 416. Frequent itemset mining applied to pharmacophore features: Constructing topological pharmacophores using open-source tools. P. J. Kowalczyk

4:00 417. Machine learning using open source tools: Data mining applied to antimalarial drug discovery. P. J. Kowalczyk

Mass Spectrometry II: New Applications and Strategies Using Ambient Ionization Methods
Raleigh Convention Center
302A

G. Glish, Organizer
J. Williams, Organizer, Presiding

1:20 418. Ambient ionization: variants, fundamentals and point-of-care diagnostics. R. G. Cooks

2:00 419. Size, m/z, and position: ion mobility spectrometry and imaging MS of ambient ions. P. Dwivedi, C. Gamage, R. Bennett, J. Keelor, F. M. Fernandez

2:40 420. Ambient tissue imaging using infrared matrix assisted laser desorption electrospray ionization mass spectrometry (IR-MALDESI MS). D. C. Muddiman, J. A. Barry, G. Robichaud

3:20 Coffee Break, Posters and Exposition.

3:40 421. New analytical opportunities in ambient surface sampling/ionization mass spectrometry: Combining laser ablation sampling and liquid phase collection. G. J. Van Berkel


105
Nanochemistry II
Raleigh Convention Center
306A

M. ter Horst, Organizer
B. Baruah, Presiding


1:40 424. Mapping optically active regions of metal-ion doped single TiO₂ nanoparticles involved in heterogeneous photocatalysis. **M. Behl**, P. K. Jain

2:00 425. "Novel Synthetic Route to 1nm Diameter Alkyne Capped Gold Nano-particles". **A. T. Hermann**, C. Gorman


2:40 Coffee Break, Posters and Exposition.

3:20 427. Surface modified monometallic and bimetallic nanoparticles, SERS substrate and analyte detection. **B. Baruah**

3:40 428. Modeling and Understanding role of shell thickness on exciton decay dynamics and charge-carrier trapping in CdSe/CdS quantum dots using time resolved photo luminescence. **G. Singh**


Organic Chemistry II
Raleigh Convention Center
203

M. ter Horst, Organizer
C. Downey, Presiding

1:20 432. Development of a one-pot, three-step thioconjugate addition-oxidation-Diels–Alder cycloaddition reaction. C. Downey


2:00 434. Determination of the mechanism for the formation of benzocyclobutenes from the flash vacuum pyrolysis (FVP) of substituted aryl propargyl ethers. J. M. Riemann, S. Safrit, Z. McMichael, Z. Dyer


2:40 Coffee Break, Posters and Exposition.

3:20 436. Improved substituent constants for the prediction of aromatic cation-pi and anion-pi binding energies. M. Lewis, C. Bagwill, S. Wireduah


4:00 438. Origin of the S_N2 benzylic effect: Contributions from resonance and induction. R. E. Rawlings, J. Karty, A. McKerlie


Biochemistry II
Raleigh Convention Center
205

M. ter Horst, Organizer
J.G. Williams, Presiding

1:40 440. Adjusting calmodulin structure and function by methionine oxidation. J. Urbauer, H. Niedermaier, R. Bieber Urbauer
2:00 441. The mechanism and function of cysteine desulfurases in the biosynthesis of thio-cofactors in *Bacillus subtilis*. **P. C. Dos Santos**

2:20 442. Sphingosine kinase 1: Insights into structure and function. **T. T. Pham**, M. A. Sparks, D. L. Baker

2:40 Coffee Break, Posters, and Exhibition.

3:20 443. UV resonance Raman detects redox-induced structural change in photosystem II-inspired biomimetic peptides. **C. V. Pagba**, B. A. Barry


4:00 445. Iron binding site in a global regulator in bacteria - ferric uptake regulator (Fur) protein: Structure, Mauer properties, and functional Implication. J. Katigbak, **Y. Zhang**

**Chemistry and Applications of Smart Molecules and Materials II**

Raleigh Convention Center
206

S. Craig, K. Franz, *Organizers, Presiding*

1:40 446. Liposomes as nanomachines. **T. Hanks**, W. Pennington


3:00 Coffee Break, Posters and Exposition.

3:40 448. Flexible, transparent, conducting networks of metal nanowires. A. Rathmell, **B. Wiley**

4:20 449. From Molecules to Materials. **C. Nuckolls**

**Computational Chemistry II**

Raleigh Convention Center
201

M. ter Horst, *Organizer*
S. Wasileski, *Presiding*

1:40 450. Impact of ligand chemistry on the interfacial properties of polymer nanocomposites. **R. Pani**, Y. G. Yingling
2:00 451. Quantum mechanical explanations for the unusual entropy increase at the transition state of bis(chromiumtricarbonyl) dibenzo[a,e]cyclooctatetraene. C. N. Ratnaweera, N. Bandara, W. P. Henry, S. R. Gwaltney


2:40 Coffee Break, Posters and Exposition.

3:40 453. Understanding non-covalent interaction in bio-nano systems with multiscale molecular modeling and simulation towards bio-medical application. Y. Wang

4:00 454. Prediction of Reaction Barriers and Thermochemical Properties with Explicitly Correlated Coupled-Cluster Methods: A Basis Set Assessment. J. Zhang, E. F. Valeev


Inorganic Chemistry III
Raleigh Convention Center
204

M. ter Horst, Organizer
C. De Silva, Presiding

1:40 456. Tetrakis 3,1-(N-phenylacetamide) dirhodium(II) adduct with 1,3-dicyanobenzene: Structural properties. C. T. Eagle, N. Atem-Tambe

2:00 457. Single crystal X-ray structure of Ba_{1.5}[Fe(C_{10}H_{13}N_2O_7)][Co(CN)_6]9H_2O. F. Quarshie, C. T. Eagle, K. K. Kpogo, J. G. Wardeska

2:20 458. Effect of sensitizer ligand on photoluminescence efficiency of Eu(III) and Tb(III) complexes: a TDDFT study of electronic structure. C. R. De Silva


3:00 Coffee Break, Posters and Exposition.

3:40 460. Investigating the existence of the pnictide analogs of cyanogen and cyanogen halides. J. W. Hall, J. R. Wasson
4:00 461. Towards Developing Organic-Radical Containing Metal Complexes to Explore Photogenerated Semiquinone-Nitronylnitroxide Excited State Dynamics. **C. Tichnell**, D. A. Shultz


**Organometallic Chemistry II**

Raleigh Convention Center
305B

M. ter Horst, *Organizer*

1:40 463. Hydrogenation and hydrogenolysis of biomass derived furan derivatives using electrophilic ruthenium bipyridine catalysts. **A. Shankara Linge Gowda**

2:00 464. Iridium-catalyzed oxidative coupling of benzoic acids with alkynes. **D. A. Frasco**, E. A. Ison, K. L. Engelman


3:00 Coffee Break, Posters, and Exhibition.


4:00 468. Mild route for the complete reduction of glucose to hexane by silane. **M. P. McLaughlin**, L. L. Adduci, J. J. Becker, M. R. Gagné

Polymer Chemistry III
Raleigh Convention Center
301B

M. ter Horst, Organizer
L. Madsen, Presiding


2:00 471. Stimuli-triggered shape response of cubical hydrogel microcapsules. V. Kozlovskaya, Y. Wang, J. Chen, Y. Chen, E. Kharlampieva


2:40 Coffee Break, Posters, and Exhibition.


4:00 475. Withdrawn

Biochemistry Poster Session
Posters are presented from 2:30 to 4:00
Raleigh Convention Center
Ballroom B/C

Y. Yingling, Organizer

2:00 - 4:30

476. Thermodynamic characterization of a thermostable antibiotic resistance enzyme, the Aminoglycoside Nucleotidyltransferase 4’. X. Jing, E. Wright, A. N. Bible, C. B. Peterson, G. Alexandre, B. D. Bruce, E. H. Serpersu

478. Investigations into the synthesis of DNA opposite 8-Oxo-2'-deoxyguanosine with Polymerase b. A. M. Weaver, M. Hamm, E. McFadden, M. Ghio

479. Physical Studies of Target Activation by Calmodulin. H. T. Niedermaier, R. J. Bieber Urbauer, C. E. Jolly, B. Jones, j. L. Urbauer

480. Evidence for the involvement of Bacillus subtilis YrvO and MnmA in the biosynthesis of 2-thiouridine tRNA. K. A. Black, P. C. Dos Santos

481. Disruption of iron metabolism by elevated nickel concentrations in E. coli: An NMR-based metabolic investigation. N. Ozonma, G. Ford, W. Outten, A. Boroujerdi

482. Characterization of the sulfur acceptor protein SufU in Bacillus subtilis. B. Selbach, P. Dos Santos

483. Role of SufBCD complex in the Fe-S cluster assembly pathway in bacteria. P. K. Pradhan, B. Selbach, B. Saitta

484. Characterization of N-acetyl-glucosamine Deacetylase and Bacillithiol S-conjugate Amidase in Bacillus anthracis. Z. Fang, A. Claiborne, C. J. Hamilton, P. C. Santos

485. Biogenesis of mitochondrial electron transport chain complex III: Role of the assembly factor Mzm1. J. L. Fox, T. Cui, P. M. Smith, O. Khalimonchuk, D. R. Winge

486. Towards the structural and functional characterization of the Aquifex aeolicus Hfq homolog. K. Stanek, J. Patterson, C. Conrad, C. Mura

487. Effect of calcium on chloride substrate inhibition in photosystem II at pH 5.5. H. Tai, A. Haddy

488. Is the iron dependent regulator from Mycobacterium tuberculosis a mixed metal regulator? L. R. Walker, B. Stapleton, T. M. Logan

489. Effects of anion inhibitors on chloride activation of oxygen evolution by photosystem II. I. Lee, P. Lee, T. (. Tran, A. Haddy

490. Syntheses of potential inhibitors of aspartate semialdehyde dehydrogenase. C. J. Halkides, W. S. Langford, M. Colner, W. S. Kish, D. M. Jansen


493. Potential Inhibition of Cytochrome P450 isozymes 3A4 and 2D6 by Acai Berry (Euterpe oleracea) Extracts. B. Hollers, G. Raner

494. DNA interactions and photocleavage by halogenated carbocyanine-based photosensitizers. C. T. Mapp, E. A. Owens, M. B. Henary, K. B. Grant

495. Impact of calcium on migration and differentiation of cultured lung myofibroblasts. H. Gipson, S. Ward, N. Fowler, S. Dahlhauser, E. Estes, B. Sharma

496. Protein Purification of Thalassiosira pseudonana. P. Curnow, A. Moody, T. Nile, S. Ratcliffe

497. Spectroscopic study Ca\(^{2+}\) induced changes in the structure, dynamics and stability of DREAM protein and its mechanism of DNA interaction. K. Pham, J. Miksovska


499. Understanding neurosteroid regulation of ionotropic glutamate receptors. S. Biello, D. Fanelli

500. Bio-Mimicking Pyruvate to Inhibit Lactate Dehydrogenase. D. N. Brockington

501. Kinetic study of inhibition mechanism of Dehaloperoxidase by 4-bromophenol and analogous molecules. J. Zhao, S. Franzen


504. Effect of osmolytes on protein association: Concanavalin A dimer to tetramer equilibrium. J. K. Myers, T. Silvers

505. Properties of the inactive ensemble of caspase-3. C. E. Cade, C. Mattos, P. Swartz, A. Clark

506. Inhibition of rabbit liver aldehyde oxidase by berberine. E. Lee, L. M. Carey, R. B. Banks

507. Dynamics of MpX insertion into model membrane vesicle bilayers. E. Schuler, S. Nagarajan, B. Dyer
Chemical Biology Poster Session
Posters are presented from 2:30 to 4:00

Raleigh Convention Center
Ballroom B/C

Y. Yingling, Organizers

2:00 - 4:30


509. Synthesis of photocaged nucleotides and morpholino oligomer subunits. Q. Liu, A. Deiters


511. Synthetic biology and photocontrol of artificial riboswitches. S. J. Walsh, G. J. Williams

512. Synthetic biology approaches to regioselectively-modified polyketides. C. Kasey, G. J. Williams

513. Reprogramming enzyme substrate specificity by yeast cell surface display. C. C. Ladner, Z. Ye, I. Koryakina, J. McArthur, G. J. Williams

514. DNA computation in live cells. J. Hemphill, A. Prokup, A. Deiters

515. Small Molecule Suppression of Oxacillin Resistance in MRSA. T. L. Harris, R. Worthington, C. Melander


517. Chemical biology approaches to probing and engineering megasynthases. Z. Ye, G. Williams


519. Photochemically Controlled DNA Computation. A. Prokup, J. Hemphill, A. Deiters


523. Studying Bacterial Indole Signaling via Biofilm Modulators. **M. J. Minvielle**, C. A. Bunders, C. Melander


525. Fluorescence and kinetic investigation of the binding of bisphenol A to mammalian dehydrogenases. **H. L. Price**, L. Lux

526. Regulation of microRNA miR-21 and miR-122 with small molecule inhibitors. **C. M. Connelly**, S. Myoung, M. Thomas, A. Deiters


528. *In vitro* photodynamic inactivation of pathogenic yeast strains. **X. Situ**, R. A. Ghiladi


530. Universal caging group for in cell detection of glutathione transferase applied to $^{19}$FNMR and bioluminogenic probes. **M. Ito**, A. Shibata, H. Abe, J. Zhang, R. Morgenstern, S. Shuto, Y. Ito

531. Design of a ratiometric fluorescent sensor for monitoring metal homeostasis in cells. **D. M. Besse**, K. J. Franz

532. Prochelator strategy to fight infection. **M. E. Helsel**, R. Festa, D. J. Thiele, K. J. Franz

533. New role for Vitamin B$_{12}$: Spatiotemporal control of oxidative damage due to hydroxyl radicals. **T. A. Shell**, D. S. Lawrence

534. Probing the kinome: Tools to study different signaling pathways. **J. R. Shell**, D. S. Lawrence


540. Structural and dynamics studies of FCCH domain. **M. Jaremko**, L. Jaremko, A. Ejchart

541. Adaptation of enzyme to different thermal conditions studied by NMR spectroscopy. **L. Jaremko**, M. Jaremko, P. Bayer, A. Ejchart


**Center for Solar Fuels (UNC EFRC) Poster Session III**

**Materials for Solar Fuels (Posters on display Wednesday through 5 pm on Thursday)**

Raleigh Convention Center
Ballroom A

T. Meyer, *Organizer*

2:40 - 3:20

545. Uncovering molecule-TiO₂ interactions with nonlinear spectroscopy. S. Miller, **P. Giokas**, K. Hanson, A. Moran

546. Calculating the electronic structure of large molecular systems via hypercontraction density fitting: an O(L⁴) CISD algorithm. **N. Shenvi**, H. Van Aggelen, W. Yang


551. Solvothermal synthesis and characterization of a new cuprous niobate single crystal and nanoparticle from a lithium niobate precursor. **J. Choi**, P. A. Maggard


556. Flux Synthesis and Photoelectrochemical Properties of p-Type CuNb3O8 and Cu2Nb8O21 Polycrystalline Films. **N. B. King**, P. A. Maggard

