

# *46<sup>th</sup> Midwest/39<sup>th</sup> Great Lakes Joint Regional Meeting of the American Chemical Society*

## *Technical Program*

Keith J. Stine, Program Chair  
Darrell Clinton, Program Co-Chair

Sheraton Westport Chalet Hotel  
Saint Louis, MO

### **WEDNESDAY AFTERNOON SESSIONS OCTOBER 19, 2011**

**Wednesday, October 19, 2011, 1:00 PM – 5:20 PM**

**Nanoscience General Session A**

**Room: Alpine I**

- 1:00** 1. Capping and passivation of aluminum nanoparticles with epoxy-alkenes. **B. J. Thomas**, K. Wentz, E. Guliants, C. E. Bunker, S. E. Hayes, P. A. Jelliss, S. W. Buckner
- 1:20** 2. Nanoneedles and Nanowires of superconducting FeSe encapsulated by carbon nanotubes. D. Nath, **S. Patil**
- 1:40** 3. Aniline capped gold colloids by solvated metal atom dispersion method. **Y. Sun**, K. J. Klabunde
- 2:00** 4. Effects of the potential energy landscape on exciton delocalization in single 1-d quantum wires. **V. L. Wayman**, R. A. Burnett, B. S. Hoener, P. J. Morrison, F. Wang, W. E. Buhro, R. A. Loomis
- 2:20** 5. Effect of doping transition metal ions on silica and titania aerogel systems. **M. N. Weerasinghe**, K. J. Klabunde
- 2:40** 6. Coaxial Silicon Coating on Vertically Aligned Carbon Nanofibers for High-Performance Lithium-Ion Batteries. **S. A. Klankowski**, J. Li, R. Rojas
- 3:00** Break.
- 3:20** 7. Characterizing the excitation-energy dependence of photoluminescence quantum yields in quantum nanostructures. **J. Hoy**, Y. Liu, L. Steinberg, W. E. Buhro, R. A. Loomis\*

- 3:40** 8. Tuning titanium dioxide nanomaterials for renewable energy applications. **X. Chen**
- 4:00** 9. Hybrid titanium dioxide nanomaterials for dye-sensitized solar cells. **H. He**, Y. Zhong, M. Dubey, M. Shrestha, L. Si
- 4:20** 10. TiO<sub>2</sub> compact layers prepared by low temperature colloidal synthesis and deposition for high performance dye-sensitized solar cells. **C. S. Kovash**, B. A. Logue
- 4:40** 11. Design of MspA-based solar cells. **A. Perera**, S. Wendel, H. Wang, S. H. Bossmann
- 5:00** 12. Solution-based synthesis of crystalline titanium disulfide nanobelts. **V. V. Plashnitsa**, P. Tongying, G. Krylova, M. K. Kuno

**Wednesday, October 19, 2011, 1:00 PM – 4:40 PM**

**Organic Chemistry General Session A**

**Room: Geneva**

- 1:00** 13. Synthesis of hybrid arylene ethynylene macrocycles via alkyne metathesis depolymerization. **D. E. Gross**, J. S. Moore
- 1:20** 14. Aromatics from pyrones: 4-Substituted alkyl benzoates from alkenes, coumalic acid and methyl coumalate. **S. J. Riley**, G. A. Kraus
- 1:40** 15. Modular Syntheses of Tetrahydro Benzoquinolines and Dihydro Benzoindoles via Sequential Copper, Ruthenium and Palladium Catalyzed Reactions. **S. N. Raikar**, H. Malinakova
- 2:00** 16. Reaction pairing: A modular approach to diversity-oriented synthesis of benzofused sultams. **J. K. Loh**, T. B. Samarakoon, A. Rolfe, S. Yoon, P. R. Hanson\*
- 2:20** 17. Carbonyl-directed catalytic asymmetric hydroboration of 1,1-disubstituted alkenes. **M. O. Bani Khaled**, S. Smith, G. Hoang, J. M. Takacs
- 2:40** 18. Dehydration of 3 and 4-methyl-1-cyclohexanols: A study of reaction rates and product distributions. **N. Toritto**, J. Friesen
- 3:00** Break.
- 3:20** 19. Predicting DNA-intercalator binding: The development of an arene-arene stacking parameter. **L. K. Hardebeck**, C. A. Johnson, Y. Ren, T. Zahrlı, B. M. Znosko, M. Lewis
- 3:40** 20. Enhancing photoreactivity of co-crystals by utilizing molecular pedal motion in the organic solid state. **R. H. Groeneman**, E. Elacqua, L. R. MacGillivray

- 4:00** 21. New insights into an alternate mechanism for oxidation of alcohols using iodine (V) reagents. B. Raya, K. K. Madne, S. Jajam, **T. K. Vinod**
- 4:20** 22. Iodine atom economic co-iodination of alkenes: Selective and differential functionalization of the two double bonds in dienes. H. Gottam, M. Kistammagiri, S. R. Pandey, **T. K. Vinod**

**Wednesday, October 19, 2011, 1:25 PM – 5:00 PM**  
**Small Chemical Businesses - True Stories of Success from Chemical Entrepreneurs**  
**Room: Alpine II**

Joseph Sabol, *Organizer*

*Supported by Division of Small Chemical Businesses*

- 1:25** Introductory Remarks.
- 1:30** 23. From sewage sludge to ebooks: An academician's ventures into the small business world. **S. E. Manahan**
- 2:05** 24. So, you want to be a consultant? Here's how to do it. **D. Webster**
- 2:40** Break.
- 3:00** 25. NUtech Ventures: Catalyzing startup success. **J. Garrity**
- 3:35** 26. Terminated to terminator. **J. Jost**
- 4:10** Panel Discussion
- 4:55** Concluding Remarks.

**Wednesday, October 19, 2011, 1:30 PM – 4:40 PM**  
**Pharmaceutical Chemistry**  
**Room: St. Moritz**

Todd Stark, *Organizer*

- 1:30** Introductory Remarks.
- 1:40** 27. Chemistry in the pharmaceutical industry, part one. **T. M. Stark**

- 2:20 28.** Synthesis of fluorophores that reveal dynamic aspects of physiology in vivo in *C. elegans*. **B. R. Peterson**, Z. R. Wodziak, A. M. Bender, L. Fu, M. Branden, N. M. Wallace, Z. Zhou, M. Visvanathan, G. H. Lushington, B. D. Ackley
- 3:00** Break.
- 3:20 29.** Pyrrole-imidazole Polyamides active against Human Papillomavirus (HPV) in cell and tissue culture. **J. K. Bashkin**
- 4:00 30.** Chemistry in the pharmaceutical industry, part two. **T. M. Stark**

A special roundtable discussion associated with this symposium will be held from 7pm – 8pm in the St. Moritz room.

“The Business of Pharmaceutical Chemistry”: A roundtable of scientists will discuss their current roles in the pharmaceutical industry that involve placing dollar values on chemistry effort, chemical compounds, and pharmaceutical products. Each panelist will describe how they arrived at their current position and together discuss the skills required to succeed in business-focused, pharmaceutical chemistry careers.

Participants:

**Todd Stark**, Business Development Manager, Johnson Matthey Pharma Services  
**Helen Anderson**, VP Commercial Development, Harvard Drug Group  
**Karthik Raghavan**, CEO, Sentio BioSciences LLC  
**Katie Grayson**, Sr Director, Technical Affairs, EAG Life Sciences division of Evans Analytical Group  
**Umashanker Sampath**, Director, New Business Development, Reliable Biopharmaceutical Corporation  
**Matthew T Reding**, Procurement Specialist Consultant II, Biologics Strategic Sourcing–Small Molecules, EMD Millipore

**Wednesday, October 19, 2011, 1:30 PM – 5:00 PM**  
**Revitalizing the Heartland's Chemical Economy**  
**Room: Davos**

John Borchardt, Lisa Balbes, *Organizers*

*Supported by Division of Professional Relations, and an ACS Innovative Project Grant for Divisional Enhancement*

- 1:30** Introductory Remarks.
- 1:35 31.** ConocoPhillips Wood River CORE project. **J. Burkinshaw**, K. Peccola
- 2:05 32.** R&D phoenix: new labs arising from the ashes. **J. K. Borchardt**
- 2:35 33.** Tech transfer & commercialization: Applied research and gap funding. **R. Silva**

**3:05** Break.

**3:25** **34.** Divergence: From startup to acquisition, a success story. **D. Rapp**

**3:55** **35.** Innovators turning into entrepreneurs: How to get started. **D. J. Broderick**

**4:25** Panel Discussion.

**4:55** Concluding Remarks.

**Wednesday, October 19, 2011, 5:00 PM – 7:00 PM**

**Chemistry of Ice Cream**

**Room: Matterhorn**

Brent Znosko, *Organizer*

*Supported by Supported by Education Division of the American Chemical Society*

**5:00** **36.** Designing ice cream quality with the aid of a microscope. **H. Goff**

The Undergraduate Ice Cream Social begins at 5:40 pm.