557. BiVO4 films for photoelectrochemical water splitting. **S. K. Holland**, D. Lawrence, T. C. DeVore

558. Metal oxynitride photocatalysts for water splitting: shape dependent catalytic properties. **K. Senevirathne**, R. Williams, A. Lachgar

559. Scanning electrochemical microscopy (SECM) of hydrogen photogenerated from platinized photosystem I modified electrodes. **D. Cliffel**, G. LeBlanc, G. Chen, K. G. Jennings


563. Structural and electronic properties of bare and capped Cd33Se33/Cd33Te33 nanoparticles. **A. E. Kuznetsov**, D. N. Beratan


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570. Crystal-Chemistry and Band Engineering in the System LiNb3O8-CuNb3O8. **P. P. Sahoo**, P. A. Maggard

571. pH effects on structure and morphology for cobalt (II) 2,9-dimethyl-1,10-phenanthroline sol-gel material hybrids. **E. M. King**, C. Taylor, M. Bertino


**Materials Chemistry II**

Raleigh Convention Center
304

M. ter Horst, *Organizer*
J. Poler, *Presiding*


4:00 576. Onset of aggregation of SWCNTs by coordination complexes. A. A. Ameen, **J. C. Poler**
THURSDAY EVENING

Analytical Chemistry Poster Session
Posters are presented from 7:00 to 8:00

Raleigh Convention Center
Ballroom B/C

Y. Yingling, Organizer

5:00 - 8:00


579. Chromatographic study of the vapors generated from melted soy beads. R. K. Zyglocke, C. E. Dahm

580. Electron transfer between small Au monolayer protected clusters. T. M. Carducci, R. W. Murray

581. Nanoparticle-doped xerogel amperometric glucose biosensors. M. H. Freeman, J. R. Hall, M. C. Leopold

582. Trace element mapping and quantitation in dried blood spots by wavelength dispersive x-ray fluorescence and sector-field inductively coupled plasma mass spectrometry. A. C. McWilliams, F. X. Weber, A. S. Essader, J. E. Medlin, A. A. Martin, K. E. Levine


588. Taking the Lab to the Field: Handheld Chemical Analysis in an Industrial Setting. J. R. Clarkson

589. Monitoring the effects of acute L-DOPA treatment on dopamine dynamics with fast-scan cyclic voltammetry at carbon-fiber microelectrodes. L. Qi, M. Spanos, L. A. Sombers

590. Quantifying omega-3 fatty acids in the yolks of chicken eggs using HPLC. S. E. Porter, J. M. Skelton, M. Bacher

591. Going greener in achiral & chiral separations: Employing sustainable technologies to reduce our environmental impact. R. M. Schmidt, C. S. Ponder, L. A. Miller, Y. Zhao

592. Photodegradation mechanism of vardenafil, the active ingredient in Levitra. L. Herbert, W. Cory


594. Investigation of the products of cetirizine solar photodegradation. A. Jenkins, W. Cory

595. Isolation of aptamer-bound thrombin using Capillary Transient Isotachophoresis and fraction collection. K. R. Riley, S. Saito, J. Gagliano, C. L. Colyer

596. Effects of L-DOPA on Dopamine Kinetics in Rat Striatal Brain Slices. E. Evbuomwan


599. Viscosity sensing based on the modulation of magnetically modulated optical particles (MagMOONs). K. T. Nguyen, J. N. Anker

600. In situ measurement of effective pH during SFC chromatography. R. J. Robinson, V. Nguyen, I. Scherer

601. Quantification of palladium contamination by using a 1.5min LC method. Y. Zhao, M. Lewandowski, E. Wentz, M. Villeneuve, L. Miller

Quantification of Fenton Chemistry. O. Banerjee, L. A. Sombers

Comparison of electrospray and nano-electrospray ionization sources for use with differential ion mobility spectrometry coupled to mass spectrometry. B. G. Santiago, G. L. Glish

Quantitative Proteomics Using SILAC to investigate the Immunomodulatory effects of Echinacea purpurea. N. B. Cech, V. Kandhi, D. C. Muddiman, S. M. Laster, S. M. Randall

CE-LIF analysis of intact marine microbes along with their constituent proteins and pigments. B. A. Vaughan, C. L. Colyer


Spectroscopic characterization of metal coordination complexes of active pharmaceutical ingredients encountered during pharmaceutical product development. B. Johnson, C. Goss, A. Wolters, K. Facchine

Application of Hydrogen-Deuterium Exchange/Mass Spectrometry(HDX/MS) for Determination of Cytochrome c Orientation on Self-Assembled Monolayers. Y. Hu


Probing site-specific optoelectronic and structural properties of doped semiconductors. M. Behl, S. L. White, P. K. Jain

Biomaterials Poster Session
Posters are presented from 6:00 to 7:00

Raleigh Convention Center
Ballroom B/C

Y. Yingling, Organizer

5:00 - 8:00

Peptide and phytohormone based building blocks as biomaterials. I. A. Banerjee, K. R. Fath, S. N. Barnaby, N. Nakatsuka

Hydrogen-bonded multilayers of silk fibroin: From coatings to shaped microcontainers. V. Kozlovskaya, B. Godin, X. Liu, E. Kharlampieva


616. Synthetic optimization and characterization of a biologically compatible poly(3,4-ethylenedioxythiophene)/alginate composite. **C. Yore**, T. Hanks

617. Characterization and optimization of biosensing diacetelyne liposomes fabricated via inkjet technology. **C. Wright-Walker**, M. Evans, T. Hanks, C. Hansen

618. Mechanically processed biologically derived biomaterial. **D. Hugar**, A. Ivanisevic

619. Rapid Diagnosis of Specific Antigen using CNT- Field Effect Transistors Direct Binding Assay. **J. K. Park**, Y. Hong, S. Choi, S. Chung


624. Effect of solvent on structure and function of *Candida antarctica* Lipase **B. H. Kim**, S. Ha, L. Sethaphong, Y. Koo, Y. Yingling
Electroanalytical Chemistry Poster Session  
Posters are presented from 7:00 to 8:00

Raleigh Convention Center  
Ballroom B/C  

Y. Yingling, Organizer

5:00 - 8:00


626. Quantifying contributions from ionic and electrical conductivity in thin films. J. A. Shetzline, J. Oh, S. E. Creager

627. Characterization of Q88K dehaloperoxidase: Controlling protein/electrode binding mechanism through site-directed mutation of a surface residue. T. K. Chen, E. F. Bowden


Energy and Fuels Poster Session  
Posters are presented from 6:00 to 7:00

Raleigh Convention Center  
Ballroom B/C  

Y. Yingling, Organizer

5:00 - 8:00

630. Studying metal-to-metal charge transfer tunability in Ti\textsuperscript{IV}/Mn\textsuperscript{II} \(\mu\)-oxo bridged heterobimetallics using Ti\textsuperscript{IV} \(\beta\)-diketiminato (NacNac) and Mn\textsuperscript{II}Salen complexes and derivatives. E. M. Goggins, W. W. Weare


633. Theoretical analysis of the Energy Transfer kinetics in Ru-Os Metal Organic Frameworks. J. LIN, P. Zhang, D. N. Beratan

634. Switching between Energy Transfer and Electron Transfer in Chromophoric Polymer Supported Ru(II) Light-harvesting Assemblies. L. Wang, E. Puodziukynaite, K. S. Schanze, J. R. Reynolds, J. M. Papanikolas

635. Uncorrelated energy transfer in pigment-protein complexes. C. Lin, A. Kell, M. Reppert, R. Jankowiak

636. GPC Analysis of Lignin and Lignin Oxidation Products. J. Mobley, N. Patil, R. Pace, M. Crocker, M. Meier

637. Electrocatalytic Carbon Dioxide Reduction by Metal-Organic Frameworks (MOFs). M. Whiting

638. Synthesis and characterization of early transition metal d^1 heterobimetallic systems for applications in solar energy conversion. A. J. Francis, W. W. Weare

639. Composite nanofibers for increased lithium-ion anode performance. M. Dufficy, P. Fedkiw, S. Khan

640. Novel materials for direct conversion of methane to methanol. L. M. Douglas, M. A. Lail, M. Pavani, J. R. Carpenter, P. Sharma

641. Controlling protein photoreduction by a quantum dot via modulation of protein interaction with quantum dot surface. B. Chica, B. Dyer

Polymer Chemistry Poster Session

Posters are presented from 6:00 to 7:00

Raleigh Convention Center
Ballroom B/C

Y. Yingling, Organizer

5:00 - 8:00

642. Ultrathin multilayer hydrogels for selective detection of amino acids. O. Zavgorodnya, V. Kozlovskaya, W. Higgins, A. Stanishevsky, E. Kharlampieva


649. Self-reinforced PCL/PCL composites. **A. Gurarslan, J. Shen**


652. Synthesis of alternating copolymers consisting of $N$-octyldodecyldithieno[2,3-b;7,6-b]carbazole and $N$-octylthieno[3,4-c]pyrrole-4,6-dione units for photovoltaic applications. **Y. YANG**, Y. Lim, S. Lee, Y. Lee


659. Changes in UV light absorption and emission of copolyesters during accelerated weathering. **A. Detwiler**
Understanding molecular motion of chemically tailored silicone elastomers. **K. Xu**, M. Roman, J. Bochinski, L. Clarke, J. Willoughby


Functionalizing and nucleating effects of Cyclodextrins on electrospun PCL nanofibers. **G. Narayanan**, A. Tonelli


**Plenary Talk: Royce W. Murray, UNC Chapel Hill**

Raleigh Convention Center
Ballroom A

L. Horne, R. Wightman, *Organizers*
J. Sweedler, *Presiding*

Vendor Exposition
8:30 a.m. – 5:00 p.m. Ballrooms B/C

Graduate School Fair
8:30 a.m. – 5:00 p.m. Ballroom Lobby

Events and Activities
12:00 p.m. – 1:30 p.m.
SERMACS Industrial Innovation Award Luncheon.
Speaker: Dr. Buck Goldstein, UNC Entrepreneur-in-Residence, “Engines of Innovation: The Entrepreneurial University in the Twenty First Century” (Ticketed event)

2:30 p.m. – 3:30 p.m.
ACS District Director’s Ice Cream Social

6:00 p.m. – 9:00 p.m.
SERMACS Awards Reception and Plenary Lecture.
Speaker: Joseph M. DeSimone, UNC Chapel Hill and North Carolina State University. “Research Alone is Not Enough: Opportunities for Chemists in Uncertain Times” (Ticketed event sponsored by Eastman Chemical)

Short Courses and Workshops
8:30 a.m. – 12:30 p.m., 1:30 p.m. – 5:00 p.m.
ACS Career Services Workshops:
    Speed Networking (8:30 - 12:30)
    Planning Your Job Search (8:30 - 9:30)
    Preparing a Resume’ (9:30 - 11:00)
    Effective Interviewing (11:00 - 12:30)
    Resume’ Reviews (1:30 - 5:00)

8:40 a.m. – 12:00 p.m.
Government Relations and Science Policy

1:00 p.m. – 5:00 p.m.
Career Connections Glass Office

1:00 p.m. – 4:00 p.m.
SENCER Workshop: Backward Course Design

41st Southeastern Magnetic Resonance Conference (SEMRC)
8:35 a.m. – 12:20 p.m.
    Structure and Dynamics by NMR/EPR I

8:20 a.m. – 12:20 p.m.
    Membrane Proteins and Peptides

1:30 p.m. – 3:00 p.m.
    SEMRC Poster Session

3:00 p.m. – 5:10 p.m.
    NMR/EPR Methods/Materials
    Contrast Methods/MRI
Friday - 16 November 2012 continued

Poster Presentations
9:00 a.m. – 11:30 a.m.
  Medicinal Chemistry
  Undergraduate: Inorganic, Organic, Organometallic

2:00 p.m. – 4:30 p.m.
  Chemical Education
  Undergraduate: Computational, Environmental, Materials, Physical, Polymer

Technical Sessions
8:00 a.m. – 12:20 p.m.
  Advanced Materials – Surface and Interfacial Chemistry  204
  Analytical Chemistry I  305B
  Atmospheric Chemistry: Gas-Particle Interactions and Climate Change I  301B
  Chemical Biology: Chemical Answers to Biological Questions I  306A
  Chemical Education I  206
  Chemistry of Bio-Nano Interfaces II  301A
  Energy and Fuels  205
  Entrepreneurial Chemistry: Academia/Industry Interactions I  402
  Frontiers in Chemistry and Medicine III  303
  Frontiers in Nucleic Acid Chemistry I  302C
  Instrumentation and Applications for Future MS III  302A
  Microorganisms: Organic Chemists Culture I  305A
  MS Information: Static Knowledge or Driving New Scientific Innovations  302B
  Organic Chemistry III  203
  Photochemistry  304
  Vendor Seminars  307

Technical Sessions
1:00 p.m. – 5:20 p.m.
  Atmospheric Chemistry: Gas-Particle Interactions and Climate Change II  301B
  Chemical Biology: Chemical Answers to Biological Questions II  306A
  Chemical Education II  206
  Chemistry of Bio-Nano Interfaces III  301A
  Dye-sensitized Solar Cells I  302B
  Emerging Environmental Contaminants MS IV  302A
  Energy and Fuels II  205
  Entrepreneurial Chemistry: Academia/Industry Interactions II  402
  Frontiers in Chemistry and Medicine IV  303
  Frontiers in Nucleic Acid Chemistry  302C
  Microorganisms: Organic Chemists Culture II  305A
  PAT and Chemometrics  305B
  Undergraduate I: Analytical, Bioanalytical  202
  Undergraduate II: Biochemistry, Biomedical  203
  Undergraduate III: Organic, Organometallic  204
Saturday Summary – 17 November 2012

Events and Activities
8:00 a.m. – 11:00 a.m.
SERMACS Regional Board Meeting

12:00 p.m. – 1:30 p.m.
Undergraduate Awards and Scholarships Luncheon
Speaker: Marty St. Clair, GlaxoSmithKline
“Thirty Years of HIV Drug Development: A Message of Hope”
(Ticketed event)

12:00 p.m. – 1:30 p.m.
ACS CHED Regional Award for Excellence in High School Teaching Luncheon
Speaker: Dr. Brian Thomas, RTI International,
“Detection of Designer Drugs and Formulations”
(Ticketed event)

Short Course and Workshops
9:00 a.m. – 12:00 p.m.
Career Connections

11:00 a.m. – 12:00 p.m.
Chemistry Demonstration

2:00 p.m. – 4:00 p.m.
Chemistry Demonstration Workshop

Graduate School Fair
8:30 a.m. – 5:00 p.m

41st Southeastern Magnetic Resonance Conference (SEMRC)
8:20 a.m. – 12:25 p.m.
Structure and Dynamics by NMR/EPR II

1:30 p.m. – 3:00 p.m.
SEMRC Poster Session

3:00 p.m. – 5:55 p.m.
NMR/EPR New Methods

Poster Presentations
9:00 a.m. – 11:00 a.m.
Project SEED and High School
Undergraduate: Analytical, Bioanalytical, Biochemical, Biomedical

2:00 p.m. – 4:30 p.m.
Agricultural and Food Chemistry, Bioanalytical,
Chemical Toxicity, Environmental, Materials, Nucleic Acid,
High School Programs

8:00 a.m. – 11:00 a.m.
- High School and ACS Project SEED Oral Presentations 305A
- High School Teacher Program Orientation with LEARN NC (invitation only) 304

9:00 a.m. – 11:00 a.m.
- High School and ACS Project SEED Poster Presentations 305B
  Panel Discussion: Preparing Students for College Chemistry 304

12:00 p.m. – 1:30 p.m.
- ACS CHED Regional Award for Excellence in High School Teaching Luncheon 304
  Speaker: Dr. Brian Thomas, RTI International, “Detection of Designer Drugs and Formulations”
  (Ticketed event)

1:20 p.m. – 5:00 p.m.
- ACS Project SEED Best Practices: What Works? 305A

3:00 p.m. – 6:00 p.m.
- High School Teacher Program Continued 304

Technical Sessions

8:00 a.m. – 12:30 p.m.
- Analytical Chemistry II 306B
- Chemistry of Bio-Nano Interfaces IV 306A
- Dye-sensitized Solar Cells II 302B
- Environmental, Agricultural, and Food Chemistry 302A
- Frontiers in Nucleic Acid Chemistry III 302C
- Undergraduate IV: Computational/Environmental 203
- Undergraduate V: Inorganic/Physical Chemistry 204
- Undergraduate VI: Materials/Polymer Chemistry 205

1:00 p.m. – 5:00 p.m.
- Bioanalytical Chemistry I 306B
- Chemistry and Applications of Colorants in the 21st Century 306A
- Chirality in Agrochemicals 302C
FRIDAY MORNING

Frontiers in Nucleic Acid Chemistry I
It's an RNA World

Raleigh Convention Center
302C

D. Graves, Organizer
L. Williams, Presiding

7:50 Introductory Remarks.

8:00 666. Ribonucleotide Incorporation during DNA Replication and Its Consequences. T. Kunkel


9:40 Coffee Break, Posters and Exposition.


11:00 671. Ironing out the RNA World. L. Williams

Analytical Chemistry I

Raleigh Convention Center
305B

M. ter Horst, Organizer
J. Grinias, Presiding

8:00 672. IR and NIR methods for chemical process monitoring from lab to plant. C. A. Goss, K. Amponsah-Manager, S. J. Sisk, B. R. Crump


9:00 675. Pillar arrayed chips for planar separation and detection. **T. Kirchner**, N. Crane, C. Freye, N. Lavrik, M. Sepaniak


9:40 Coffee Break, Posters and Exposition.


11:00 679. Speciation and Determination of Vanadium compounds using UPLC-ICP-SFMS and UPLC-ICP-QMS. **N. Kilibarda**, K. Levine, F. Yan, S. Afton


**Chemical Education I**

Raleigh Convention Center
206

M. ter Horst, Organizer
C. Siburt, Presiding

8:00 682. Specialty advising—why and how. **S. Myers**, T. Crute


8:40 684. Development and implementation of guided inquiry experiments for physical chemistry. **R. M. Whitnell**, S. S. Hunnicutt, A. Grushow

9:00 685. Too Much Information: Reducing Content and Increasing Impact in Your Chemistry Course. **K. Cossey**, J. K. Padden Metzker
9:20  686. Teaching intervention to promote visualization skills in an inorganic context. M. T. Oliver-Hoyo, H. Schiltz

9:40 Coffee Break, Posters and Exposition.


10:40  688. Development of a Biginelli MCR cascade in the organic chemistry lab. W. A. Wallace

11:00  689. Reducing lecture and increasing impact in an organic I course: Redesign and implementation. K. Cossey

11:20  690. Infusing forensic science into undergraduate chemistry laboratory curriculum. T. M. Gerald, F. Yan, F. W. Lewallen, J. Ellenson

11:40  691. Overcoming challenges in teaching organic chemistry to non-majors. V. J. Mukku

Entrepreneurial Chemistry: Academic/Industry Interactions I
Assistance for Entrepreneurs
Raleigh Convention Center
402

Sponsored by ACS Division of Small Chemical Business, ACS Local Section Corporate Grants
S. Kulkarni, Organizer, Presiding

8:00  692. What Makes an Entrepreneur? R. D. Thomas

8:20  693. Opportunities in Entrepreneurship for Scientists and Engineers. C. J. Oldham

8:40  694. What's behind the Business Plan? R. Debo

9:00  695. Outsourcing the drug discovery and development services- Challenges and opportunities. B. Venepalli

9:20 Coffee Break, Posters and Exposition.

10:00  696. Incubators for Chemical Entrepreneurs. R. Closner


10:40  698. Innovation, Entrepreneurship and Chemistry: support from SCHB / ACS. M. S. Chorghade
Chemical Biology: Chemical Answers to Biological Questions I

Raleigh Convention Center
306A

Supported by North Carolina Biotechnology Center, CEM, GlaxoSmithKline, ACS Division of Biological Chemistry, Glen Research
Sponsored by ACS Division of Organic Chemistry, NC State University Department of Chemistry
P. Thompson, Organizer
A. Deiters, Organizer, Presiding

8:15 Opening Remarks.

8:20 699. The Role of CXCR4 Modulators in Controlling HIV Entry, Inflammation and Certain Types of Cancer. D. C. Liotta

9:00 700. Selective Chemical Approaches to Probe Cysteine Redox Biology. K. S. Carroll

9:40 Poster Talk 1.

9:50 Coffee Break, Posters, and Exhibition.

10:20 701. Small molecule suppression of antibiotic resistant phenotypes. C. Melander

11:00 702. Development of proof-of-concept chemical probes targeting novel biological targets. W. R. Roush

11:40 Poster Talk 2.

Frontiers in Chemistry and Medicine III: Novel Approaches for Peptide Drug Discovery

Raleigh Convention Center
303

Sponsored by GlaxoSmithKline
M. Bishop, Organizer
V. Srivastava, Organizer, Presiding

8:15 Introductory Remarks.

8:20 703. Omontys (peginesatide): from discovery to approval of a PEGylated dimeric EPO receptor agonist for the treatment of anemia in CKD patients on dialysis. C. P. Holmes

9:00 704. Chemoselective strategies for the synthesis of proteins and labeling of nanoparticles. P. Dawson
9:40 Coffee Break, Posters and Exposition.

10:15 Introductory Remarks.

10:20 705. Stapled Peptide Drugs: Platform to Pipeline. T. K. Sawyer

11:00 706. Guanylate Cyclase C: A Target for the Treatment of Functional Intestinal Disorders. M. G. Currie

11:40 Concluding Remarks.

Advanced Materials- Surface and Interfacial Chemistry for Sustainable Innovation

Raleigh Convention Center
204

Supported by MeadWestVaco
J. Jur, J. Willoughby, Organizers, Presiding

8:20 707. Withdrawn

8:40 708. The Targeted Synthesis of Single Site Heterogeneous Catalysts. C. Barnes, J. Abbott, N. Chen

9:00 709. Amphipathic Films for Water Collection. J. Lee, T. Sundaresan


9:40 Coffee Break, Posters and Exposition.

10:20 711. Silicone Materials for Improved Efficiency and Durability of Photovoltaic Modules. A. Norris, B. Ketola, N. Powell

10:40 712. Probing trap dynamics of CdS quantum dots using temperature-dependent TRPL. D. Woodall, M. Guericke, M. Jones

11:00 713. Surface modification of lignin and hydrophobic substrates by adsorption of soy proteins. C. L. Salas, O. J. Rojas, M. A. Hubbe, L. Lucia

11:20 714. Viewing Solid-Liquid Catalytic Interfaces with Attenuated Total Reflection Infrared Spectroscopy. C. T. Williams
Atmospheric Chemistry: Gas-Particle Interactions and Climate Change - I

Raleigh Convention Center
301B

Sponsored by RTI International
R. Jayanty, Organizer, Presiding

8:20 715. Toward a greater understanding of the global impacts of mineral dust aerosol: Atmospheric chemistry, climate, biogeochemistry and health. V. Grassian


9:40 Coffee Break, Posters and Exposition.


Mass Spectrometry III: Instrumentation and Applications for the Future

Raleigh Convention Center
302A

Sponsored by ThermoFisher Scientific
G. Glish, Organizer, Presiding


8:55 720. Insights into ion trap resonance ejection using graphic card based trajectory simulations. P. M. Remes

9:30 721. Laser desorption/ionization mass spectrometry (LDI-MS) for the multiplexed tracking and imaging of nanoparticles in biological samples. B. Yan, Z. Zhu, V. M. Rotello, R. W. Vachet

10:05 Coffee Break, Posters and Exposition.

11:00 723. Structural mass spectrometry strategies for deciphering systems biology. J. A. McLean


Mass Spectrometry Informatics: Static Knowledge or Driving New Scientific Innovations?
Raleigh Convention Center
302B
A. J. Williams, Organizer, Presiding


8:40 726. Supporting Medicinal Chemistry and Lead to Hit Screening in Pharmaceuticals – A project of result accuracy, automation, infrastructure, time to result and reducing complaints. M. A. Bayliss, M. Führ, U. Jagusch, S. Oberbörsch

9:00 727. High-throughput metabolomics: Applications in mass spectrometry automation. C. DeHaven, A. Evans

9:40 Coffee Break, Posters and Exposition.

10:20 728. Considerations for automated data processing of high resolution LC/MS data. T. R. Croley, A. M. Knolhoff, J. Simpkins, S. Murphy, M. Bayliss

10:40 729. Model-driven statistical analysis of isobaric tag data. J. Hoefkens, P. Haberl, A. Ceroni

11:00 730. How simple can new mass spectrometry software be for complicated analyses? G. A. McGibbon, V. Lashin, A. Aminov

11:20 731. Structure verification and elucidation using the ChemSpider database. A. J. Williams, V. Tkachenko, A. Pshenichnov

Microorganisms: Organic Chemist's Culture

Raleigh Convention Center
305A

Sponsored by ACS Division of Organic Chemistry
Supported by Mycosynthetix, Teledyne ISCO
N. Oberlies, Organizer, Presiding

8:20 Introductory Remarks.

8:30 732. New perspectives on the diversity, distributions, and applications of endophytic fungi. A. Arnold

9:30 733. The history and chemistry of one of the world's largest fungal libraries. C. Pearce

10:10 Coffee Break, Posters and Exposition.

11:10 734. Eroding a Pathogen's Defenses by Disrupting Candida Biofilms with Fungal Natural Products. R. H. Cichewicz

Photochemistry

Raleigh Convention Center
304

Sponsored by the Physical Chemistry Division of the ACS and the Inorganic Chemistry Division of the ACS
M. Forbes, Organizer, Presiding


9:20 737. Upconversion photochemistry: Sensitized triplet fusion. F. N. Castellano

9:40 738. Computational studies of the hole transfer in oxidized porphyrin dyads: The role of non-coplanar conformation. E. Jakubikova

10:00 Coffee Break, Posters and Exposition.

**11:00 740.** Experimental determination of the reorganization energy for spin-state conversion in six-coordinate Fe(II) complexes. A. M. Brown, L. L. Jamula, J. K. McCusker*

**11:20 741.** Trifluoropropynyl as a surrogate for the cyano ligand and intense room temperature phosphorescence from one of its rhodium(III) complexes. P. S. Wagenknecht, C. Sun, P. U. Thakker, L. Khulordava

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**SEMRC - Membrane Proteins and Peptides**

Raleigh Convention Center
306C

Sponsored by NC State University Department of Chemistry, Doty Scientific
Supported by Bruker Biospin EPR Division, North Carolina Biotechnology Center, National High Field Magnet Laboratory, Cryogenic Limited, Norell, Wilmad Lab Glass, Sigma-Aldrich Isotec, New Era Enterprises, Cambridge Isotope Laboratories
A. Nevzorov, I. Nesmelova, Organizers

**8:20 742.** Combining Structural Restraints from Oriented Sample and Magic Angle Spinning Spectroscopy for Membrane Protein Structures. T. A. Cross

**9:00 743.** Structure and oligomerization of Anabaena Sensory Rhodopsin determined by solid state NMR spectroscopy. V. Ladizhansky, S. Wang, R. Munro, L. Shi, T. Okitsu, A. Wada, K. Jung, S. Kim, L. S. Brown


**9:40 745.** Tertiary structural models for a three helix membrane protein in a bilayer environment from aligned sample solid state NMR data. D. T. Murray, J. Griffin, I. Hung, T. A. Cross

**9:55** Coffee Break, Posters and Exposition.

**10:20 746.** Peptide Amphiphile Macromolecular Assembly. A. K. Mehta, L. Li, R. Ni, S. Childers, D. Lynn

**10:45 747.** NMR and EPR studies of protein-mediated lipid organization, structure, and dynamics in lung surfactant. J. R. Long, S. Farver, A. Kuznetsova, A. Turner, G. Fanucci

**11:10 748.** Site-directed spin labeling reveals multiple modes for regulating protein-protein interactions in bacterial outer membrane transport. D. S. Cafiso

**11:35 749.** Structure, dynamics, and membrane binding of NOD peptides: a spin-labeling EPR study. M. Quinones, V. A. Bankaitis, T. I. Smirnova
11:50 750. Ionic strength modulates β-barrel membrane protein loop dynamics and interactions and dramatically affect NMR spectra quality. R. H. Lo, D. A. Fox, L. M. Columbus


SEMRC - Structure and Dynamics by NMR/EPR Session 1
Raleigh Convention Center
306B
Sponsored by NC State University Department of Chemistry, Doty Scientific
Supported by Bruker Biospin EPR Division, North Carolina Biotechnology Center, National High Field Magnet Laboratory, Cryogenic Limited, Norell, Wilmad Lab Glass, Sigma-Aldrich Isotec, New Era Enterprises, Cambridge Isotope Laboratories
A. Nevzorov, I. Nesmelova, Organizers


9:00 753. Small molecule directed studies of enzyme dynamics. A. L. Lee, M. J. Carroll, R. V. Mauldin

9:25 754. Actin binding is allosterically linked to vinculin tail domain dimerization and actin filament bundling through a kinked helix. P. M. Thompson, S. L. Campbell

9:40 755. Effects of Altered Salt-bridge Formation on HIV-1 Protease Flap Conformational Sampling. X. Huang, J. L. Kear, G. E. Fanucci

9:55 Coffee Break, Posters and Exposition.


11:10 758. Characterization of the electronic structure of P450 compound I. A. Silakov, E. Onderko, C. Krest, M. T. Green

11:35 759. Evidence for Two Oxygen Induced Radical Intermediates in nNOS using Pulsed EPR. A. A. Cruce, M. D. Kryzyaniak, A. Tsai, V. Berka, M. K. Bowman


**Government Relations and Public Policy**

Raleigh Convention Center
202

M. ter Horst, *Organizer*
R. Davison, *Presiding*

8:40 Federal Policy Update. **R. Davison**, ACS Advocacy Manager

9:00 Report from Raleigh, TBD

9:20 Questions and answers

**Chemistry of Bio-Nano Interfaces II**

Raleigh Convention Center
301A

Y. Yingling, A. Smirnov, *Organizers, Presiding*

8:40 762. Epitope presentation using gold nanoparticles for immunoassay development and in vivo studies. **D. Cliffel**, A. Agrawal, A. Travis


9:40 Coffee Break, Posters and Exposition.