**WEDNESDAY EVENING SESSIONS**  
**OCTOBER 19, 2011**

**Wednesday, October 19, 2011, 7:00 PM – 9:00 PM**

**SciMix Poster Session**

**Versailles Ballroom**

37. Valence-bond determination of bond lengths of polycyclic aromatic hydrocarbons. **J. R. Dias**
38. In search for natural tau fibrillization inhibitors: Preliminary evaluation of horse apple fruit extract. S. Awan, A. Abraha, **E. A. Abourashed**
39. RNA CoSSMos: Characterization of Secondary Structure Motifs- A searchable database of secondary structure motifs in RNA three dimensional structures. **P. L. Vanegas**, G. A. Hudson, A. R. Davis, S. C. Kelly, C. C. Kirkpatrick, B. M. Znosko
40. Chemical synthesis of  $\alpha$ -deuterated amino acid, biosynthesis of *Clostridium symbiosum* glutamic dehydrogenase (*cs*-GDH) and study of kinetic isotope effect of dehydrogen reaction of glutamic acid catalyzed by *cs*-GDH. **X. Chen**, S. J. Maniscalco, H. F. Fisher
41. Time-averaging approximation in the interaction picture for absorption line shape and vibrational energy transfer in liquid water. **M. Yang**, J. L. Skinner
42. Control of surface functionality via photopatterning: Self-assembled monolayers for small molecule and protein attachment. **M. Hynes**, J. Maurer
43. Contribution of core/shell and core/shell/shell lattice interfaces on the optical properties of quantum dots? **B. O. Omogo**, M. Benamara, C. D. Heyes
516. Increasing biochar surface area: Effects of various milling parameters. **S. C. Peterson**, M. A. Jackson, S. Kim, D. Palmquist
45. Characterization of arsonic acid self-assembled monolayers (SAMs): A new class of monomers. **N. A. LaFranzo**, J. A. Maurer
46. Mineral Levels in Mature Soybean Seed Are Not Altered by Glyphosate Treatment or the Glyphosate Tolerance Trait. **D. R. Lundry**, R. M. Alba, A. H. Culler, M. S. Bleek
47. Self-assembly and dynamics in pore formation by amphiphilic heptapeptides. **S. Negin**
48.  $^{19}\text{F}$  NMR studies reveal pH susceptibility of domain 2 of anthrax PA. **F. Chadegani**, J. Bann

49. Free Energy Changes and the Vibrational Partition Function. P. E. Smith, **S. Dai**
50. Photophysical Properties and Electronic Structure of Stable, Tunable Synthetic Bacteriochlorins: Extending the Features of Native Photosynthetic Pigments. **E. Yang**, C. Kirmaier, M. Krayner, M. Taniguchi, H. Kim, J. R. Diers, D. F. Bocian, J. S. Lindsey, D. Holten
51. Theoretical studies on the optoelectronic properties of *N*-fused quinazolinimaniums. **O. Alawode**, S. Rayat
52. Synthesis of potent inhibitors of YopH in *Yersinia pestis*: Pathogen responsible for the Black Death. **M. P. Paudyal**, C. D. Spilling
53. Morphology-controlled synthesis of nanosize cuprite (Cu<sub>2</sub>O). **K. M. Shrestha**, K. J. Klabunde
54. Computational investigation of the extrusion of PhSi:<sup>+</sup> from a 7-phenyl-7-silanorbornadienyl cation in solution. **S. E. White**, P. P. Gaspar
55. In situ generation of bromine for micelle-assisted bromination and oxidation. **A. Mishra**, Z. Wang, D. S. English, E. Talaty
56. Reaction of hemiacetals with Pd  $\pi$ -allyls: Stereoselective synthesis of cyclic ethers. **S. Dawadi**, C. D. Spilling
57. AFM imaging analysis of pUC19 DNA on modified mica. **N. Nezamabadi**, J. C. Goeckner, C. Wei, E. J. Voss
58. NMR observations of optical pumping events in si-GaAs and GaAs quantum wells. **D. Wheeler**, E. Sesti, W. Worthoff, C. Stanton, S. E. Hayes
59. Elucidating the energy-transfer mechanisms at the interface between the chlorosome and FMO protein in green sulfur bacteria. **G. S. Orf**, D. Bina, R. E. Blankenship
60. Spectroelectrochemical investigations of metalloporphyrin carbonyl and nitrosyl complexes. **M. J. Shaw**, K. Sharmah-Gautam, K. W. Rodgers, C. Felchlia, A. Daryaei, P. Ashitey
61. Prospecting for NMR Structures with Sparse, Unassigned Data. **A. E. Nesbitt**, M. Tang, M. C. Brothers, K. M. Nuzzio, G. Comellas, L. J. Sperling, C. M. Rienstra
62. Preparative Studies of Re(I)-Terpyridine Complexes. **D. R. Black**, S. E. Hightower
63. Tether-Mediated Ring-Closing Metathesis Studies. **S. Maitra**, R. Chegondi, J. Markley, P. R. Hanson\*

64. Selective sialylations by the use of C-5 modified S-benzoxazolyl sialyl donors. **C. Gobble**, C. De Meo, M. Stark, P. Patel, B. Harris
65. Electronic structure of platinum fluoride, PtF, by intracavity laser absorption spectroscopy. **K. A. Womack**, L. C. O'Brien, J. J. O'Brien
66. Spectral analysis of the three major isotopologues of PtC. **J. Raskas**, **D. Schultz**, J. J. O'Brien, L. C. O'Brien
67. Cobalt(III) Schiff base complexes as zinc finger transcription factor inhibitors. **M. C. Heffern**, A. S. Harney, N. Yamamoto, T. J. Meade
68. Reductive Photoelimination of Bromine from a Pt(IV) Perylene Complex. **M. Masjedi**, A. Raphael Karikachery, P. R. Sharp
69. Synthesis and reactivity of bidentate phosphine platinum(II) peroxo compounds. **M. A. Moody**, P. R. Sharp
70. Triflic acid promoted synthesis of various azapolycyclic aromatic compounds. **A. Kethe**, A. Li, R. Naredla, D. A. Klumpp\*
71. Assignment of proton resonances for damaged DNA using two-dimensional nuclear magnetic resonance. **S. P. Kramer**, B. Medrano, G. Meints
72. Synthesis toward molecular "tweezers". **T. R. Bowen**, Z. Yan
73. Nanorattles: Silver nanoparticles entrapped in porous polymer nanocapsules. **S. N. Shmakov**, E. Pinkhassik
74. Synthesis and functionalization of Rhenacarboranes as drug-delivery vehicles. **D. Pruitt**, P. Jelliss
75. Studies towards the electrooxidative coupling of heterocycles to olefins. **J. A. Smith**, K. D. Moeller
76. New cucurbitane analogs: Potential anticancer candidates for the treatment of prostate cancer. **N. Rice**, F. Halaweish
77. Optimization of synthesis toward the development of an anion binding molecule. **A. Dawson**, C. Bagwill, S. Garvey, E. Sullivan, M. Lewis
78. Anodic olefin coupling reactions: Probing reaction mechanisms and relative reaction rates via competition experiments. **J. M. Campbell**, H. Xu, K. D. Moeller
79. New BODIPY based fluorescent indicator for elective detection of Pb<sup>2+</sup> ions in living cells. **M. Baruah**, E. Huntimer, S. Mahmoud, A. Hoppe, F. Halaweish



80. Protease-activated receptor (PAR)-1 inhibiting nanoparticles for modulation of vascular inflammatory signaling. **B. Sinha**, H. Pan, C. F. Semenkovich, S. A. Wickline
81. Amphiphilic Behavior of Alkyl-chained Resorcinarenes. **P. Ogirala**
82. Synthesis and photochromicity of extended cinnamaldehyde derivatives from phosphorous ylides. **J. M. Saathoff**, S. M. Fortin, E. M. Treadwell
83. Hydrogen atom abstraction from rhodium hydrides by nitroxyl radicals and generation of  $\text{LRh}^{2+}$ . **J. F. Dunne**, A. Bakac
84. Microelectrode array-based chemistry. J. Bartels, **S. Uppal**, K. D. Moeller

**THURSDAY MORNING SESSIONS**  
**OCTOBER 20, 2011**

**Thursday, October 20, 2011, 8:00 AM – 12:00 PM**

**Biological Mass Spectrometry**

**Room: Alpine I**

Henry Rohrs, Joshua Coon, Michael Gross, *Organizers*

*Supported by Advion, Leco, Waters, JEOL, Thermo Scientific, Bruker, AB Sciex, Agilent Technologies, Shimadzu, and Division of Analytical Chemistry*