11:00 765. Electrostatics of bio- and nano-materials' interfaces by EPR of pH-sensitive nitroxides. **M. A. Voynov**, A. I. Smirnov

**Energy and Fuels I**

Raleigh Convention Center
205

M. ter Horst, *Organizer*
A. Schrand, *Presiding*
8:40 766. Withdrawn


9:20 768. Structural evidence for inter-residue hydrogen bonding observed for cellobiose in aqueous solution. W. B. O'Dell, D. C. Baker, S. E. Mcclain

9:40 769. Photoelectrochemical Performance of CdS Electrodeposited on Nanostructured Ti Nanowires Decorated with Gold Nanoparticles. Z. Shan, S. Pan

10:00 Coffee Break, Posters and Exposition.

10:40 770. Deoxygenation of guaiacol and anisole over carbon-supported Pd and Re catalysts. S. T. Thompson, H. H. Lamb

11:00 771. Metal Traps for Mitigating Vanadium in Fluid Catalytic Cracking. S. Sithambaram

11:20 772. Quantum dots as tools for catalytic initiation of hydrogenases and multi-electron enzyme reduction. B. L. Greene

11:40 773. Optimizing cattail microwave pre-treatment before enzyme treatment to produce cellulosic biofuel and biobased organic compounds via saccharification. J. Emrani, A. Shahbazi

**Medicinal Chemistry Poster Session**

Posters are presented from 9:30 to 11:00

Raleigh Convention Center
Ballroom B/C

Y. Yingling, Organizer

9:00 - 11:30


778. Synthesis and Characterization of Opioid Peptides with a Head-to-Side Chain Lactam Cyclization and Halogen Substitution at the Para Position of Phenylalanine. **C. Flowers, A. Wormsbecher, S. Hutchison, E. Williamson, K. R. Wilson**


784. Synthesis, antioxidant and antimicrobial properties of substituted N-(5-methylisoxazol-3yl)cinnamides. **M. Kuchana**


789. Computational design and development of non-ATP competitive inhibitors targeting the cyclin binding groove of cell cycle CDKs. **P. N. Premnath, T. Perkins, S. Liu, C. McInnes**
790. Evaluation of synergism from combination of some cyclopeptides and antibiotics. J. Dumond, L. Rudd, J. Rigaud, M. Ngu-Schwemlein


792. Fungal blood: Natural products chemistry of an endophytic *Penicillium* sp. (G85) from milk thistle (*Silybum marianum* (L.) Gaertn.). M. Figueroa, N. H. Oberlies


795. High resolution MS, MS/MS and UV library of fungal secondary metabolites as a dereplication protocol for bioactive natural products. T. El-Elimat, B. M. Ehrmann, N. B. Cech, C. J. Pearce, N. H. Oberlies

796. Minimizing the environmental footprint of natural product extracts. R. Bukhari

797. Toxins and Beyond - Chemical Investigations of *Microcystis* Blooms in the Cape Fear River. J. Isaacs, A. Barbera, M. McIver, M. Mallin, W. K. Strangman, J. L. Wright

798. Multidisciplinary approaches for the isolation of new chemistry from marine actinomycetes. A. K. Stewart, E. Skellam, J. L. Wright


Organic Chemistry III

Raleigh Convention Center
203

M. ter Horst, Organizer
A. E. Gorden, Presiding

9:00 800. Enantioselective Synthesis of Biphenols, Bismurrayaquione: A “Traceless” Chirality Relay Approach. F. Guo


10:00 Coffee Break, Posters, and Exhibition.

10:40 803. Use of 3-methoxy N-acylpyrazinium salts towards the synthesis of praziquantel. A. L. Williams, V. R. St. Hilaire

11:00 804. One-step diastereoselective synthesis of bis-furan alcohol of Darunavir and Brecanavir: Dramatic impact of fluoro alcohols on selectivity. S. Xie, B. E. Cooley, J. A. Corona, T. C. Lovelace, A. Millar, Y. Zhang


Undergraduate Poster Session: Inorganic Chemistry
Odd numbered posters are presented from 9AM to 10AM; Even numbered posters are presented from 10AM to 11AM

Raleigh Convention Center
Ballroom B/C

I. Shin, Organizer

9:00 - 11:00


809. Reaction of nitromethane with a Pd(II) acetate thiacrown supported complex. L. Keller, J. P. Lee, G. J. Grant

810. Synthesis and characterization of potentially chemotherapeutic gold(III) compounds involving thiacrown ethers. D. Colangione, G. J. Grant, J. P. Lee

811. Ligand-assisted oxygen reduction reaction in (nitro)cobaltpfluorophthalocyanine: a cyclic voltammetry and DFT computational study. J. Simmons, R. Kimble, T. Risher, E. Magee, J. A. Goodwin

812. Unique properties of U(VI) demonstrated in metal mediated synthesis of 2,3-diaminophenazine. K. S. Lynn, B. A. Maynard, A. E. Gorden
Effect of an iron(II) chelator on the growth rate of *Escherichia coli* under oxidative stress in the presence of ascorbate and desferrioxamine. **A. Eid, M. C. McDonald, J. I. Wirgau**

Water soluble N-confused tetraphenylporphyrin. **P. Salehi, A. Stovall, J. L. Shaw**

Synthesis and coordination studies of Si(bipy)2(dpca)2+. **D. A. Lee, S. K. Moon, A. N. Sizeland, N. W. Gould, T. A. Schmedake**

Photophysics of phosphorescent trifluoropropynyl complexes. **L. Khulordava, C. Sun, P. S. Wagenknecht**


Catalytic activity of copper(II) and nickel(II) complexes with N-[3-trimethoxysilyl)propyl]ethylenediamine. **B. O. Adaka, P. R. Alburquerque**

Controlled Formation of Metal Silicate Monolayers on Silicon Surfaces. **D. Bume, C. Barnes**

Synthesis of halogen bonded complexes through ball-milling. **A. kropilak, T. Hanks**

Synthesis and luminescence of an EDTA-based terbium chelate with capsaicinoid antennae. **J. Bullock, B. Johnson, C. G. Gulgas**


Heterobimetallic systems containing hexacoordinate chromium complexes. **J. Nguyen, T. Lekich, A. Francis, W. W. Weare**

Chemical Tuning of the charge transfer characteristics of Zn(II) polypyridyl thiol complexes. **M. E. Mundy, D. R. Striplin**

Cation binding selectivity and cooperative ion-pair binding of PAIn, a synthetic ion-pair receptor. **C. Okrah, A. Contractor, F. A. Khan, M. Fujita**

Metal-organic frameworks utilizing fluorous ligands. **W. Lenox, S. Hickman, J. Kelley, L. Peterson, Jr., M. D. Smith, H. zur Loye**

Exploring Metal Binding Properties of SIH-related Chelators. **K. P. Martinez, D. Besse, K. Franz**

Investigation of an Axial Pyridine Ligand for the Surface Immobilization of Cobaloxime Catalysts. **C. S. Eubanks, M. S. Hambourger, D. E. Wheeler**
Undergraduate Poster Session: Organic Chemistry
Odd numbered posters are presented from 9AM to 10AM; Even numbered posters are presented from 10AM to 11AM

Raleigh Convention Center
Ballroom B/C

I. Shin, Organizer

9:00 - 11:00

829. New one-pot reductive workup procedure for sec- and tert-alcohol Grignard adducts. J. M. Gibson, H. V. Clontz, M. I. Moore, A. P. Honeycutt


831. Reactions of benzaldehyde in boiling water. B. E. Belachew, C. E. Dahm


833. The Impact of Conjugation Length on Benzobisazole Cruciforms. A. Tomlinson, C. Collins

834. Progress towards the synthesis of a pyrimidodiazepine-based folate as a potential inhibitor of glycinamide ribonucleotide formyltransferase. M. Aminou, L. Gonzalez, P. S. Ray

835. Addition of thiols to electron-deficient cyclopropanes catalyzed by a calcium (II) complex. A. M. Shema, C. M. Braun, K. Nolin

836. Synthesis of 2-amino-7-benzyl-6-hydroxy-7H-purin-8(9H)-one derivatives as a potential inhibitors of folate requiring enzymes. E. E. Brazil, P. S. Ray

837. Design and synthesis of sphingosine kinase inhibitors with improved bioavailability. L. M. Mount, T. Grattan

838. Design and synthesis of modified sphingosine kinase inhibitors to improve oral bioavailability. S. R. Woodson, T. Grattan


841. Investigation of the Differences in Reaction Time and Peptide Purity in a Head-to-Side Chain Lactamization of Opioid Peptides Containing Either Glutamic Acid or Aspartic Acid. A. Wormsbecher, C. Flowers, S. Hutchison, E. Williamson, K. R. Wilson


844. Synthesis of 2,3,6,11-Tetrabromo-1,4-naphthacenedione. W. J. Collier, R. Martin, S. Miao

845. Tandem Meyer-Schuster Rearrangement-Conjugate Addition Reactions Catalyzed by a Re(V)-oxo Complex. A. E. Garst, A. D. Badiceanu, K. A. Nolin

846. Progress Towards the Synthesis of a Donor-Acceptor Complex. L. Harvey, A. Coffman

847. Aldehydes to Lactones: A synthetic strategy towards asymmetric lactones. B. Weaver, S. Franz, R. Watkins, G. Gumina, B. Feske

848. Progress towards the synthesis of a temperature-responsive polyethylene glycol dendron. M. R. Achard, A. H. Coffman


850. Sophomore Organic Laboratory Experiment: Acid-base Extraction and Isolation integrated with Spectral Analysis. K. Banerjee, B. Bill


855. Development of o-vanillylidene anilines for application in the high school laboratory. S. N. Ganrude, C. G. Gulgas


857. Synthesis of a new indole chalcone. C. M. Bridges, H. L. Holt

Isolation of lactams from a classical 2-aminopyrrole synthesis. **E. K. Hong**, C. E. Stephens

Internal conformational elements to force lactamizations in the synthesis of bis-hetero-2,5-diketopiperazines. **K. A. Martin**, K. Ha

Microwave Dehydration of Tertiary-Butyl Alcohol. **J. R. Wells**, M. B. Wells

Abiotic Synthesis of Nucleobases in Alternative Solvents. **P. Lee**, G. Springsteen

Colorimetric Boronic-Acid-Based Sugar Sensors. **G. Gaydos**, G. Springsteen

Total synthesis of hibiscone C. **J. L. Efird**, W. L. Packer

Sensory and Chemical Differences Between Naturally and Artificially Carbonated Beer. **M. Kerestes**, E. Allain

Highly Efficient Synthesis of Tropane Skeleton. **r. smitherman**

Liquid Chromatographic Approach to Study of Suwannee River Humic Acid Adsorptive Fractionation and Desorption Interactions with Anion Exchange Resin. **R. R. Joyce**, S. S. Sutton, D. Kreller


**Undergraduate Poster Session: Organometallic Chemistry**

Odd numbered posters are presented from 9AM to 10AM; Even numbered posters are presented from 10AM to 11AM

Raleigh Convention Center
Ballroom B/C

I. Shin, *Organizer*

9:00 - 11:00

Synthesis of Ru(II) bromide complexes supported by bis(pyrazolyl)acetic acid: Intermediates to potential olefin hydroarylation catalysts. **M. Trivitayakhun**, S. Kennedy, M. Sharma, N. Tyler-Hashemi, B. Quillian

Fluorescent imidazolium salts and their corresponding NHCs: Synthesis and characterization. **D. Tapu**, Z. **McCarty**, L. **Hutchinson**


**Undergraduate Oral Presentations: Biochemistry/Biomedical Chemistry**

Raleigh Convention Center
203

I. Shin, *Organizer*
J. Pierce, *Presiding*

1:00 **873.** Making musical serialism using mass spectrometry and nuclear magnetic resonance. **L. Tomlinson**, C. Fuller, S. S. Pierce

1:20 **874.** Uncovering the link between Bcl-2 proteins and chemoresistance. **R. E. Wilson**, V. Del Gaizo Moore

1:40 **875.** Characterization of Manganese-dependent ribonucleotide reductase from Coryneform ammoniagenes. **C. Seacrist**, P. Riggs-Gelasco

2:00 **876.** Investigation into ROS oxidation products of dopamine. **A. Fischer**, K. Matera

2:20 **877.** Determination and alteration of the loci of aggregation in amyloid beta and insulin. **K. Knaus**, K. Matera

2:40 Coffee Break, Posters and Exposition.

3:20 **878.** Honeycomb electrospun fiber scaffold for expending cancer stem cells. **J. Hsieh**, X. Duan, Q. Wang

3:40 **879.** BCL-2 protein regulation of apoptosis in diabetic cardiomyopathy. **K. M. Van Dalfsen**, V. Del Gaizo Moore

4:00 **880.** Inhibitory effects of Congo red dye on amyloid-beta plaque formation. **A. Helman**

4:20 **881.** Inhibition of the HMGA A/T hook. **E. Hardy**, K. Buchmueller

4:40 **882.** Assessment of apoptotic protein modifications during cellular stress. **J. A. Crum**, V. Del Gaizo Moore
FRIDAY AFTERNOON

SERMACS Industrial Innovation Award Luncheon and Keynote Lecture
Honoring Awardee Christian Melander, NCSU and Agile Science

Raleigh Convention Center
402

S. Kulkarni, *Organizer, Presiding*

12:00 883. Engines of Innovation: The Entrepreneurial University in the Twenty-First Century. **B. Goldstein**

Frontiers in Nucleic Acid Chemistry II
Nucleic Acid Damage and Repair

Raleigh Convention Center
302C

D. Graves, *Organizer*
K. Hayden, *Presiding*

1:00 884. Structures of human exonuclease I complexes with DNA suggest a common mechanism for 5' nuclease family. E. McSweeney, J. Orans, R. Iyer, Y. Shi, M. Hast, H. Hellinga, P. Modrich, **L. Breese**

1:40 885. RNA ligation by the Schistosoma hammerhead ribozyme in frozen solution. **L. Lie**, R. M. Wartell

2:20 886. The enzyme G4 Resolvase 1 (G4R1), the protein product of the DHX36 gene, specifically binds and unwinds DNA and RNA quadruplex structures. P. J. Smaldino, E. D. Routh, S. A. Akman, **J. P. Vaughn**

2:40 Coffee Break, Posters and Exposition.


4:20 889. Major groove DNA bis-alkylation products arising from diepoxiybutane. **M. P. Stone**

5:00 Wrap-Up of Day 1.
Undergraduate Oral Presentations: Analytical/Bioanalytical Chemistry

Raleigh Convention Center
202

I. Shin, Organizer, Presiding

1:00 890. GC-MS, UV-VIS, and HPLC analysis of nicotine in e-cigarette filling solutions. J. M. Justice, A. R. Balestrino, C. R. Dockery, G. E. Potts

1:20 891. Determination of explosives in aqueous solution using electrochemiluminescence quenching. C. L. Smith, K. D. Sienerth

1:40 892. Natural product toxin effects on fission yeast as observed by imaging flow cytometry. J. Heisler, L. Elvir, E. Charles, R. Pyati

2:00 893. Quantification of dye-mediated photodamage during single-molecule DNA imaging. C. F. Dial, M. A. Tycon, C. J. Fecko

2:20 Coffee Break, Posters and Exposition.


3:40 896. Investigation of sample matrix effects using spinning sampling chamber laser ablation ICPMS. M. W. Boyce, J. L. Malloy, S. E. Long

4:00 897. Development of a rapid covalent-labeling and mass spectrometry-based technique to study the mechanism of aggregate inhibition of Beta-amyloid (1-40). J. W. Griffin, P. A. Martino

Undergraduate Oral Presentations: Organic/Organometallic Chemistry

Raleigh Convention Center
204

I. Shin, Organizer
G. Wahl, Presiding

1:00 898. Synthesis of a Large Dihydroheteroacene. D. J. Stone, S. Miao


2:00 901. Reversible hydroboration of stilbenes and stilbenoids favoring the E-isomer. **L. E. Rabenold**, E. E. Gray, B. C. Goess


2:40 Coffee Break, Posters and Exposition.


3:40 904. Chromophores Built on a 1,4-Fluorenylene Scaffold. **M. K. Burdette**, S. El Homsi, B. J. Laughlin, R. C. Smith


**Frontiers in Chemistry and Medicine IV: Drug Delivery- Biologics and Small Molecules**

Raleigh Convention Center
303

Sponsored by GlaxoSmithKline
C. Gersbach, V. Srivastava, **Organizers**
S. Lai, **Organizer, Presiding**

1:15 Introductory Remarks.


2:00 908. Micromolded Particle Engineering for Therapeutic Drug Formulation and Delivery. **P. Mack**

2:40 Coffee Break, Posters and Exposition.

3:15 Introductory Remarks.
3:20 909. Genetically engineered polypeptide nanoparticles for drug delivery. A. Chilkoti

4:00 910. Living cells as drug delivery vehicles for CNS delivery. E. V. Batrakova, M. J. Haney, Y. Zhao, S. Li, N. Klyachko, R. Mosley, H. E. Gendelman, A. V. Kabanov

4:40 Panel Discussion.

5:10 Concluding Remarks.

Atmospheric Chemistry: Gas-Particle Interactions and Climate Change - II

Raleigh Convention Center
301B

Sponsored by RTI International
R. Jayanty, Organizer, Presiding


2:00 912. Agricultural Air Quality: Emissions, Consequences, And Management. V. P. Aneja

2:40 Coffee Break, Posters and Exposition.

3:20 913. Understanding the Aerosol Particle Nucleation and the Aerosol Direct Radiative Forcing at A Forest Site in the South East United States. P. R. Pillai, V. P. Aneja

4:00 914. Characterization of fine particulate matter (PMfine) in urban areas of Pakistan. A. Rasheed, V. P. Aneja, A. Aiyyer, U. Rafique

Chemical Biology: Chemical Answers to Biological Questions II

Raleigh Convention Center
306A

Supported by North Carolina Biotechnology Center, CEM, GlaxoSmithKline, ACS Division of Biological Chemistry, Glen Research
Sponsored by ACS Division of Organic Chemistry, NC State University Department of Chemistry
A. Deiters, Organizer
P. Thompson, Organizer, Presiding

1:20 916. Using rapid chemical kinetics to probe biological systems. K. Chang, R. W. Alexander


2:40 Poster Talk 3.

2:50 Coffee Break, Posters and Exposition.

3:10 918. Catalyzing chemical biology through strategic compound sets. W. Zuercher

3:50 919. A chemical biology route for imaging, isolation and culturing of cancer stem cells. X. Duan, Q. Wang

4:30 Poster Talk 4.

4:40 Break.

5:00 920. Thiostrepton: New Tricks for an Old Antibiotic. W. L. Kelly

5:40 921. Examining the interplay between the LSD1 histone demethylase and the estrogen receptor alpha in breast cancer pathobiology using chemical biology approaches. D. McCafferty

6:20 Concluding Remarks.
Chemical Education II
Raleigh Convention Center
206

M. ter Horst, Organizer
D. Canelas, Presiding

1:20 922. Developing a Study Abroad course in Historical Aspects of Chemistry. R. C. White, J. H. White

1:40 923. Teaching the history of chemistry as a civilizations and cultures class with e-portfolio. D. Y. Pharr

2:00 924. Creative writing exercises in the general chemistry curriculum. D. W. Carpenetti II

2:20 925. Providing a global perspective for science students. M. Z. Hoffman

2:40 926. Engaging students with art-based activities: an NSF-TUES sponsored endeavour. A. C. Gaquere-Parker

3:00 Coffee Break, Posters, and Exhibition.

3:40 927. How to use the book African American Women Chemists to teach chemistry and history. J. E. Brown

4:00 928. Development and assessment of an introductory chemistry course for students with limited backgrounds in chemical problem solving. D. A. Canelas, R. A. MacPhail

4:20 929. Creative Exercises: Creative student-centered testing in traditional and active classrooms. D. G. Sauder, S. E. Lewis

4:40 930. Four experiment series for use in a one semester chemistry course for health professionals. T. J. Fuhrer

5:00 931. Moved to Thursday 11:20 am, Room 302B. ChemIDplus, a public chemical information database at the U.S. National Library of Medicine (NLM). G. F. Hazard, M. A. Miller, S. M. Jordan, J. C. Fang, C. Lan
Dye-sensitized Solar Cells I
Raleigh Convention Center
302B
A. El Shafei, Organizer, Presiding


2:05 934. Charge transfer processes with {001} facet-dominating anatase TiO$_2$ in dye-sensitized solar cells. M. Maitani, Y. Wada

2:25 Coffee Break, Posters and Exposition.


3:25 936. Earth-abundant solar cells: Can iron complexes serve as photosensitizers in DSSCs? E. Jakubikova


Energy and Fuels II
Raleigh Convention Center
205
M. ter Horst, Organizer
X. Fan, Presiding

1:20 938. Synthesis and characterization of early transition metal d$^1$ heterobimetallic systems for applications in solar energy conversion. A. J. Francis, W. W. Weare


2:00 940. Interfacial nano-scale modification of photoanodes for the optimization of parameters of dye-sensitized solar Cells. T. Luitel, F. P. Zamborini

2:40 Coffee Break, Posters, and Exhibition.

3:20 942. Evaluation of catalysts for hydrogen production: The importance of extracting the efficiencies for each reaction in photochemical water reduction systems. B. Shan, **R. Schmehl**

3:40 943. Printable CIGS thin films for solar cells. **X. Fan**, T. Samples

4:00 944. ZnO 3D hierarchical nanostructures for photocatalysis application. **J. Zhao**, Q. Yang, X. Zhang, A. Bagal, C. Chang, G. N. Parsons

**Microorganisms: Organic Chemist's Culture II**

Raleigh Convention Center  
305A

Sponsored by ACS Division of Organic Chemistry  
Supported by Mycosynthetix, Teledyne ISCO  
N. Oberlies, **Organizer, Presiding**

1:20 945. Bioactive natural products from targeted fungal groups: some recent highlights and insights. **J. B. Gloer**

2:20 Coffee Break, Posters and Exposition.

3:00 946. Poisons, Peptides and Polyethers: A tale of toxins. **J. L. Wright**

**SEMRC - Poster Session Friday**  
**Friday Posters Presenting/ALL Poster Viewing**

Raleigh Convention Center  
North Hallway, 306 B/C Lobby

A. Nevzorov, A. Smirnov, I. Nesmelova, **Organizers**

1:30 - 3:00

947. Microscopic properties of the amorphous solid mesophase in frozen sucrose-water solutions revealed by electron paramagnetic resonance techniques. **H. Chen**, L. **Sun**, K. Warncke

948. NMR study of binding interface in chemokine heterodimer. **S. A. Patil**, L. N. Mukhamedova, I. V. Nesmelova


951. Steady-state and time-resolved EPR investigation of nanostructures in catanionic mixtures of SDS/DTAC. L. E. Jarocha, M. D. Forbes

952. HYSCORE measurements of the astaxanthin carotenoid radical cation on solid supports. A. Magyar, A. Focsan, M. Krzyaniak, L. Kispert

953. HIV-1 membrane analysis by multi-frequency EPR at 9, 95 and 240 GHz. L. Yu, H. Van Tol, L. Song


955. Site-specific structural determination of human proinsulin within bacterial inclusion bodies by MAS-ssNMR and REDOR. E. P. Vogel, D. P. Weliky


957. Effects of lipid composition on bilayer insertion of transmembrane helices of CesA. L. Li, M. A. Voinov, A. I. Smirnov

958. Dark-stable multiline EPR signal from the calcium-depleted oxygen evolving complex of photosystem II. A. Haddy, B. M. Ore, R. A. Reed


961. Solid-state MAS NMR study of the proton transfer heart - His37 tetrad in M2 full length protein. Y. Miao, H. Qin, R. Fu, T. A. Cross


963. NMR in the physical chemistry lab: H- bonding in dilute solutions of methanol - acetone. T. C. DeVore, A. C. Bagley
964. Characterization of Rainwater DOC by 1D and 2D NMR Techniques. P. J. Seaton, O. Brennan, R. J. Kieber, J. D. Willey, G. B. Avery

965. Magnetization enhancement in static solids and uniaxially diffusing membrane proteins at low RF powers: Adiabatic transfer vs. repetitive cross polarization. S. N. Koroloff, W. Tang, A. A. Nevzorov

966. Local structure and global patterning of Cu^{2+} binding in fibrillar amyloid-β protein. W. A. Gunderson, J. Hernández-Guzmán, J. W. Karr, L. Sun, V. A. Szalai, K. Warncke

967. Aromatic carbon clusters in thermally-treated lignocellulosic biomass. J. Park, K. Lim, O. J. Rojas, S. Park

968. NMR solution structure of Opa60: a Neisserial membrane protein that mediates host phagocytosis. D. A. Fox, L. Columbus

969. NMR Studies of Aggregation of Organic Dyes. C. J. Lopez, J. D. Walls

970. Protein structure determination from challenging sets of RDCs using REDCRAFT. M. Simin, H. Valafar

971. Does the gold nano particle conjugation affect the structure of the bombesin peptide: A 2D NMR study. T. L. Mackey

Chemistry of Bio-Nano Interfaces III
Raleigh Convention Center
301A

Y. Yingling, A. Smirnov, Organizers, Presiding

1:40 972. Mapping of the Properties of Inner Limiting Membranes from Human Eyes. A. Ivanisevic


2:40 974. Protein scaffold for tunable nano-structured biohybrid materials. N. A. Carter, T. Z. Grove

3:00 Coffee Break, Posters and Exposition.

3:40 975. Small, Soft, and Electric: The next generation of biomedical materials. C. J. Bettinger

Process Analytical Technology and Chemometrics

Raleigh Convention Center
305B

Sponsored by Mettler Toledo Autochem
F. Vogt, Organizer, Presiding

1:40 977. Using chemometrics and ambient mass spectrometry for oncometabolomics diagnostics applications. A. Gray, C. Jones, T. Long, M. Monge, J. McDonald, F. Fernandez


3:00 Coffee Break, Posters and Exposition.


4:00 981. Recent advancements in organic chemistry: In situ reaction analysis. S. Rea, B. Wittkamp


4:40 983. Camera as an Analytical Instrument: From simple to process control. R. L. McGill

Chemical Education Poster Session
Posters are presented from 2:30 to 4:00

Raleigh Convention Center
Ballroom B/C

Y. Yingling, Organizer

2:00 – 4:30

984. Electrophoretic Analysis of Lysozyme Modifications Induced By Chloro-p-benzoquinone. A. Zyglewska, C. Cho, J. Kim

985. Comparison of high school dual-enrollment and traditional introductory chemistry class outcomes. D. R. Zuidema

987. Applying cognitive science to study how students develop understanding of the practice of chemistry. **J. Dunn**, S. Cullipher, S. M. Landge, H. Sevian


989. Developing Young Scientists. **A. Loch, K. E. Martin**, T. J. Boyle, B. A. Hernandez-Sanchez, J. Brinker, C. Ashley, R. A. Kemp, W. F. Hammetter, A. Tapia


991. Use of worksheets as study aids in an introductory organic chemistry course. **M. E. Yacuzzo, M. T. Gallardo-Williams**

992. Isomer enumeration: An exercise in group theory. **T. S. Whiteside**, C. W. Padgett


994. Organic solvent miscibility in the water-acetic acid system. **J. W. Hall**, C. E. Phipps


996. Council on Undergraduate Research: A faculty development organization. **R. E. Bachman**

997. Approximations in general chemistry. **E. M. Epp**

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**Entrepreneurial Chemistry: Academic/Industry Interactions II**

**Entrepreneurs in Action**

Raleigh Convention Center

402

Sponsored by ACS Division of Small Chemical Business, ACS Local Section Corporte Grants

S. Kulkarni, Organizer, Presiding

2:00 998. The SCYNEXIS Story: From Small Spin Out To Global Leader. **Y. J. Ribeill**

2:40 999. Serial Entrepreneurship: Lessons Learned. From Chemir to Avomeen. **S. Thanedar**

3:20 Coffee Break, Posters and Exposition.

4:00 1000. Agile Sciences, From Academic Discovery to Building a Commercialization Entity. **C. C. Melander**

**Mass Spectrometry IV: Emerging Environmental Contaminants**

Raleigh Convention Center  
302A

S. Richardson, G. Glish, *Organizers, Presiding*


2:40 1004. The detection and fate sucralose in the aquatic environment. **R. N. Mead**

3:00 Coffee Break, Posters and Exposition.