- 8:00** Introductory Remarks.
- 8:05** **85.** Redox profiling and protein characterization via MS to investigate thiol-based regulatory mechanisms induced by oxidative stress in plants. **L. M. Hicks**, J. M. Jez, S. Alvarez, A. Galant, Z. Liu
- 8:50** **86.** Functional proteomics in *Arabidopsis* G-protein signaling in response to ABA. **S. Alvarez**, L. M. Hicks, S. Pandey
- 9:20** **87.** Integrated metabolomics provides novel insight into legume natural product biosynthesis. D. S. Yang, J. H. Snyder, D. V. Huhman, V. Tzin, S. Allen, Y. Tang, **L. W. Sumner**
- 10:05** Break.
- 10:25** **88.** Mass spectrometry based protein footprinting: the fourth pillar of proteomics. **M. L. Gross**, D. Rempel, J. Chen, B. Gau, H. Zhang, R. Huang, C. Frieden, K. Gerai
- 11:10** **89.** The use of hydrogen/deuterium exchange-mass spectrometry in VDR modulator development. **J. Zhang**

**Thursday, October 20, 2011, 8:00 AM – 12:00 PM**

**Nanoscience General Session B**

**Room: Basel**

- 8:00** **90.** Formation of Hydrogen-Bonded Nanostructures through the Self-Assembly of Mixed Macrocycles. **C. R. Pfeiffer**, A. K. Maerz, D. A. Fowler, M. Mistry, C. L. Barnes, J. L. Atwood

- 8:20 91.** Encapsulation of Fluorescent Reporter Molecules within Hydrogen-Bonded Dimeric Pyrogallol[4]arene Nanocapsules. **D. A. Fowler**, K. K. Kline, S. A. Tucker, J. L. Atwood
- 8:40 92.** Nanocapsules with programmed nanopores. **E. Pinkhassik**
- 9:00 93.** Liposome-templated polymer nanocapsules: from synthetic methods to smart containers. **S. A. Dergunov**, M. D. Kim, E. Lindner, E. Pinkhassik
- 9:20 94.** Controlled Polymer Property Manipulation via Nano and Other Technologies. **D. E. Bowen III**, E. A. Eastwood
- 9:40** Break.
- 10:00 95.** Polymeric “single molecule magnet” nanoparticle as a magnetic resonance imaging contrast agent. **D. Pan**, B. Kim, A. H. Schmieder, A. J. Stacy, S. A. Wickline, G. M. Lanza
- 10:20 96.** Morphology control of cadmium selenide nanocrystals: Insights into the roles of di-*n*-octylphosphine oxide (DOPO) and di-*n*-octylphosphinic acid (DOPA). **F. Wang**, W. E. Buhro
- 10:40 97.** Characterization of protein immobilization on nanoporous gold using atomic force microscopy and scanning electron microscopy. **Y. Tan**, A. V. Demchenko, K. J. Stine
- 11:00 98.** Pseudocapacitive behavior of electrodeposited nickel hydroxide films on laser ablated nickel electrodes. **T. G. Smith**, C. Zuhlke, T. Anderson, D. Alexander, R. Y. Lai
- 11:20 99.** Balancing stability and the SERS activity of caged nanoparticles. **M. Konne**, M. Pierre, A. J. Haes
- 11:40 100.** Synthesis of Fe/Fe<sub>3</sub>O<sub>4</sub>/Au core/shell nanoparticles for magnetic hyperthermia and MRI application. **H. Wang**, T. B. Shrestha, M. T. Basel, R. K. Dani, L. Maurmann, V. Chikan, D. L. Troyer, S. H. Bossmann

**Thursday, October 20, 2011, 8:00 AM – 12:00 PM**

**Natural Products Synthesis**

**Room: Zurich**

Christopher D. Spilling, *Organizer*

*Supported by Division of Organic Chemistry, Reliable Biopharmaceutical, Covidien*

- 8:00 101.** Approaches to Tetrahydrofuran-Containing Natural Products. **C. D. Spilling**

- 8:30 102.** Semi-synthetic opioids from diene natural products. **T. Mannino**
- 9:00 103.** Natural product synthesis through tandem cationic reactions. **D. F. Wiemer**
- 9:30 104.** Phosphate tether-mediated protocols for natural product synthesis. **P. R. Hanson**
- 10:00** Break.
- 10:20 105.** Progress toward the synthesis of Antascomicin B. J. M. Hutchison, D. R. Clay, J. Rivero, **M. C. McIntosh**
- 10:50 106.** Total synthesis of marine alkaloids. **C. J. Lovely**
- 11:20 107.** Natural products as leads for anticancer drug discovery. **G. I. Georg**

**Thursday, October 20, 2011, 8:00 AM – 11:40 AM**

**Organic Chemistry General Session B**

**Room: Geneva**

- 8:00 108.** Iodine Lewis acid catalysis in organic chemistry: Iodine bonding between molecular iodine and triethyl orthoformate. **S. Coyle**, R. Glaser
- 8:20 109.** Biomass deconstruction using ionic liquids. **T. Guney**, G. A. Kraus
- 8:40 110.** Intramolecular hydroamination of olefins using a novel salicylaldehyde calcium complex. **K. Kunchithapatham**, J. P. Stambuli
- 9:00 111.** A four step route to a benzannulated benzocarbazole. **J. Beasley**, G. A. Kraus
- 9:20 112.** Strategic benzylic cross-coupling via Pd-mediated decarboxylation. **R. R. Torregrosa**, J. A. Tunge
- 9:40** Break.
- 10:00 113.** Supported patterned lipid bilayers on glycol-terminated monolayers: Formation and characterization. **M. K. Strulson**, J. A. Maurer
- 10:20 114.** Improved substituent constant for predicting the strength of cation- $\pi$  binding. **S. Wireduah**, T. M. Parker, C. C. Kirkpatrick, M. Lewis
- 10:40 115.** Investigation of silicon analog of fluorescein as pH responsive fluorescent probe. **N. Sattenapally**, Q. A. Best, C. Liu, C. Bailey, D. Dyer, L. Wang, M. McCarroll, C. G. Scott

**11:00 116.** Anodic electrochemistry: New reaction development and the use of solar power. **A. M. Redden**, K. D. Moeller

**11:20 117.** Effects of antioxidants on atomic oxygen O(<sup>3</sup>P) induced cleavage of DNA. **J. Korang**, R. D. McCulla

**Thursday, October 20, 2011, 8:00 AM – 11:40 AM**

**Physical Chemistry General Session A**

**Room: Zermatt**

**8:00 118.** CREPES, a tool for conformational searching on a potential energy surface. **M. P. Ver Haag**, T. A. Holme

**8:20 119.** Development and testing of torsional potentials for peptides and proteins. **Y. Jiao**, F. Chen, P. E. Smith

**8:40 120.** Microwave spectroscopic study of C-H...X (X =  $\pi$ , Cl, F or Br) interactions in a series of weakly bound dimers. **R. A. Peebles**, S. A. Peebles, B. J. Bills, C. L. Christenholz, A. A. Elliott, L. F. Elmuti, D. A. Obenchain, J. M. Sexton, B. H. Pate, M. T. Muckle, J. L. Neill, A. L. Steber

**9:00 121.** Calixarene and pyrogallolarene "suction cups" for the tethering of peptides. **M. D. Breite**, J. E. Adams

**9:20 122.** Dynamic stability of hydrogen-bonded pyrogallolarene capsules in the gas phase and in solution. **A. C. Webb**, J. E. Adams

**9:40** Break.

**10:00 123.** Cobaloxime hydrogen catalysts: A comprehensive EPR and computational investigation of the effect of ligand substitution on electronic structure. **K. L. Mardis**, J. Niklas, D. M. Tiede, O. G. Poluektov

**10:20 124.** TDDFT studies of optical properties of silver nanoparticles: Octahedra, truncated octahedra, and icosahedra. **G. Bae**, C. M. Aikens

**10:40 125.** Structural and single particle and ensemble spectroscopic studies of various core-shell biofunctional quantum dots: Implications for biological imaging. **C. D. Heyes**

**11:00 126.** Attempts to fabricate high efficiency chalcogenide solar cells through patterned growth of nanowires. **M. Nath**, S. Patil

**11:20 127.** Fluorescence intermittency of CdSe nanorods in PMMA/P3HT polymer blend. **S. Roy**, D. A. Higgins, V. Chikan

**11:40 449.** Batch pH oscillations in the Belousov-Zhabotinsky reaction. **G. A. Frerichs**, X. Huang, J. Jones, M. Gebrekidan, J. Burch, M. Yuan

**Thursday, October 20, 2011, 8:00 AM – 12:00 PM**

**Plant Biotechnology : Blurring the Line between Chemistry and Biology**

**Room: Bern**

Joseph Jez, Xuemin Wang, *Organizers*

*Supported by Pioneer – A Dupont Business, EPL Analytical Services, Divergence, VWR, Integrated DNA Technologies, Inc., Monsanto, Sequoia Sciences*

**8:00** Introductory Remarks.

**8:05 128.** Carbonyl chemistry-based biorenewable chemicals: Diversifying fatty acid synthesis with polyketide synthesis biocatalysts. **B. J. Nikolau**