**Undergraduate Poster Session: Computational Chemistry**

Odd numbered posters are presented from 2PM to 3PM; Even numbered posters are presented from 3PM to 4PM

Raleigh Convention Center  
Ballroom B/C

I. Shin, *Organizer*

2:00 - 4:00

1008. Hydroxamate Linker Results in Fastest Interfacial Electron Transfer Rates in Fe(bpy)$_2$(CN)$_2$ – Sensitized Solar Cell. **L. J. Barnes**, D. N. Bowman, E. Jakubikova

1010. DFT study of eroxocarbonate relevant to oxygen reduction in solid oxide fuel cells. **K. Haines**, C. Qin

1011. Computational study of synergistic effects of chlorine and fluorine as catalysts for fullerene formation. **C. Pregot**, T. J. Fuhrer

1012. Computational and crystallographic studies of N-oxide halogen bonds. **S. Bailey**, C. W. Padgett

1013. Understanding the genetic predispositions to Parkinson's disease: A computational model of the impact of L449S nsSNP in the histamine H1 receptor. **B. T. Nguyen**, Z. Zhang, E. Michonova-Alexova


1018. Any systematic differences between x-ray crystallography and NMR determined protein structures? a case study. **S. A. Nance**, X. Tao

Undergraduate Poster Session: Environmental Chemistry
Odd numbered posters are presented from 2PM to 3PM; Even numbered posters are presented from 3PM to 4PM

Raleigh Convention Center
Ballroom B/C

I. Shin, Organizer

2:00 - 4:00

1020. Biosorption of mercury from aqueous solutions utilizing highly characterized peats. A. M. Rizzuti, K. A. Wilson

1021. Spatial variation of volatile organic compounds associated with gas production operations in southwestern Pennsylvania. B. L. Mitchell, B. Miller, R. Swarthout, Y. Zhou, B. C. Sive

1022. Synthesis, Characterization, and Catalytic Activity of Core Shell Fe₃O₄@C Nanoparticles. C. A. Arnott, C. Deshmane, M. Wright, A. Lachgar


1024. Analysis of trichloroethene (TCE) accumulation by hybrid poplar trees planted in soil and grown hydroponically at a property contaminated with TCE. L. Svetlova, J. Wilcox, S. A. Wasileski


1028. Solid phase micro-extraction (SPME) to extract polar haloacetamides from drinking water. B. D. Jessie, C. N. Dalton

1029. Development of a protein-based system for the detection of organophosphates using the pH dependence of enhanced green fluorescent protein. A. Henson, J. Harris, L. Puckett

Undergraduate Poster Session: Materials Chemistry
Odd numbered posters are presented from 2PM to 3PM; Even numbered posters are presented from 3PM to 4PM

Raleigh Convention Center
Ballroom B/C

I. Shin, Organizer

2:00 - 4:00

1030. A comparison of SAM formation on mica using a variety of alcohols. J. R. Klecker, L. L. Wright, T. Hanks
1031. A comparison of SAM formation of carboxylic acids on mica and glass. M. Milkovska, L. L. Wright, S. Arrowood

1032. Structural analysis of Bosch heated exhaust gas oxygen sensors after voltage treatments. R. Blackman, A. Alshowaier, E. P. Murray

1033. Surface modifications of alginate-conducting polymer composites. K. Hajny, H. Gordhan, T. Hanks

1034. Leakage of encapsulated fluorophores from polydiacetylene liposomes. E. Nyers, C. Wright-Walker, T. Hanks

1035. Photoelectrochemical performance of tungsten doped BiVO₄ films. M. Dutter, S. K. Holland, D. Lawrence, T. C. DeVore

1036. Redox and spin state control of bis-terpy Fe(II) via steric & inductive influence of ligand substituents. C. Pasko, H. Wallace, S. Slattery


1041. In-situ synthesis and characterization of conjugated polymer/carbon nanotube materials. H. P. Barrett, D. S. Boucher


1043. Metal flavonolate complexes for luminescent liquid crystal applications. K. C. Hall, P. J. Pryor, T. A. Bradshaw, D. J. Timmons

1044. Extending the flavone core to construct liquid crystals. R. S. Dilley, A. M. Gernhardt, D. J. Timmons

1045. Lignin as a material platform for bio-derived macromolecules and fibers. M. Wilt, M. Mazloumpour, O. Rojas, J. Willoughby

1046. Surface chemistry on upconverting particles for cell targeting. S. E. Neville, J. Ayres, M. Therien
1047. Impact of solvent on the interactions between poly(methyl methacrylate) and a single walled carbon nanotube. **C. E. Davy**, S. Tallury, M. A. Pasquinelli


Also includes **1218.** Characterization of $p$-GaAs$_{1-x}$Bi$_x$ and $p$-InP semiconductors for photoelectrochemical water splitting. **E. Brahm**, T. Deutsch

**Undergraduate Poster Session: Physical Chemistry**
**Odd numbered posters are presented from 2PM to 3PM; Even numbered posters are presented from 3PM to 4PM**

Raleigh Convention Center
Ballroom B/C

I. Shin, **Organizer**

2:00 - 4:00


1051. Assembling graphene layers to create plate, parallel plate, and double parallel plate models to represent molecule-pore interactions. **M. C. Trentle**, T. R. Rybolt, M. J. Rice, H. E. Thomas


1053. Investigating the effects of trioctylphosphine (TOP) ligand on the fluorescence dynamics of CdSe quantum dots. **K. M. Dipple**, M. Jones, A. Tobias, M. Guericke


1057. Toward controlled polymer self-organization in solution. **C. E. Johnson**, D. S. Boucher


1061. Preparation and characterization of palladium, platinum, and ruthenium catalysts on alumina support. M. Anderson, L. Richardson, S. Ferguson, M. Boykin, C. Smith, A. Banerjee

1062. Understanding the steam reformation process of ethanol over an iron catalyst. P. J. Drew, J. T. Lyon

1063. Superoxide Production in Fructose Treated Hepatocytes. V. E. Nordman, H. Xu

1064. Charge Transfer Phenomena at the Molecular Donor/Acceptor Interface. K. E. Martin, J. Gao, J. K. Grey

1065. Molecular Dynamics Simulations of a Nanobiosensor Made From Bee Venom. S. Sadagopan, M. A. Pasquinelli


1068. Capillary Electrophoretic Studies of a Squarylium-Based Dye (SQ-BA) with Sugars. B. G. Taylor, C. L. Colyer

1069. Development of sensing systems to monitor the hydrolysis of β-lactam antibiotics. K. P. Rzasa, N. M. Reilly, L. G. Puckett
Undergraduate Poster Session: Polymer Chemistry

Odd numbered posters are presented from 2PM to 3PM; Even numbered posters are presented from 3PM to 4PM

Raleigh Convention Center
Ballroom B/C

I. Shin, Organizer

2:00 - 4:00

1070. Cross-linked Self-Assembled Monolayers as a Protective Overcoating for Silvered Telescope Mirrors. J. D. Askey, K. L. Brodhacker


1072. Poly(dimethylsiloxane) metal coordination polymer networks with ruthenium(II), copper(II), iron(II), or cobalt(II) tris(bipyridine) complex cross-links. M. A. Mcvannel, M. L. Pippin, K. M. Vailonis, M. G. Hyatt, A. D. Schwab

1073. Probing Diels-Alder adducts of anthracene and maleimide as mechanically active functional groups. M. G. Hyatt, Z. S. Kean, B. Lee, S. L. Craig

1074. Approaches toward a Triaryl Lactone. O. Diop, S. Mitchell, D. Thompson, ,. Sarden, K. Clark, K. S. Aiken


1077. Origami folding of polymer sheets by local light absorption. B. Shaw, Y. Liu, J. Genzer, M. D. Dickey

1078. Characterization Between Chemically Polymerized and Electropolymerized Polyaniline. T. M. Sprinkle, R. Gregory


1080. Formation and characterization of an inclusion complex (IC) between Poly (2-hydroxyethyl methacrylate) (PHEMA) and Gamma Cyclodextrin (γCD). I. P. Kichak, A. S. Joijode, A. E. Tonelli, J. Genzer
1081. Controlling the chain conformation of conjugated polymers. C. L. Smith, K. Plunkett

1082. Self-healing stretchable wires for reconfigurable circuit wiring and 3D microfluidics. S. M. Reece, E. Palleau, S. C. Desai, M. E. Smith, M. D. Dickey


1085. Molecular dynamics simulations of the interactions between a series of polythiophenes with single-walled carbon nanotubes. J. A. Moo-Young, M. A. Pasquinelli

SEMRC - Contrast Methods/MRI
Raleigh Convention Center
306C

Sponsored by NC State University Department of Chemistry, Doty Scientific
Supported by Bruker Biospin EPR Division, North Carolina Biotechnology Center, National High Field Magnet Laboratory, Cryogenic Limited, Norell, Wilmad Lab Glass, Sigma-Aldrich Isotec, New Era Enterprises, Cambridge Isotope Laboratories
A. Nevzorov, I. Nesmelova, Organizers

3:00 1086. MR studies of fatty tissues with hyperpolarized xenon gas. R. Branca

3:25 1087. ELECTRON SPIN RELAXATION IN MRI CONTRAST AGENTS. R. G. Bryant, G. Diakova

3:50 1088. Polarization-lifetime extension using singlet states in symmetric spin systems. T. Theis, Y. Feng, W. S. Warren


4:30 1090. MR Imaging of Impaired Pulmonary Gas Exchange with Hyperpolarized $^{129}$Xe. Z. I. Cleveland, M. S. Freeman, S. S. Kaushik, Y. Qi, B. Driehuys


5:00 1092. Magnetic nanoclusters with hydrophilic spacing for dual drug delivery and sensitive magnetic resonance imaging. N. Pothayee, N. Pothayee, S. Balasubramaniam, N. Jain, N. Hu, R. M. Davis, N. Sriranganathan, A. P. Koretsky, J. S. Riffle
3:00 1093. High-field EPR studies of molecular magneto-structural correlations under pressure. S. Hill, C. C. Beedle, K. Thirunavukkuarasu, C. Morien, S. W. Tozer, A. Prescimone, S. Parsons, E. K. Brechin, S. Winter, R. T. Oakley, J. A. Schlueter, J. L. Manson


SATURDAY MORNING

Analytical Chemistry II
Raleigh Convention Center
306B

M. ter Horst, Organizer
G. Potts, Presiding

8:00 1099. NIR monitoring and control of a constant volume distillation. B. E. Cooley

8:20 1100. Spectroscopic and Voltammetric Determination of Hemoglobin in Tooth and Bone. S. Hooper Marosek, A. Suroviec

8:40 1101. Probing intermolecular interactions in polyelectrolyte scaffolds for molecular assembly. A. Mallet, M. Bonizzoni


9:40 Coffee Break, Posters, and Exhibition.


10:40 1105. Hydrogen-bonding forces at the gas-surface interface: Methyl salicylate desorption from amorphous silica. J. Abelard, A. Wilmsmeyer, J. R. Morris

11:00 1106. Novel palladium-coated gold nanorod catalysts studied with super-resolution single molecule imaging. L. Zhao, P. Cobb, Y. Zhao, G. Wang


High School and Project SEED Student Oral Presentations

Raleigh Convention Center
305A

Sponsored by NIEHS and SERMACS
A. Tonelli, Organizer, Presiding

8:00 1109. Synthesis of novel HDAC6 inhibitors Tubastatin A and NQN-1. M. Zhou

8:15 1110. Effects of Human Serum Albumin Model Peptides on the oxidation state of copper. U. Nwanaji-Enwerem

8:30 1111. The Effect of the Gene Expression of Alleles on Penstemon neomexicanus and Penstemon barbatus Heterozygous F2s' Color. R. Smithwick


9:00 1113. Validation of SIS1 and FAS1 as Tamoxifen Targets. D. R. Bryant

9:15 1114. Determining the Role of the Sirtuin Deactylases in Saccharomyces cerevisiae on the Regulation of Metabolic Flux for Biofuel Production. M. V. Lucas

9:30 1115. Decadal Trend of Coastal Water Quality in Orange County Beaches and Management Efficacy at Improving Public Health Protection. S. Lim, Y. Jeong

9:45 Coffee Break, Posters and Exposition.

10:15 1116. Engineering a whole-cell calcium ion biosensor in yeast to detect signaling malfunctions as a rapid cancer diagnostic and potential therapy screening tool: in silico studies and beyond. W. J. Feng

10:30 1117. Synthesis, Morphology, and Optical Properties of ZnO Nanostructures for LEDs. K. D. Dawkins

10:45 1118. Using the photodecomposition of triarylsulfonium hexafluorophosphate salt to develop a novel method for fabricating and enhancing properties of conductive copper nanowire films. J. Howell
Undergraduate Oral Presentations: Polymer Chemistry/Materials Chemistry

Raleigh Convention Center
205

I. Shin, Organizer
D. Argyropoulos, Presiding

8:00 1119. MicroMRI transport study of polymer beacons for combined DNA delivery and image contrast. M. D. Boatwright, X. Wang, S. Kelkar, T. M. Reineke, L. A. Madsen


9:20 Coffee Break, Posters and Exposition.


10:20 1124. Characterizing electrochemical manipulation of eutectic gallium-indium in microchannels. C. Trlica

Frontiers in Nucleic Acid Chemistry III
It's Not Your Watson and Crick Nucleic Acids Anymore

Raleigh Convention Center
302C

D. Graves, Organizer
Z. Xu, Presiding

8:10 1125. Effects of 5-methylcytidine incorporation on i-motif-forming sequences of DNA. R. M. Wadkins, Y. P. Bhavsar-Jog, E. V. Dornshuld, G. S. Tschumper

8:40 1126. Interaction of PEG-PLL copolymers with DNA oligonucleotides. L. A. Marky, H. Lee, I. Khutsishvili

9:20 1127. Modified peptide nucleic acids. C. Achim, S. Bezer, J. Kong
10:00 Coffee Break, Posters and Exposition.


11:00 1130. RNA Dynamics at Atomic Resolution: Role in Gene Regulation by Riboswitch. Q. Zhang


12:20 Concluding Remarks.

Environmental, Agricultural and Food Chemistry

Raleigh Convention Center
302A

M. ter Horst, Organizer
K. Levine, Presiding


8:40 1133. Photochemical release of free and combined amino acids from resuspended sediments. J. C. Nguyen, G. B. Avery, R. J. Kieber, S. A. Skrabal, R. N. Mead, J. R. Helms

9:00 1134. Copper photodissolution from resuspended estuarine sediments. A. M. Wetterauer, S. A. Skrabal, R. J. Kieber, G. B. Avery, R. N. Mead

9:20 1135. Labile phosphorous levels in Kentucky soils amended with various biochar types. S. Burris, A. Reddy, C. Bolster

9:40 Coffee Break, Posters and Exposition.


SEMRC - Structure and Dynamics by NMR/EPR Session 2

Raleigh Convention Center
306C

Sponsored by NC State University Department of Chemistry, Doty Scientific
Supported by Bruker Biospin EPR Division, North Carolina Biotechnology Center, National
High Field Magnet Laboratory, Cryogenic Limited, Norell, Wilmad Lab Glass, Sigma-Aldrich
Isotec, New Era Enterprises, Cambridge Isotope Laboratories
A. Nevzorov, A. Smirnov, I. Nesmelova, Organizers

8:20 1138. EPR studies of natural and artificial water-oxidation catalysts. G. W. Brudvig

9:00 1139. Determinants of catalytic specificity in a DNA-modifying enzyme by DEER
spectroscopy. S. K. Saxena

9:25 1140. Local Structure and Global Patterning of Cu$^{2+}$ Binding in Fibrillar and Oligomeric
Forms of Amyloid-β Protein. K. Warnecke, J. Hernández-Guzmán, J. W. Karr, L. Sun, V. A.
Szalai, W. A. Gunderson

9:50 Coffee Break, Posters and Exposition.

10:20 1141. Site-specific monoubiquitination activates Ras by impeding GTPase activating
Locasale, L. C. Cantley, B. Kuhlman, H. G. Dohlman

10:45 1142. Role of protein disorder in substrate recognition by ubiquitin ligases. W. K. Nkari,
Schulman, J. D. Forman-Kay, T. Mittag

A. Mueller, E. F. DeRose, S. A. Gabel, L. C. Pedersen, M. J. Cuneo

11:35 1144. Characterization of dynamic processes in substrate recognition by cytochrome P450

12:00 1145. Structural and Biochemical Characterization of Allergens. G. Mueller, L. Pedersen,
L. Edwards, F. Lih, K. Tomer, J. Glesner, M. Chapman, A. Pomes, D. Ghosh, S. Gupta-
Bhattacharya, H. Haas, R. London
Chemistry of Bio-Nano Interfaces IV
Nanoparticles
Raleigh Convention Center
306A

Y. Yingling, A. Smirnov, Organizers, Presiding

8:40 1146. Probing non-covalent interactions between DNA and gold nanoparticles/nanoclusters at the single-molecule level. L. A. Peteanu, S. Chowdhury, S. Kumar, S. K. Dey, R. Jin

9:20 1147. Surface-mediated production of hydroxyl radicals as a mechanism of iron oxide nanoparticle biotoxicity. T. I. Smirnova, M. A. Voinov, A. I. Smirnov

10:00 Coffee Break, Posters and Exposition.

10:40 1148. Towards Intelligent Materials. D. Lynn

11:00 1149. SERS Nanoparticles: Large Scale Synthesis and their Applications in Diagnostics. J. Thomas

Dye-sensitized Solar Cells II
Raleigh Convention Center
302B

A. El Shafei, Organizer, Presiding

8:40 1150. Plasmonic nanoparticle Applications in solar energy conversion and in Nanomedicine. M. El-Sayed

9:20 1151. Nanostructured MoS₂ electrodes for polysulfide reduction in QDSSCs. S. T. Finn, J. E. Macdonald


10:00 Coffee Break, Posters and Exposition.


11:00 1154. DSSC Performance Properties of New Sensitizers Based on Heteroaryl Spacers. H. S. Freeman, B. Kim


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Undergraduate Oral Presentations: Computational Chemistry/Environmental Chemistry
Raleigh Convention Center
203
I. Shin, Organizer

8:40 1156. Role of deprotonation in flavonoid activity: A computational investigation. K. Smith, E. Williams, J. Metzker

9:00 1157. Halogen bonding interactions between group 14 halomethane analogues and Lewis bases. M. Tawfik, K. J. Donald


9:40 Coffee Break, Posters and Exposition.

10:20 1159. Analysis of humic acid interference on estrogenic activity using an estrogen-sensitive yeast assay. M. Bedard, V. Del Gaizo Moore, K. Sienerth


Undergraduate Oral Presentations: Inorganic Chemistry/Physical Chemistry
Raleigh Convention Center
204
I. Shin, Organizer
C. Eagle, Presiding


9:40 Coffee Break, Posters and Exposition.

High School Student Poster Presentations
Odd numbered posters are presented from 9AM to 10AM; Even numbered posters are presented from 10AM to 11AM

Raleigh Convention Center
Ballroom C
Y. Yingling, Organizer

9:00 - 11:00


1166. Investigating “natural” homemade soaps as effective alternatives to commercially available soaps using traditional wet chemistry techniques. J. M. Speer, M. A. Vu, D. M. Athavale, B. W. Corbett


1168. Investigation into thermal and rheological properties of oil-based CuO nanofluids: Applications in heat transfer. N. S. Mundkur, J. L. Tatarko, G. A. Willing


1170. Distribution and efferent projections of the galanin coexpressing subpopulation of the locus coeruleus. F. C. Ashworth, J. de Marchena, M. Halpin, P. Jensen


1173. Use of bioinformatics tools in amyotrophic lateral sclerosis (ALS) pathway analysis: Updates to KEGG pathway map. K. A. Morris

Preparing Students for College Chemistry Panel Discussion
Raleigh Convention Center
305B

9:00 AM to 11:00 AM
L. Coker, Presiding

Project SEED Poster Session
Odd numbered posters are presented from 9AM to 10AM; Even numbered posters are presented from 10AM to 11AM
Raleigh Convention Center
Ballroom C
A. Tonelli, Organizer

9:00 - 11:00

1175. American Chemical Society Project Seed Program at the University of South Carolina. C. Tang

1176. Construction of phenylethynylene macrocycles and experiments involving guest loading into macrocyclic hosts. C. Maddox, S. Salpage, L. Shimizu


1178. Application of Computational Chemistry in the SEED Program. R. Prabhakar

1179. Bis(picolyl)selone complexes of tin(IV). A. Fowler, B. L. Gray, D. Rabinovich

1180. Using the photodecomposition of triarylsulfonium hexafluorophosphate salt to develop a novel method for fabricating and enhancing properties of conductive copper nanowire films. J. Howell

1181. Synthesis of novel HDAC6 inhibitors Tubastatin A and NQN-1. M. Zhou

1182. Studies on the Self-Assembly of Achiral and Chiral Helical Polymer Nanocomposites Containing Graphene Oxide Nanoribbons. C. Evans, I. Khan, M. Gaines, X. Wang

1184. The Effect of the Gene Expression of Alleles on Penstemon neomexicanus and Penstemon barbatus Heterozygous F2's Color. **R. Smithwick**

1185. Synthesis, Morphology, Optical Properties of ZnO Nanostructures for LEDs. **K. D. Dawkins**

1186. Environmental effects on pollen-pistil incompatibilities in the genus Cakile. **K. E. Bunch**

1187. Effects of Human Serum Albumin model peptides on the oxidation state of copper. **U. Nwanaji-Enwerem**


1190. Probing the Bases of Polymer Glass Transitions. **M. Ndukwe**

1191. PCR based assay for evaluating MHC I expression in Zebrafish. **C. R. Rivera**

1192. Sustainability of cleaning Cellulose surfaces through computer simulations. **A. C. Sumner**, M. A. Pasquinelli


1194. Development of an efficient cycloaddition reaction towards the synthesis of 5-membered carbocycles. **A. Bethea**

1195. The Validation of SIS1 and FAS1 as Tamoxifen Targets. **D. R. Bryant**

1196. Determining the Role of the Sirtuin Deactylases in Saccharomyces cerevisiae on the Regulation of Metabolic Flux for Biofuel Production. **M. V. Lucas**

1197. The Determination of the Binding Affinity of the A3 Receptor for 3-Nitrotyrosine. **M. J. Reese**

Undergraduate Poster Session: Analytical/Bioanalytical Chemistry
Odd numbered posters are presented from 9AM to 10AM; Even numbered posters are presented from 10AM to 11AM

I. Shin, Organizer

9:00 - 11:00


1202. Understanding the Mechanism of Luminescence in Paint Concealed Bloodstains. A. Brown, B. Borowski, S. Parrish

1203. Electrodeposition of sol-gels for spectroelectrochemical sensing: Three modes of selectivity - one small device. J. Hayes, K. Warner, R. Dansby-Sparks

1204. Quantification of antibiotic release from a polymeric nanofiber mesh applicable to limb salvage. C. Quinn, M. Morgan, S. Symes, T. Currey

1205. Determination of the concentration of iron in local soil samples by atomic absorption spectrophotometry. W. A. Carter, R. Fietkau

1206. Analysis of municipal water by as a function of distance from the water treatment plant. C. O. Hale, R. Fietkau

1207. First and second derivative UV-Vis spectroscopy of potassium permanganate calculated and plotted using spreadsheet. S. C. Hawkins, R. Fietkau


1209. Degradation of a polymeric nanofiber mesh to be used in the treatment of bone repair. M. Morgan, C. Quinn, S. Symes, T. Currey

1210. Low cost instrumentation and procedures for electrochemical detection and quantification of metals. A. Shuey, J. C. Beimborn, E. N. Azoulay, K. Huff, J. S. Summers
1211. Measurement of L-Ascorbic Acid (Vitamin C) in oranges and orange juice using HPLC. A. Walker, A. Murray, G. G. Brown

1212. Silica nanoparticles as a carrier of fluorescence molecule. U. Kalapathy, M. O. Olagunju

1213. Automated spectrophotometric titrations and extraction of equilibrium constants. J. Hammond, J. A. Lynch

1214. Synthesis and Characterization of Branched Amino Acid Based Surfactants for the Separation of Chiral Compounds in Capillary Electrophoresis. F. Billiot, E. Billiot, M. Garza, J. Georgiadis

1215. Characterization of the particulate phase of mainstream hookah smoke. T. Oh, J. Annonio, C. D. Hauser

1216. Ambient ionization tandem mass spectrometry for the analysis of aerosols produced by the pyrolysis of natural products. C. A. Tyler, B. G. Santiago, S. E. Spencer, G. L. Glish


1218. Moved to Friday 2:00-4:00 pm, Ballroom B/C Characterization of $p$-GaAs$_{1-x}$Bi$_x$ and $p$-InP semiconductors for photoelectrochemical water splitting. E. Brahm, T. Deutsch

1219. Investigating ion transmission in differential ion mobility spectrometry. K. J. Stevens, S. L. Isenberg, G. L. Glish

1220. Probing the topography of rigid $\alpha$-conotoxin GI using a newly proposed mass spectrometry-based covalent labeling method. J. E. Denny, P. A. Martino


Undergraduate Poster Session: Biochemistry/Biomedical Chemistry
Odd numbered posters are presented from 9AM to 10AM; Even numbered posters are presented from 10AM to 11AM

Raleigh Convention Center
Ballroom C

I. Shin, Organizer

9:00 - 11:00


1224. Studies into the Mutagenic Potential of OdGTP using Nucleotide Analogues. M. Ghio, M. Hamm

1225. Investigations into the mutagenic potential of 8-oxo-2'-deoxyguanosine using nucleotide analogues. K. Kindler, M. Hamm, M. Lindell, C. Ligon

1226. Investigation of stem-loop DNA for potential use in SELEX. S. Boone, G. Springsteen, A. C. Spencer

1227. Solid-phase peptide synthesis and solid state NMR analysis of GRF (1-29). A. L. Corona, S. Wang, Y. Ishii

1228. Effects of a cavity-filling mutation in the enzyme choline acetyltransferase. C. D. Ester, D. Rodgers

1229. NMR-Based Metabolic Profiling of Different Tissues of Watermelon. J. O. Lee, M. Watanabe, K. Shaker, K. Chowdhury, A. Boroujerdi


1231. Investigations into the Mutagenic Potential of 8-Oxo-2'-deoxyguanosine with the Y-Family Polymerase Dpo4. J. S. Silberg, K. Crowley, M. Hamm

1232. Effects of pyridine nucleotide transferase activity by varying nitrile concentrations. H. M. Fogg, M. F. Santiago

1233. Regulation of Aspartate Transcarbamoylase from cells of Pseudomonas diminuta. L. E. Pedersen, M. F. Santiago

1234. Reactivity models for oxidative stress; Copper(II) complexes of 2-S-succinyl modified cysteine compounds. B. Hickman, B. M. Foster, J. S. Summers
Characterizing substrate-specificity in the aldo-keto reductase, YDL124w via modified Alanine-scanning mutagenesis. J. Hall, B. Stevenson, C. Poole, B. Feske, S. C. Mateer


Effects of varying trace metal concentrations on pyrimidine enzyme activities. H. N. Lynch, M. F. Santiago

Purple Urine Bag Syndrome: Regulation of pyrimidine enzymes by nitriles. A. N. Broadway, S. R. Whitson, K. B. Whitson, M. F. Santiago

Structure prediction using a homology model of YOL151W. P. T. Nguyen, M. West, S. C. Mateer, B. D. Feske, C. W. Padgett


Fmoc Solid Phase Synthesis of Circular Histone H4 Peptides for Epigenetic Enzyme Inhibition. J. Truong, L. Yan, B. Canup, K. Qian, Y. G. Zheng

Investigations into the mutagenic potential of 8-oxo-2'-deoxyguanosine using Polymerase β. E. J. Mcfadden, A. Weaver, M. Ghio, M. Hamm


The role the 4-methoxy analog of tetrahydrobiopterin plays in nitric oxide synthase. J. Lamkin, D. Little, A. Rogers

The role the 3-methyl analog of tetrahydrobiopterin plays in nitric oxide synthase. D. Little, L. Jonathan, A. Rogers


Alzheimer's Disease: Analysis of Amyloid-beta Aggregation. M. Dalgetty, K. Matera

Effect of the sonication of alpha-amylase during the hydrolysis of blue starch. B. Hussein, A. M. Arruda, A. C. Gaquere-Parker

Purification, characterization, and crystallization of inorganic pyrophosphatase from Thermococcus thioreducens. H. M. French, M. Morris, C. Wood, J. D. Ng

Changes in heat capacity as a probe for the competition between A/T hook and netropsin for DNA. C. Quandt, A. Gorensek, K. Buchmueller
1251. Expression of the Organic Anion Transporter in E.coli. S. M. Comadoll, J. P. Cecile

1252. Capillary Electrophoresis for the Detection of Drug Interactions with Organic Anion Transporters. B. Pearce, J. P. Cecile

1253. Characterization of manganese(III) and manganese(IV) porphyrin complexes with methoxide and imidazole ligands by UV-Vis absorption spectroscopy. L. Arnold, H. Swaffar, S. Zelman, G. B. Ray


1255. Generation of stable thin films of plant virus particles for stem cell research. L. Lucas

1256. Effect on anticoagulant activity of thrombin-binding aptamers by tethering them to DNA weave-tiles using flexible linkers. B. Goodfred, A. Rangnekar, T. H. LaBean

1257. Iron-sulfur cluster assembly and transport to apo-aconitase in the *Bacillus subtilis* SUF system. C. H. Bloomer, P. C. Dos Santos

1258. Monitoring and imaging hypoxic cells and tissues with perfluorinated near-infrared fluorescent micelles. K. Margita, S. Achilefu, R. Tang

1259. Docking studies of 2:1 DNA minor groove binder. R. Whitmire, L. Jobe, C. Bruce

1260. Delivery of paclitaxel with elastin-like polypeptides. C. Caudill, J. Bhattacharyya, A. Chilkoti


1262. Microbial fuel cell utilizing *Saccharomyces cerevisiae*. D. W. Goodlett


1264. Selectivity of human phosphatase, PPM1A (PP2C-alpha), towards artificial substrates. C. M. Loy, D. F. McCain

1265. Dynamic activity and crosstalk modeling with pheromone and glucose sensing pathways in *Saccharomyces cerevisiae*. Z. A. Duck, J. Brigati, G. Wilhite, S. Wright


1268. Ribonuclease Sa as a Model System for Measuring the Effects of Electrostatic Interactions in Denatured States. M. N. Newell, J. Myers
SATURDAY AFTERNOON

Chirality in Agrochemicals
Raleigh Convention Center
302A

Sponsored by BASF Crop Protection
E. Ulrich, W. McCall, Organizers, Presiding

1:20 1269. Chiral pesticides 101. E. M. Ulrich

1:40 1270. Chiral pesticides in chiral biological environments: Do we need to move beyond our achiral perspective? J. F. Kenneke

2:20 1271. Industry view on risk assessment of chiral pesticides. M. Radzom

3:00 Coffee Break, Posters and Exposition.

3:20 1272. Stereochemistry considerations can improve pesticide safety and sustainability. A. W. Garrison

4:00 1273. Consideration of chiral chemistry in Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) ecological risk assessments. J. A. Hetrick, R. D. Jones

Project SEED Best Practices
Raleigh Convention Center
305A

Sponsored by NIEHS and SERMACS
Supported by ACS Innovative Projects Grants
A. Tonelli, Organizer, Presiding

1:00. National SEED. S. Bonetti and C. Hernandez

1:20 1274. Challenges for a successful Project SEED experience: Identifying promising students and projects. T. Burkey

2:00 1275. Clark Atlanta University ACS Project SEED: Program activities that work. I. Khan, J. Reed, M. Williams

2:40 Coffee Break, Posters and Exposition.