**8:45 129.** Engineering proteins to improve biological function: Applications to Ag Biotech. **S. J. Franklin**

**9:05 130.** From climate change to proteins: redox proteomics of ozone-induced responses in soybean. **J. M. Jez**, A. Galant, R. P. Koester, E. A. Ainsworth, L. M. Hicks

**9:25 131.** Vacuolar glyphosate-sequestration correlates with glyphosate resistance in ryegrass (*Lolium spp.*): a <sup>31</sup>P-NMR investigation. **X. Ge**, D. A. d'Avignon, J. J. Ackerman, A. Collavo, E. L. Ostrand, R. D. Sammonse

**9:45** Break.

**10:10 132.** Tailoring plant biomass for biofuel production. **Z. Ye**

**10:40 133.** Improvement of soybean nutritive value by overexpression of a key enzyme involved in the sulfur assimilatory pathway. W. Kim, J. M. Jez, **H. B. Krishnan**

**11:00 134.** Carbons for lipids or carbohydrate: identifying a potential point of metabolic modulation. **M. Li**, S. Bahn, L. Guo, W. Musgrave, A. Saettele, M. Tang, H. Berg, R. Welti, X. Wang

**11:20 135.** Visualizing lipid compositions in plant tissues, cells and subcellular compartments: Could location be a factor in oilseed engineering? P. J. Horn, P. B. Neogi, A. R. Korte, K. Strupat, T. Arrey, V. Shulaev, Y. Lee, **K. D. Chapman**

**Thursday, October 20, 2011, 8:15 AM – 11:30 AM**

**Small Chemical Businesses - What Every Small Business Owner Needs to Know about Patents, Trademarks, and Intellectual Property**  
**Room: Alpine II**

Harry J. Guttman, *Organizer*

*Supported by Division of Small Chemical Businesses*

- 8:15** Introductory Remarks.
- 8:20** **136.** Small business IP – red flags and core concepts. **H. J. Guttman**
- 9:05** **137.** Patent information research and its role in managing intellectual property. **E. S. Simmons**
- 9:50** Break.
- 10:10** **138.** So you have an invention, now what? Important considerations when filing a patent application (*develop a patent strategy!*). **C. M. Tellez**
- 10:55** **139.** When is your molecule or method eligible for patent protection? Lessons from recent court cases and practical business guidance. **S. M. Lee**

**Thursday, October 20, 2011, 8:30 AM – 10:00 AM**

**General Poster Session I**

**Versailles Ballroom**

- 140.** Synthesis and Electrochemical Properties of Various Pd(II) Complexes. **S. Park**, F. Tang, L. M. Mirica
- 141.** Recycling gold from electronics. **A. W. Hummer**, H. J. Gregg, T. L. Troyer
- 142.** Pressure-Induced Structural and Optical Changes in  $\text{YIn}_{1-x}\text{Mn}_x\text{O}_3$ . **D. Freeman**, Z. Hayes, K. Chapman, P. Chupas, G. Halder, C. Josefson, P. Barnes
- 143.** Biomimetic studies of manganese (II) dioxygenase and cobalt-substituted enzymes. **J. Transmeier**, F. E. Jacobsen, T. A. Jackson
- 144.** Synthesis, electronic structure, and properties of organometallic indium porphyrins. **J. R. Sabin**, P. V. Solntsev, S. J. Dammer, V. N. Nemykin
- 145.** Preparation and testing of nanoparticle materials and thin films for use as substrates in dye-sensitized solar cells. **C. A. Nicholson**, E. A. Wovchko

146. Complexation studies of Ru(II) and Re(I) pendant polyamine host complexes. **A. M. Putt**, M. Harris
147. Preparation and investigation of gallium-based materials for hydrogen storage. **A. A. Fratantuono**, E. A. Wovchko
148. Novel synthesis and characterization of various pyrazolylsilane compounds. **N. C. Boyde**, S. Mason
149. Estimating the HOMO-LUMO gaps of siloles by cyclic voltammetry. **E. A. Weber**, B. E. Eichler, D. E. Weisshaar
150. Synthesis and characterization of biomimetic Rieske complexes. **C. J. Windorff**, C. T. Saouma, J. M. Mayer
151. Predicting the dimensionality of metal halides and oxides. **S. R. Cowin**, A. M. Beatty
152. Synthesis and binding studies of anion-responsive terpyridine functionalized calixarenes. G. Chen, **N. Y. Edwards**
153. Synthesis of some new tridentate ligands to complex silver. **L. R. Verheyen**, E. Bosch
154. The (1,1) band of the  $b^1\Sigma^+ - X^3\Sigma^-$  transition of O<sub>2</sub> by intracavity laser absorption spectroscopy. **L. C. O'Brien**, E. C. O'Brien, J. J. O'Brien
155. Reciprocal kinetic curves in electrochemical systems. **M. Hankins**, I. Kiss, G. Yablonsky
156. Calibration of model complexes and pyrogallol for metal-coordinated pyrogallol[4]arene capsules. **C. M. Mayhan**, A. V. Mossine, A. E. Kroeger, C. W. Dye, J. L. Atwood, C. A. Deakyne
157. Raman scattering of deuterated DNA nucleoside and solid DNA structure. **C. Hagan**, M. Hayes, S. Nichols, G. Meints
158. Using Knudsen effusion to measure the vapor pressure of compounds. **Y. Li**, C. Greenlief, G. A. Baker
159. Accurate monitoring of  $x$ ,  $y$ , and  $z$  magnetization at any point in an NMR pulse sequence. **E. T. Satterfield**, K. Woelk
160. Low-field NMR spin-lattice relaxation time-constant distributions of shale. **R. E. Gerald II**, L. Chi, H. Zhang, K. Woelk
161. Solid-state NMR of inorganic nanomaterials. **K. M. Wentz**, B. Thomas, D. W. Hammerstroem, S. W. Buckner, P. A. Jelliss, S. E. Hayes



162. Spontaneously synchronized current oscillations of nickel electrodisolution in an epoxy-based dual electrode microchip flow cell. **Y. Jia**, I. Z. Kiss
163. Using streamlined mutagenesis and screening to increase electron transfer to the B-branch pathway in bacterial photosynthetic reaction centers. **K. M. Faries**, P. D. Laible, L. Kressel, M. Wander, D. Holten, D. K. Hanson, C. Kirmaier
164. Photoreactions in the solid state: An NMR study. **S. J. Mattler**, D. A. Hirsh, K. Harstein, S. E. Hayes
165. Ship-in-a-bottle assembly of molecules in porous hollow nanocapsules. **S. N. Shmakov**, S. A. Dergunov, E. Pinkhassik
166. Ytterbium nanocolloids as a potential molecular contrast agent for computed tomographic imaging. **A. Senpan**, D. Pan, A. H. Schmieder, C. Schirra, X. Yang, S. A. Wickline, G. M. Lanza
167. Nucleic Acid-Directed Self-Assembling Nanoparticles for Imaging and Therapy. **Z. Li**, J. A. Taylor
168. Enhancement of commercial antibiotics by synthetic ion channels. **J. Atkins**, M. Patel
169. Coadsorbent effects on DSSC performance and dye loading. **J. Kofford**, B. Logue
170. Self-catalyzed growth of semiconducting samarium sesquisulfide nanowires. **C. M. Marin**, H. Liu, M. S. Thompson, C. Cheung
171. Impact of “click” functionalization on the toxicity of titanium dioxide nanoparticles in zebrafish embryos. **S. P. Yang**, K. M. Louis, O. Bar-Ilan, R. J. Hamers, R. E. Peterson, W. Heideman, J. A. Pedersen
172. Conjugated polymers as photocatalysts to promote homolytic pinacol coupling of aryl-aldehydes: Effects of Lewis and Brønsted acids. **W. D. Rouch**, M. Zhang, R. McCulla
173. Charge delocalization and enhanced acidity in tricationic superelectrophiles. **R. R. Naredla**, S. O. Nilsson Lill, C. Zheng, D. A. Klumpp\*
174. Superelectrophilic chemistry of various nitriles. **E. K. Raja**, D. Klumpp\*
175. Rapid access to exocyclic allenes by double hydride reduction of 3-trimethylsilylethynyl-2-cycloalkenones. J. M. Kum, A. K. Urick, **M. Hulce**
176. Synthesis and spectra of methyl-3 $\alpha$ -carboethoxy-7 $\alpha$ -(4-iodobenzoyloxy)-5 $\beta$ -cholanoate. **H. Veeramachaneni**, M. Turkyilmaz, H. Karabulut, J. R. Dias

177. Neutral picket fence porphyrins that bind the head group of phosphatidylglycerol, a phospholipid found in bacterial membranes. **A. Alliband**, D. H. Burns
179. From NP-HPLC to RP-UPLC: Ultra performance liquid chromatography for in-process analytical support of narcotics in the pharmaceutical industry. **H. Zhong**
180. Building addressable libraries: UV-Cross-linkable di-block copolymer strategy for functional reaction surfaces on microelectrode arrays. **L. Hu**, K. D. Moeller
181. Band-gap engineering of carborane-containing conducting polymers: A computational study. **E. Harak**, J. Varberg, P. Bobadova-Parvanova
182. Synthesis and characterization of polyionic mixed polymer nanobrushes on gold by ATRP and surface-initiated photopolymerization techniques. **B. Mitrovic**, C. Scott
183. Soybean-based epoxy-anhydride thermoset coatings. **A. Paramarta**, T. Nelson, X. Pan, D. Webster
493. A batch pH oscillator: The Belousov-Zhabotinsky reaction. **J. Jones**, X. Huang, M. Gebrekidan, J. Burch, M. Yuan, G. A. Frerichs
185. Synthesis, extraction and analysis of molecularly imprinted quercetin polymers. **A. Heck**, B. Schenavar, G. Mwangi
186. Synthesis of Photoactive Polymer Brush by RAFT polymerization: Applications in isolation of biological macromolecules. **M. D. Bisen**, M. J. Pabich, D. Dyer, C. Scott
187. Reactivity of cyclic carbonates as substrates for non-isocyanate polyurethanes. **O. Bilic**, I. Javni, D. Hong, J. Hong, Z. S. Petrovic

**Thursday, October 20, 2011, 8:55 AM – 12:00 PM**

**Chemical Education Research and Practice**

**Room: Davos**

Steve Kinsley, Susan Wiediger, *Organizers*

**8:55** Introductory Remarks.

**9:00** **188.** High school students' attitude towards chemistry as a science and chemistry studies. **F. Mumba**, V. M. Chabalengula, A. Banda, S. M. Mbewe

- 9:20 189.** Successes and challenges in the implementation of the laboratory components of a dual credit general chemistry course. **J. L. Torres y Torres**, B. D. Caldwell, M. W. Ducey
- 9:40 190.** Evaluating the probability of success in general chemistry coursework using placement testing and course prerequisite information. **Y. Law**, E. G. Olmstead, Jr
- 10:00 191.** Targeting diverse learning needs in general chemistry with a buffet redesign model. **K. Woelk**
- 10:20** Break.
- 10:40 192.** Teaching chemistry in inclusion classrooms: Implications for chemistry teacher education. **F. Mumba**
- 11:00 193.** Zambian pre-service science teachers' ranking of chemistry education goals. **A. Banda**, F. Mumba, V. M. Chabalengula, S. Mbewe
- 11:20 194.** Teaching assistants' successes and challenges in Assessment, Review and Instruction System (ARIS) program. G. Kinsel, **V. Wong**, F. Mumba
- 11:40 195.** Impact of computer-based structured learning workshop on graduates teaching assistant's specific chemistry content. V. Wong, **K. K. Priyasantha**, G. Kinsel, F. Mumba

**Thursday, October 20, 2011, 8:55 AM – 12:00 PM**

**Supramolecular Chemistry in Membranes**

**Room: St. Moritz**

George W. Gokel, Jerry L. Atwood, *Organizers*

*Supported by Division of Organic Chemistry*

- 8:55** Introductory Remarks.
- 9:00 196.** Synthetic organic transporters that function in bilayer membranes. **G. Gokel**, S. Negin, M. Daschbach, J. Atkins, M. Patel, P. Ogirala, J. Autry, N. Curvey
- 9:30 197.** Transmembrane ion transporters made from various natural products and their analogs. S. Bahmanjah, N. Zhang, S. Rastogi, **J. T. Davis**
- 10:00 198.** Protein-binding molecular switches: Designs based on supramolecular and nucleic acid chemistry. **J. Jayawickramarajah**, D. C. Harris, X. Su
- 10:30 199.** Nor-seco-cucurbit[n]uril molecular containers. **L. Isaacs**

**11:00 200.** Assembly and binding properties of deep-cavity cavitands in water. **B. C. Gibb**

**11:30 201.** New strategy of transforming pharmaceutical crystal forms. **J. L. Atwood**, J. Tian, S. J. Dalgarno

**Thursday, October 20, 2011, 10:30 AM – 12:00 PM**

**General Poster Session II**

**Versailles Ballroom**

- 202.** Encapsulation of cantharadin in gold nanoshells for use as a potential cancer therapeutic agent. C. M. Klimavicz, **L. Baxter**, P. W. Barnes, G. D. Bennett
- 203.** Investigating solution-phase architecture of copper-seamed C-heptadecylpyrogallol[4]arene nanocapsules. **N. J. Schuster**, H. Kumari, S. R. Kline, C. L. Barnes, J. L. Atwood
- 204.** Self-assembled nanoparticles from non-lanthanide metal oleates for magnetic resonance imaging application. D. Pan, **C. Yalaz**, A. Senpan, A. H. Schmieder, S. A. Wickline, G. M. Lanza
- 205.** Synthesis and biological evaluation of irregular-shaped micelles prepared from amphiphilic di block co polymer. D. Pan, **B. Kim**, A. H. Schmieder, S. A. Wickline, G. M. Lanza
- 206.** Infrared studies of photochemistry of adsorbed species over semiconducting nanoparticles. **J. Kristalyn**, J. VanAuker, S. Bandaru, D. K. Paul, K. J. Klabunde
- 207.** Low-temperature photoluminescence spectroscopy of single semiconductor quantum wires. **R. A. Burnett**, R. A. Loomis, V. L. Wayman, W. E. Buhro, J. J. Glennon, Y. Liu, B. S. Hoener
- 208.** Analytical strategies for monitoring and quantifying interactions of gold nanoparticles with thiolated molecules in solution. **C. Burke**, M. Roca
- 209.** Construction of functional group arrays on SAMs with the guanidium-sulfonate macromolecular synthon. **G. Ruan**, M. Hynes, A. Munir, J. A. Maurer
- 210.** Attachment of a Fluorescent Dye to Core-Shell Quantum Dots. **K. Luepke**, S. Adrian, B. Eichler
- 211.** Does the reaction of thiol with surface cluster atoms of Au nanoparticles, prepared by the solvated metal atom dispersion (SMAD) method, yield RS-H or RS<sup>-</sup> interactions? **J. E. Matthiesen**, K. J. Klabunde, D. Jose, Y. Kuo

212. Degradation of Rhodamine B Using TiO<sub>2</sub> Nanofibers Calcined in O<sub>2</sub> and H<sub>2</sub>. **J. Benoy**, E. Obuya
213. Effects of two commercial nanoparticles on two unique environmental bacteria. **K. Ruedinger**, K. Crawford, S. Mueller-Spitz
214. Investigations into Metal-Seamed Dimeric Capsules of Aryl-Pyrogallol[4]arenes. **S. M. Hirner**, D. A. Fowler, A. K. Maerz, C. A. Deakyne, J. L. Atwood
215. Study of the relation of nanoporous gold structure to optical and electrochemical responses to protein binding. **J. K. Bhattarai**, Y. Tan, A. V. Demchenko, K. J. Stine
216. Electroanalytical studies to determine the surface morphology of nanoporous gold. **A. Sharma**, Y. H. Tan, J. Bhattarai, A. V. Demchenko, K. J. Stine, B. Pandey
217. Surface area and pore size characteristics of nanoporous gold subjected to thermal, mechanical, or chemical modifications studied using BET isotherm analysis, cyclic voltammetry, and scanning electron microscopy. **J. A. Davis**, Y. Tan, A. V. Demchenko, K. J. Stine
218. The effect of 1-methyl, 2,3 dimethylimidazolium tetrafluoroborate BDMIMBF<sub>4</sub> ionic liquid as a mobile phase additive on the adsorption behavior of tryptophan. **T. Ahmad**, K. Aluguvelli
219. Investigation of the effect of 1-butyl -3-methyl imidazolium tetrafluoroborate ionic liquid on the separation of basic drugs. **T. Ahmad**, K. Aluguvelli, T. Ahmad, S. Salam
220. Dye-loaded porous polymer nanocapsules as new optical sensor platform. **M. D. Kim**, S. A. Dergunov, E. Lindner, E. Pinkhassik
221. Surface chemistry studies of CO<sub>2</sub> with the MgO(100) surface. **J. Wang**, C. Greenlief, T. R. Marrero
222. Analysis of variance components in spectroscopic imaging data. **J. Kwak**, R. Reddy, S. Sinha, R. Bhargava
223. Improving the compatibility of macrocyclic polyamide compounds within ion-selective membranes for fluoride analysis. **Q. Zhang**, J. T. Mitchell-Koch, K. Bowman-James
224. Method for testing antibiotic residues in milk, fish, and distiller grain. **J. Baldwin**
225. Transmission Raman tomography for determining the position and size of targets buried in light scattering media. **M. R. Kole**, M. V. Schulmerich, M. K. Gelber, R. Bhargava