3:20 1276. ACS Project SEED summer research program at UNC Charlotte. T. A. Schmedake, K. S. Asala
4:00 1277. The NC-ACS Project SEED: Beyond the summer research model. K. A. Cutler

4:40 Award Presentations.

SEMRC - Poster Session Saturday
Saturday Posters Presenting/ALL Poster Viewing

Raleigh Convention Center
North Hallway, 306 B/C Lobby

A. Smirnov, A. Nevzorov, I. Nesmelova, Organizers

1:30 - 3:00

1278. Insights into the mechanisms of drug resistance in HIV-1 protease from pulsed EPR and NMR spectroscopy. I. S. de Vera, X. Huang, M. E. Blackburn, A. N. Smith, A. M. Veloro, B. M. Dunn, G. E. Fanucci

1279. Monitoring the unstructured-to-structured transition of IA₃ using site-directed spin labeling and electron paramagnetic resonance. E. Milshteyn, N. L. Pirman, M. B. Chandler, G. E. Fanucci

1280. Selective Oxidation of Manganese centers in Bacillus subtilis Oxalate Decarboxylase. U. Twahir, W. Kellet, N. G. Richards, A. Angerhofer*

1281. Dipolar Relaxation of Trityl Radicals at Low Temperatures. H. D. Chen, M. D. Krzyaniak, M. K. Bowman

1282. Spin Relaxation Measurements of the Oxygen-Induced Radicals in neuronal Nitric Oxide Synthase. M. D. Krzyaniak, V. Berka, A. Tsai, M. K. Bowman


1284. Investigating the effect of lung surfactant peptide SP-B₁₋₂₅ on lipid dynamics. A. N. Smith, R. S. Farver, J. M. Wilson, J. R. Long


1286. Rapid freeze for pulsed EPR studies of ATP hydrolysis. Y. V. Tkachev, J. Ge, Y. E. Nesmelov

1287. Solution NMR structures of the Rev1 C-terminal domain and its complex with the polymerase κ Rev1-interacting region. J. Wojtaszek, J. Liu, S. Wang, Y. Xue, P. Zhou
1288. Spin trap studies on radical formation in Oxalate decarboxylase. C. Lee, U. Twahir, A. Angerhofer

1289. Mechanism of core radical rearrangement and coupled hydrogen transfer reactions in an adenosylcobalamin-dependent enzyme from 190-300 K. A. Bovell, C. Zhu, H. Chen, K. Warncke

1290. Protein structure determination from unassigned NMR data. A. Fahim, M. Simin, H. Valafar

1291. Effect of non-aggregating membrane-spanning WALP peptide on self-association of CesA transmembrane helices 4 and 5. L. Li, M. A. Voinov, L. Sethaphong, Y. Yingling, A. I. Smirnov

1292. Pulse sequence for optimal signal-to-noise over wide spectral ranges: A long-range $^1$H-$^{15}$N correlation experiment using frequency-swept radiofrequency pulses. T. D. Spitzer, R. D. Rutkowske, G. F. Dorsey

1293. Mg$^{2+}$-Dependent Hierarchical Folding Underlies Ligand Recognition by Fluoride Riboswitch. B. Zhao, J. Yu, M. Ramanan, D. Kim, Q. Zhang


1295. Using intermolecular multiple quantum coherences (iMQCs) to measure temperature during cancer hyperthermia. R. M. Davis, W. S. Warren


1297. NMR Investigation of a peptide toxin Mellitin and the peptide chaperone in age related cataract formation. L. S. Mansell, T. Kinscale


Bioanalytical Chemistry I
Raleigh Convention Center
306B

M. ter Horst, Organizer
J. Mazlo, Presiding

1:40 1299. Spectroscopic study of micelle-enhanced ligand exchange of gallium (III)/4-(2-pyridylazo) resorcinol complex by calf thymus DNA. F. Yan, C. L. Spurgeon

2:00 1300. Manipulation and characterization of single DNA molecules in nanofluidic devices. L. D. Menard, J. Zhou, J. M. Ramsey

2:20 1301. C-peptide stimulated nitric oxide production in a cultured pulmonary artery endothelium is erythrocyte-mediated and requires Zn$^{2+}$. P. A. Vogel, A. W. Giebink, D. M. Spence

2:40 Coffee Break, Posters and Exposition.


3:40 1303. Modulating the physical properties of micelles for membrane protein investigations. R. C. Oliver, R. H. Lo, D. A. Fox, J. Lipfert, L. Columbus

Chemistry and Applications of Colorants in the 21st Century
Raleigh Convention Center
306A

R. Shamey, H. Freeman, Organizers, Presiding

1:40 1304. Color Yes, Toxicity No: Systematic Approaches to Meeting this Challenge. H. Freeman


2:40 Coffee Break, Posters and Exposition.

3:20 1307. Sustainable cotton dyeing. P. J. Hauser
3:40 1308. Ionic liquids for the dyeing of polyester fabric. **H. Boyter, Jr., S. Li**

**Agricultural and Food Chemistry Poster Session**

Posters are presented from 2:30 to 4:00

Raleigh Convention Center
Ballroom C

Y. Yingling, Organizer

2:00 - 4:30

1309. Impacts of Food Proteins on the Thermal Stability of Polyphenols Extracted from Muscadine Grape Pomace. **S. Ji, J. Yu**

1310. Fatty Acid Composition of Grape Seed Oils from Some Grape Cultivars in North Carolina. **J. Yu, I. Smith**


1312. Use of sweet potato (Ipomoea batatas) to develop a medium for cultivation of lactic acid bacteria. **S. A. Hayek, A. Shahbazi, S. A. Ibrahim**

1313. Viability of Lactobacillus reuteri and Bifidobacterium in skim milk in the presence of shiitake mushroom extract during refrigerated period. **O. Hassan, S. Ibrahim, O. O. Isikhuemhen, A. Shahbazi, A. Abughazaleha**

1314. Impact of different gums on the growth of Lactobacillus reuteri in laboratory medium. **B. Karlton-Senaye, A. Shahbazi, S. Ibrahim**

1315. Effect of exercise : Diet program on obesity among students of Saudi Arabia. **S. O. Aljaloud, S. Ibrahim, M. S. Al.Ansari**


1317. Stability of biogenic amines in relation to the quality of three fish species commonly consumed in Kuwait. **A. Anderson**


1319. Comparisons of dietary fiber and polyphenol composition of grape pomaces from four grape cultivars grown in North Carolina. **A. McMillan, I. Smith, J. Yu**

1321. %Trans-fat in select food items purchased from Long John Silver's: A Preliminary Study. **S. K. Jenkins, P. Campbell**

1322. %Trans-Fat in donuts purchased from supermarkets, gas stations, and bakeries: A preliminary study. **S. K. Jenkins, P. Campbell**

1323. Impact of metoprolol, common elderly medicine on the survival of *Bifidobacterium*. **T. O. Obanla, R. Gyawali, S. A. Ibrahim**

**Bioanalytical Chemistry Poster Session**

Posters are presented from 2:30 to 4:00

Raleigh Convention Center
Ballroom C

Y. Yingling, **Organizer**

2:00 - 4:30

1324. Cellular responses to anti-cancer drugs in 3D and 2D cell cultures. **G. Trivedi, W. Tyson, L. Yang**

1325. Modified FRAP methodology with millisecond time resolution for the investigation of heterogeneous RNA polymerase II diffusion dynamics. **M. A. Tycon, C. J. Fecko**

1326. The spectrochemical characterization of novel Vis-NIR dyes as fluorescence probes for developing new bioanalytical techniques to study the catalytic activity of alkanesulfonate monooxygenase. **G. Beckford, M. Henary, H. Ellis, G. Patonay**


1330. Developing biotin and histidine tagged protein-protein interaction assay platforms for the quartz crystal microbalance with dissipation (QCM-D) technology. M. Dixon, F. Andersson, J. Wilkstrom, M. Ferrarelli

1331. Planar nanogap electrical detector for Single Molecule sensing and Biopolymer sequencing. F. I. Uba, J. Wu, S. Park, S. A. Soper


Chemical Toxicology, Health, and Safety Poster Session
Posters are presented from 2:30 to 4:00

Raleigh Convention Center
Ballroom C

Y. Yingling, Organizer

2:00 - 4:30


1336. Trans lesion synthesis DNA polymerase assays of dietary mutagen 2-amino-3-methylimidazo-[4,5-]quinoline (IQ). A. D. Millsap, E. K. Hawkins, C. J. Rizzo
Environmental Chemistry Poster Session
Posters are presented from 2:30 to 4:00

Raleigh Convention Center
Ballroom C

Y. Yingling, Organizer

2:00 - 4:30

1337. Occurrence and removal of pharmaceuticals and personal care products in different wastewater treatment plants. J. Kwon, J. Rodriguez, A. Brown

1338. A Method using Ultrasonication Coupled with Solid Phase Microextraction (SPME) in the determination of Polybrominated Diphenyl Ethers (PBDEs) in House Dust. W. Weathers, A. Hines, M. Colon

1339. Optimized evaluation of isotopic fractionation of N2O in the atmosphere. J. D. Weibel, Y. L. Yung, R. Shia


1341. Changes in Fe(II) concentration and stability in rain water in Wilmington, NC. B. C. Rice, J. D. Willey, R. J. Kieber, G. Avery, R. N. Mead


1344. The Development of a Lisianthus with Characteristics of the Elusive Blue Rose. C. M. Lariviere, H. D. Schreiber


1346. Through the quadropole: An investigation into the chemical composition and source origin of summertime aerosols using aerosol mass spectrometry. M. Link, B. Taubman

1347. Comparison of EDC determination in natural waters by stir-bar sorptive extraction and solid phase extraction. A. Fleming, B. Lacy, P. A. Ruiz-Haas

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1348. The effects of endocrine disrupting compounds on Red Breasted Sunfish (Lepomis auritas) as determined by the presence of testicular oocytes. B. Lacy, A. Fleming, P. Ruiz-Haas


1350. Aerobic formaldehyde oxidation catalyzed by the polyvanadotungststates. W. Guo, Z. Luo, H. Lv, C. L. Hill

1351. Fall to spring seasonal and environmental analysis on the water quality for the headwaters of the Little Shoe Heel Creek in Scotland County, NC. M. S. Morton, R. Brandenburg, D. Carbonell

1352. Effects of nutrient additions on benthic metabolism in the Southern Everglades. M. S. Noguera

1353. Understanding the endogenous and exogenous effects of reactive aldehydes. B. Moeller, K. Lu, N. Herr, W. Bodnar, L. Recio, J. A. Swenberg


Materials Chemistry Poster Session
Posters are presented from 2:30 to 4:00

Raleigh Convention Center
Ballroom C

Y. Yingling, Organizer

2:00 - 4:30

1356. Fabricating porous gallium nitride with dip pen nanolithography. S. Wilkins, A. Ivanisevic

1357. Square graphene domains and graphene hybrids using chemical vapor deposition. G. Dai, K. Vinodgopal, D. K. Taylor, M. H. Wu


1359. Composition tunable absorption and emission properties of Ge_xSn_{1-x} alloy nanocrystals. R. J. Esteves, I. U. Arachchige
1360. Sol-Gel Methods for the Assembly of Hollow Metallic Spheres into Metal Aerogel Frameworks. X. Gao, K. Ranmohotti, I. U. Arachchige

1361. Incorporation of graphene nanoplatelets to PDMS. N. Farahbakhsh, J. S. Jur


1367. Synthesis of flavones with mesogenic properties. D. J. Timmons


1369. Electropolymerization of polymer-coated silver nanoparticles: Incorporation of particles into a polymer network. S. C. Paul, V. Cammarata

1370. Investigation of hybrid film formation mechanism via sequential vapor infiltration. H. I. Akyildiz, J. S. Jur

1371. Barriers to rotation in 2-butyne and analogous compounds. O. Omorodion, M. Bober, K. J. Donald

Nucleic Acid Chemistry Poster Session
Posters are presented from 2:30 to 4:00
Raleigh Convention Center
Ballroom C
Y. Yingling, Organizer

2:00 - 4:30


SEMRC - NMR/EPR New Methods
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A. Nevzorov, A. Smirnov, I. Nesmelova, Organizers

3:00 1376. Increasing CP-MAS NMR Resolution Using Single Crystals. S. Dugar, R. Fu, N. Dalal

3:25 1377. Application of Sparse Sampling in Biomolecular NMR. P. Zhou


4:15 1379. $^1$H Dynamic nuclear polarization based on an endogenous radical. A. Miller, T. Maly, D. Cui, R. Griffin


5:05 1381. Electronic spin relaxation at high fields. J. van Tol, J. Wang, Z. Wang

5:30 SEMRC Business Mtg.
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Welcome to... Downtown Raleigh

If you are interested in:
- seeing and doing more in Greater Raleigh, start with the Visitor Information Center (VIC);
- visiting North Carolina, start with the N.C. Division of Tourism (C,2);
- relocating to Greater Raleigh, start with the Chamber of Commerce (C,14);
- touring the Capital area with 10 or more, start with Capital Area Visitor Information (C,3)

Parks
- Nash Square (B, 4)
- Moore Square (D, 4)

Civic/Government
- N.C. State Capitol (C, 3)
- Wake County Courthouse (C, 5)
- N.C. State Legislative Building (C, 3)
- Federal Government Complex (D, 4)
- City of Raleigh Municipal Complex/Parks Department (B, 4)
- N.C. Executive Mansion (D, 3)
- Greater Raleigh Chamber of Commerce (C, 7)
- N.C. State Archives (D, 3)
- Capital Area Visitor Information (C, 3)
- Greater Raleigh Convention and Visitors Bureau (C, 6)
- N.C. Division of Tourism, Film & Sports Development (C, 2)

Attractions
- Artspace (D, 5)
- City Market (D, 5)
- City Plaza (C, 6)
- Contemporary Art Museum
- Haywood Hall (D, 3)
- Marbles Kids Museum/Wachovia IMAX® Theatre (D, 4)
- N.C. Museum of History (C, 3)
- N.C. Museum of Natural Sciences (C, 3)
- Raleigh AmphiTheater and Festival Site (B, 6)
- Raleigh City Museum (C, 4)

Greater Raleigh Visitor Information Center

Transit
- Amtrak Rail Station (A, 5)
- City Bus Terminal (D, 4)
- Greyhound Bus Terminal (B, 3)
- R-LINE Stops
- R-LINE after 6:30pm route

Hotels
- Clarion State Capital (B, 3)
- Days Inn Downtown (B, 2)
- Raleigh Marriott City Center (C, 6)
- Oakwood Inn & B&B (E, 2)
- Sheraton Raleigh Hotel (C, 5)

Symbols
- Parking
- Parking entryway indicator
- Information
- Railroad tracks
- Flow of traffic
- Post offices
Y'all come!

Building Chemical Bonds: Academia-Industry-Government

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