226. Application of three chromatographic techniques in the bioanalysis of a new thiazolodiazepin ultra-short-acting hypnotic. **E. A. Abourashed**, M. Hefnawy, H. I. El-Subbagh
227. Determination of DNA base pairs by surface-enhanced Raman scattering spectroscopy. **M. W. Stutelberg**, B. A. Logue
228. Effect of sodium hydroxide and sodium pyrophosphate on the extraction of humic acid and humin from different source materials. **C. Johnson-Edler**, G. Chilom, J. Rice
229. Solvent dependent cluster formation of thioamide-based Pd and Pt pincer complexes. **R. A. Begum**, Q. Wang, V. W. Day, K. Bowman-James
230. Free energy correlations of platinum(II) biphenyl complexes containing 2,2'-bipyridine derivatives. W. Huang, D. Rillema, K. Siam, **A. J. Cruz**, D. Base.
231. Developing oligourea-based anion ligands inspired by metal coordination. **C. Jia**, S. Li, B. Wu, K. Bowman-James
232. Diffusion of tin from TEC-8 conductive glass into mesoporous titanium dioxide in dye sensitized solar cells. **J. Cabell**, R. J. LeSuer
233. (Triphos)Ir(III)-Complexes for photo Chemistry Study. **A. Ross**, P. R. Sharp, C. Barnes
234. Elucidating the mechanism of electrocatalytic dioxygen reduction with copper complexes. **M. A. Thorseth**, C. S. Letko, T. B. Rauchfuss, A. A. Gewirth
235. Rhenium complexes as photocatalysts in the reduction of CO<sub>2</sub> to CO. **E. Oweggi**, V. Komreddy, D. Rillema
236. Preparation, characterization and photocurrent efficiency of Re(I) and Ru(II) bipyrazine complexes. **V. Komreddy**, N. Subbaiyan, E. Oweggi, D. Rillema, C. Wilkinson
237. Effect of graphene nanofillers on flexible molded polyurethane foam properties. **N. Bilic**, I. Javni, Z. S. Petrovic
238. Synthesis of comb-like polymers with rigid-rod side chains. **X. Bai**, X. Chen, J. Dias, T. Sandreczki
239. Foam from cashew nut shell liquid. **D. Hong**, M. Ionescu, I. Javni, Z. S. Petrovic
240. Dynamic solid phase microextraction sampling for monoterpenes in the presence of ozone. **W. Hua**, K. E. Huff Hartz
241. Plastic debris: Is Lake Superior invaded by synthetic polymers? **L. M. Rios**

242. Self-assembled polyelectrolyte complex: Sericin/DDAB. R. Chollakup, **W. Smitthipong**, K. Mougín, M. Nardin
243. Surface modification of silk fabric using polyelectrolyte technique. **R. Chollakup**, W. Smitthipong, R. Tantatherdtam, M. Nardin
244. Dual control of selectivity in the synthesis of donor-acceptor cyclopropanes via the addition of alcohols to *in situ* generated cyclopropenes. **P. G. Ryabchuk**, J. P. Matheny, I. A. Babkov, M. Rubina, M. Rubin
245. Investigating the mechanism of formation of phenanthridine fused quinazoliniminiums from heteroenyne-allenes. **K. Robb**, S. Rayat
246. Molecular Scaffold in Biocatalysis. X. Song, W. Niu, **J. Guo**
247. Studies towards the synthesis of protected derivatives of 4(5)-benzylhistidine suitable for peptide synthesis. D. D. Smith, **V. M. Crowley**, W. Gergens, P. W. Abel, A. T. Gallagher, M. Hulce
248. Synthetic applications of indole aryne cycloadditions. New strategies for the construction of complex natural products. N. Chandrasoma, **A. Nerurkar**, L. Maina, N. Brown, D. Luo, A. Brassfield, J. DeCapo, S. Suarez, K. R. Buszek
249. Parallel Synthesis of Alkyl and Aryl *S-tert*-butylthioethers. **R. Norcross**, J. Stanfield, R. W. Fitch

**THURSDAY AFTERNOON SESSIONS**  
**OCTOBER 20, 2011**

**Thursday, October 20, 2011, 1:00 PM – 4:40 PM**

**Analytical Chemistry General Session A**

**Room: Basel**

- 1:00 250.** Enhanced Fourier transform infrared (FT-IR) spectroscopic imaging. **R. K. Reddy**, P. S. Carney, R. Bhargava
- 1:20 251.** Towards the design of an enzymatic breath sensor for acetone. **N. Hausmann**, S. D. Minteer
- 1:40 252.** Measuring protease concentrations in dog urine: A new diagnostic method for cancer detection? **L. K. Bossmann**, D. Udukala, C. Robinson, H. Wang, M. Kalita, M. T. Basel, M. Pyle, D. McCaw, D. L. Troyer, S. H. Bossmann
- 2:00 253.** Sub-diffraction determination of changes to the actin network by stimulated emission depletion microscopy. **M. D. Lesoine**, S. Bose, J. W. Petrich, E. A. Smith
- 2:20 254.** Measurements of integrin mobility in the membrane of cultured cells using fluorescence recovery after photobleaching (FRAP) and single molecule imaging. **D. Mainali**, N. Arora, E. Smith
- 2:40** Break.
- 3:00 255.** Scanning Angle Total Internal Reflection Raman Microscopy of Plant Cell Wall Biopolymers. **E. A. Smith**, K. McKee, M. Meyer, J. Lupoi
- 3:20 256.** Design and characterization of a dual-signaling DNA sensor based on target hybridization-induced change in DNA probe flexibility. **W. Yang**, R. Y. Lai
- 3:40 257.** Multivariate spectral analysis of phase partitioning in methacrylate-based dentin adhesive. **Q. Ye**, P. Spencer, R. Parthasarathy, J. Park, J. S. Laurence, A. Misra
- 4:00 258.** Quantitative investigation of surface functionalization of cylindrical nanopores derived from polystyrene-poly(methylmethacrylate) diblock copolymers. **F. Li**, R. Diaz, T. Ito
- 4:20 259.** In vitro simulation studies for the development of a nocturnal hypoglycemic alarm based on near-infrared spectroscopy. **S. Ranasinge Pathirajage**, G. W. Small



**Thursday, October 20, 2011, 1:00 PM – 5:00 PM**

**Biochemistry General Session**

**Room: Bern**

- 1:00 260.** Utilizing enzyme cascades for deep oxidation of a variety of biofuels. **D. Sokic-Lazic**, S. D. Minteer
- 1:20 261.** Optimizing the growth of *M. smegmatis* with respect to cell mass yield and fermentation cost. **S. O. Wendel**, A. S. Perera, P. H. Pfromm, P. Czermak, S. H. Bossmann
- 1:40 262.** High resolution imaging mass spectrometry of sphingolipid and cholesterol distributions in intact mammalian plasma membranes. **J. F. Frisz**, K. Lou, H. Klitzing, R. Wilson, W. P. Hanafin, R. Kim, V. Lizunov, P. K. Weber, J. Zimmerberg, M. L. Kraft
- 2:00 263.** Diffusion dynamics of single molecules confined in biomimetic crowded environment. R. Welty, J. Bentley, D. Wickramasinghe, **A. A. Heikal**
- 2:20 264.** New molecular biomarkers for cancer detection. **C. D. Nusbaum**, S. Almowallad, S. A. Wolfe, J. E. Mayfield, J. G. McAfee
- 2:40** Break.
- 3:00 265.** Membrane topology and mechanistic view of a disulfide bond generating membrane protein by a structural model of membrane-embedded DsbB. **M. Tang**, A. E. Nesbitt, L. J. Sperling, D. A. Berthold, C. D. Schwieters, R. B. Gennis, C. M. Rienstra
- 3:20 266.** Microglial activation by A $\beta$ (1-42) protofibrils. **G. S. Paranjape**, L. K. Gouwens, D. C. Osborn, M. R. Nichols
- 3:40 267.** Secondary structure comparison of the early onset Parkinson's disease related mutants and wild-type  $\alpha$ -synuclein fibrils. **L. R. Lemkau**, G. Comellas, L. K. Rikardson, S. W. Lee, W. S. Woods, J. M. George, C. M. Rienstra
- 4:00 268.** Rapid and accurate determination of entrapped volume and permeability in liposomal suspensions. **J. T. Buboltz**
- 4:20 269.** Zinc and Manganese Homeostasis in *Streptococcus pneumoniae* and *Myxococcus xanthus*. **F. E. Jacobsen**, L. Brumley, K. Kazmierczak, M. Winkler, D. Giedroc, R. Taylor
- 4:40 270.** Archaeal Histones: Homo- or Heterodimers? **L. Gray**, J. Kristalyn, M. Miller, J. G. McAfee, I. S. Zegar

**Thursday, October 20, 2011, 1:00 PM – 4:50 PM**

**Biological Mass Spectrometry**

**Room: Alpine I**

Henry Rohrs, Joshua Coon, Michael Gross, *Organizers*

*Supported by Advion, Leco, Waters, JEOL, Thermo Scientific, Bruker, Ab Sciex, Agilent Technologies, Shimadzu, and Division of Analytical Chemistry*

- 1:00 271.** New mass spectrometry technology for protein sequence analysis and beyond. **J. J. Coon**
- 1:45 272.** Characterization of D-amino acid-containing peptides (DAACPs) in the central nervous system. **L. Bai**, E. V. Romanova, I. Livnat, J. V. Sweedler
- 2:15 273.** Protein interaction reporter: “News” on protein topologies in cells. **J. E. Bruce**, J. D. Chavez, C. Zheng, L. Yang, C. Weisbrod
- 3:00** Break.
- 3:20 274.** Directed mass spectrometry: Molecular dissection of androgen signaling networks in human disease. J. J. Hsaio, H. D. Martinez, **M. D. Wright**
- 4:05 275.** Mass spectrometry characterization of a therapeutic antibody conjugate. **J. B. Sperry**, J. C. Rouse, J. A. Carroll

**Thursday, October 20, 2011, 1:00 PM – 2:30 PM**

**General Poster Session III**

**Versailles Ballroom**

- 276.** Helical dimanganese-(salen) complexes and application in asymmetric epoxidation of olefin. **T. Liu**, C. Levy, J. Desper
- 277.** Anisotropy tensor alignment in  $\{\text{Fe}^{\text{III}}_n\text{Ni}^{\text{II}}_m\}$  cyanometalate-based single-molecule magnets. **P. J. Janini**, Y. Zhang, U. P. Mallik, N. Rath, R. Clérac, S. M. Holmes
- 278.** Coordination of bqp on Rhenium(I). **C. J. Bosworth**, D. J. Losey, D. R. Black, S. E. Hightower
- 279.** Electronic communication and reaction chemistry of dinuclear anthracene bridged platinum complexes. **Y. Li**, P. R. Sharp

280. Reductive Photoelimination of Chlorine from Organoplatinum(IV)Chloro Complexes. **T. A. Perera**, M. Moody, P. R. Sharp
281. Cloning, Purification and Characterization of Acetate Kinase from Methicillin resistant *Staphylococcus aureus* Mu50 strain. **T. McCune**, C. Wu
282. An Exploration on Purification of putative Fructose 1, 6-Bisphosphate Adolase from Methicillin resistant *Staphylococcus aureus* Mu50 strain. **E. Girad**, C. Wu
283. Comparative analysis of protein phosphorylation in the Protein Databank: What have we known? **M. Zha**, J. Warnke, H. Zhong
284. Synthesis of 3-pyridylmethyl glucosinolate from 3-pyridylacetonitrile. **J. W. Keppen**, J. J. Clark, J. R. Mays
285. Synthesis and RP-HPLC Monitored Hydrolysis of Non-natural Glucosinolates. **K. J. Vastenhout**, J. R. Mays
286. Exploring the Significance of F427 in Anthrax Protective Antigen using <sup>19</sup>F-NMR. **L. J. Ferris**, J. G. Bann
287. Optical and DNA binding studies of *N*-fused heterocyclic cations based on quinazoline scaffold. **C. Galloway**, C. A. Larson, O. Alawode, V. K. Naganaboina, S. Rayat
288. A putative mammalian riboswitch in the spermine biosynthetic pathway. **K. Del Vecchio**, J. Monahan, M. McDevitt, G. Soukup, J. Soukup
289. *glmS* ribozyme mechanism and development of artificial agonists as candidate antibiotics. **E. Johnson**, M. McDevitt, D. Renner, X. Fei, D. Berkowitz, G. Soukup, J. Soukup
290. Thermodynamic contribution of pseudouridine·adenosine base pairs in oligoribonucleotides. **G. A. Hudson**, R. Bloomingdale, W. Qu, V. E. Ponnusamy, B. M. Znosko
291. Establishment of photo-activated localization microscopy (PALM) for imaging signaling complexes on the surfaces of cells. **B. E. Iverson**, A. Hoppe
292. Evaluating transgenic *Xenopus* as a model system for the expression of secreted proteins. **K. R. Marshall**, M. A. Dean, J. G. Laird, S. A. Baker
293. Potential for using waste glycerol from biodiesel production as a carbon source for heterotrophic algal feedstock production. **C. Wooldridge**
294. Thermodynamic Parameters for the Formation of RNA Duplexes with Triple Nucleotide Bulges. **M. H. Murray**, J. A. Hard, A. R. Davis, B. M. Znosko

295. Effects of non-nearest neighbors on the stability of RNA GNRA tetraloops. **P. L. Vanegas**, T. S. Horwitz, B. M. Znosko
296. Fluorescence polarization imaging of sub-resolution membrane curvature during endocytic events. **E. D. Swanson**, J. G. Kerkvliet, H. D. Adam
297. Determination of adenine nucleotide levels in rat urine by HPLC to elucidate the role of resveratrol in reducing cisplatin toxicity. **H. J. Gregg**, A. W. Hummer, T. L. Troyer, M. A. Valentovic
298. Investigation of alcohol-tolerant deoxyribozymes. **A. K. Behera**, K. O. Alila, D. A. Baum
299. Synthesis of 1-butyl-3-methylimidazolium derivatives. **M. E. Amundson**, A. R. Letcher, G. W. Earl, D. E. Weisshaar
300. Synthesis and Characterization of Hydrophobic and Hydrophilic Siloles for Cytotoxicity Studies and Applications in Printable Radio-frequency Antennas. **E. Gardner**, B. Eichler
301. Synthesis and Characterization of Novel 2,3,4,5-Tetraarylsilacyclopentadienes. **J. Drenkow**, B. Eichler
302. Soluble Luminescent 2,3,4,5-Tetraarylsiloles Synthesis and Characterization for Use in OLED Devices. **B. Jackson**, B. Eichler
303. Synthesis of matrix metalloprotease chemical probes to profile enzyme activity. **M. E. Boursier**, K. Nandy, A. T. Wright
304. Synthesis of isothiocyanates with electron-deficient aromatic rings. **Z. Erickson**, J. R. Mays
305. Selective COX-2 inhibition and anticancer activity of diarylalkynylsulfonamides complexed with hexacarbonyl dicobalt. **P. Mancina**, S. Debbert
306. Synthesis of novel alkyne hexacarbonyldicobalt complexes and their effect on human breast and prostate cancer cells. **C. Vornholt**, S. Debbert
307. Synthesis of a new monomer for a fluorescent conjugated polymer to act as a chemosensor. **A. Pfeifle**, J. Duffy-Matzner, S. Pinnock, M. Fegley, A. Oakes
308. Synthetic efforts towards a selective photodynamic therapy agent. **F. A. Venable**, Q. A. Best, C. N. Scott
309. Preparation of sulfones utilizing a new green ruthenium/aluminum oxide heterogeneous catalyst. **G. Meyer**, J. Heath, T. Williams, L. Clippard, M. Ali, B. Olesen, B. Ranu

- 310.** Preparation of sulfones utilizing a new green ionic liquid oxidizing reagent. T. Williams, **L. Clippard**, J. Heath, G. Meyer, M. Ali, B. Olesen, B. Ranu
- 311.** Synthesis and DNA or RNA intercalation of 4-substituted naphthalimides. **Y. Ren**, T. Zahrl, L. K. Hardebeck, M. Lewis
- 312.** Optimization of a Multistep Synthesis of Acyl Pyrazolidinones. **P. E. Flores Gallardo**, C. P. Jasperse
- 313.** Toward  $^{18}\text{F}$ -naproxen radiotracer synthesis via reductive elimination of a diaryliodonium salt. **K. S. Glaspy**, J. C. Easdon, L. Qin, K. Neumann, S. DiMagno
- 314.** Interference by matrix esters during headspace-gas chromatography analysis of volatile alcohols. **G. M. Fischer**, M. D. Power
- 315.** Mechanistic Investigation of the  $\gamma$ -C-alkylation of  $\beta$ -Ketoesters using Equilibrating Conditions. **J. G. Hinman**, W. B. Bosma, B. Andersh
- 316.** Utilization of  $\beta$ -Ketoester Monoanions for Amide Formation. **J. J. Remsza**, B. Andersh
- 317.**  $\gamma$ -C-alkylation of  $\beta$ -Ketoesters using Equilibrating Conditions: The Identity of the  $\beta$ -Ketoester. **M. E. Roark**, B. Andersh
- 318.** Synthesis and characterization of novel high-nitrogen energetic materials. D. E. Romonosky, **C. M. Hadsall**, G. D. Bennett, P. W. Barnes
- 319.** Synthesis of 3-oxo- $\delta$ -lactones via  $\gamma$ -C-alkylation of  $\beta$ -Ketoesters using Equilibrating Conditions. **F. S. Couri**, B. Andersh
- 320.** Towards the synthetic development of an anion binding molecule. **E. Sullivan**, S. Garvey, A. Dawson, C. Bagwill, M. Lewis
- 321.** Synthesis and Characterization of Peptide-capped ZnS Nanoparticles. **K. L. Holt**, W. A. Patton
- 322.** Optimization of polymer coatings for building addressable libraries on microelectrode arrays. L. Hu, **M. Graaf**, K. Moeller
- 323.** Efficient and general approach for safe oxidation of alkyl and aromatic sulfides to sulfones. **M. R. Lutz Jr**, K. Boyer, D. Baehr, E. Blumenthal, I. Likhovtorik

**Thursday, October 20, 2011, 1:00 PM – 4:40 PM**  
**Organic Chemistry General Session C**  
**Room: Geneva**

- 1:00 324.** “Click, Click, Click, Cyclize” strategy to novel tricyclic sultams. **K. Jeon**, P. R. Hanson\*
- 1:20 325.** Tether-mediated, one-pot metathesis processes: Application in small molecule and total synthesis. **P. K. Venukadasula**, G. M. Suryan, R. Chegondi, S. Maitra, P. R. Hanson\*
- 1:40 326.** Resveratrol: Efficient synthetic method and selective delivery method to target cancer cells. **H. C. Manawadu**, T. B. Shrestha, D. L. Troyer, S. H. Bossmann
- 2:00 327.** Buckytriplet: Cyclotrimerization of Corannulyne. **M. Yanney**, A. Sygula, F. Fronczek, W. P. Henry, D. Beard
- 2:20 328.** Synthesis of benzimidazolium ions for dye-sensitized solar cells. **R. C. Hawkins**
- 2:40** Break.
- 3:00 329.** Comparing Reductive Cleavage Methods in the Structure Determination Of Natural Products. **K. P. Manfredi**
- 3:20 330.** Isolation and characterization of novel natural products isolated from plants utilized in traditional folk medicine. **K. N. Whitlatch**, J. D. Wagoner, J. Sparks, L. G. Huggins, T. L. Troyer
- 3:40 331.** Phosphate tether-mediated synthetic studies towards the total synthesis of fostriecin and analogs. **S. Jayasinghe Mudiyansele**, J. P. McParland, P. R. Hanson
- 4:00 332.** Synthetic studies towards (–)-lyngbouillose and phosphate tether-mediated ring-closing metathesis studies . **R. Chegondi**, S. Maitra, J. Markley, P. R. Hanson
- 4:20 333.** Recent developments on the homoallylation reaction and its application in the synthesis of the tetrahydrofuran ring. **M. P. Paudyal**, C. D. Spilling

**Thursday, October 20, 2011, 1:00 PM – 5:00 PM**

**Supramolecular Chemistry in Membranes**

**Room: St. Moritz**

George W. Gokel, Jerry L. Atwood, *Organizers*

*Supported by Division of Organic Chemistry*

- 1:00 334.** Crystal engineering cocrystals: Application in the structure determination of a chiral ladderane. **L. R. MacGillivray**
- 1:30 335.** Structural variations, dynamics, and molecular intercalation and transport in layered ammonium carboxylates. **A. M. Beatty**

- 2:00 336.** Molecular pipes and boxes: Containers for anions. Q. Wang, V. W. Day, **K. Bowman-James**
- 2:30 337.** Supramolecular concepts in mechanochemical synthesis. **T. Friscic**
- 3:00 338.** Exploring the surface modifications of macrocycles via copper catalyzed azide-alkyne cycloaddition “click” coupling. **S. M. Grayson**, Y. Li, B. Gibb
- 3:30 339.** Responsive nanoassemblies. **S. Thayumanavan**
- 4:00 340.** Glowing rotaxanes: a new paradigm for optical imaging. **B. D. Smith**
- 4:30 341.** Metal-organic calixarene assemblies. **S. J. Dalgarno**

**Thursday, October 20, 2011, 1:00 PM – 3:00 PM**  
**Technical Symposium on Plant Chemistry**  
**Room: Davos**

Brent M. Znosko, *Organizer*

*Supported by Education Division of the American Chemical Society, Principia College*

- 1:00 342.** Evolution of herbicide resistance. **D. Sammons**
- 1:40 343.** Plant natural products in a modern drug discovery program. **R. B. Williams**
- 2:20 344.** Post-genomic elucidation of plant natural product pathways. **T. M. Kutchan**, D. Ruzicka, M. Rolf

**Thursday, October 20, 2011, 1:30 PM – 4:45 PM**  
**High Sensitivity Spectroscopy**  
**Room: Zermatt**

James J. O'Brien, *Organizer*

*Supported by Division of Physical Chemistry, Division of Analytical Chemistry, Coherent*

- 1:30** Introductory Remarks.
- 1:35 345.** High sensitivity absorption spectra using broadband intracavity laser spectroscopy. **J. J. O'Brien**, L. C. O'Brien

- 2:10 346.** Fiber laser-induced fluorescence and laser-induced phosphorescence spectroscopy for atmospheric measurements. **F. Keutsch**
- 2:45 347.** New approaches to high-resolution, high-sensitivity spectroscopy of molecular ions. **B. J. McCall**
- 3:20** Break.
- 3:35 348.** Single-conformation spectroscopy of synthetic foldamers, peptides, and model lignin compounds. E. G. Buchanan, J. C. Dean, **T. S. Zwier**
- 4:10 349.** Transient absorption microscopy studies single metal and semiconductor nanostructures. **G. V. Hartland**

**Thursday, October 20, 2011, 1:30 PM – 5:00 PM**  
**Small Chemical Businesses - What Every Small Business Owner Needs to Know about Patents, Trademarks, and Intellectual Property**  
**Room: Alpine II**

Harry. J. Guttman, *Organizer*

*Supported by Division of Small Chemical Businesses*

- 1:30** Introductory Remarks.
- 1:35 350.** Who owns patented technology? A review of the U.S. Supreme Court's recent decision in *Stanford v Roche* and how it applies to federally-funded research. **S. C. Hall**
- 2:20 351.** Patent law reform legislation: Survival tips for academic and entrepreneurial scientists. **J. Stipkala**
- 3:05** Break.
- 3:25 352.** Small businesses and their assets: Building an intellectual property wall. **T. J. Welch**
- 4:10** Panel Discussion.
- 4:55** Concluding Remarks.

**Thursday, October 20, 2011, 3:00 PM – 4:30 PM**  
**General Poster Session IV**  
**Versailles Ballroom**



353. Development and Practice of “Air Pollution” Educational Material Unit Aiming at Education for Sustainable Development (ESD) in Korea. **Y. Kong**
354. Comparison on Elementary Science Achievement between Korea and Japan in TIMSS 2007. **Y. Kong**
355. Tutorial on the facile determination of the number of Kekulé and Dewar resonance structures in conjugated systems. **J. R. Dias**
356. Impact of participation in the Indiana Science Initiative on teachers' beliefs about student learning in science. **N. Cook**, G. C. Weaver, B. Walker
357. Discovering  $^{13}\text{C}$ -NMR,  $^1\text{H}$ -NMR and IR spectroscopy in the General Chemistry laboratory through a sequence of guided-inquiry exercises. **D. C. Justice**, H. Iler
358. Kinetic study of the reaction  $\text{H}_2\text{O}_2 + 3 \text{I}^- + 2 \text{H}^+ \rightarrow \text{I}_3^- + 2 \text{H}_2\text{O}$  employing spectroscopic methods. **H. R. Krueger**
359. Teaching Precipitation Titration without the Buret: A Coulometric Method for the Determination of Chloride. **D. W. Harak**, M. Kimbrough
360. Project SEED in Kansas City. **E. W. Hellmuth**
361. Buffer standards for the zwitterionic buffer (ACES) at  $I = 0.16 \text{ mol}\cdot\text{kg}^{-1}$  from 5 to 55 °C. **I. B. Henson**, J. M. Stegner, J. J. Dinga, L. Dieterman, L. N. Roy, R. N. Roy
362. Buffer standards for the physiological pH of *N*-[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]glycine (TRICINE) from  $T = (278.15 \text{ to } 328.15) \text{ K}$ . **J. A. Veliz**, J. M. Stegner, C. E. Summers, G. L. Suhrheinrich, L. N. Roy, R. N. Roy
363. New microboiling point technique for the undergraduate laboratory. **W. J. King**, J. A. Lehman, M. Hood, K. N. Whitlatch, J. D. Wagoner, T. L. Troyer
364. Using Non-Silver photography as a discovery based lab for non-science majors. J. Yukna, **M. Sparks**
365. Theoretical studies of a cyclic peroxide reactive intermediate. **S. Christian**, W. W. Winn, J. N. Woodford
366. Kinetics of Pore Formation and Receptor (CMG2) Dissociation from the Anthrax Protective Antigen. **K. K. Andra**
367. Structure and function of the Alternative Complex Three from the photosynthetic bacteria *Chloroflexus aurantiacus* and *Roseiflexus castenholzii*. **E. L. Wunderlich Majumder**, R. E. Blankenship

- 368.** Probing the effect of the electron density distribution in the primary electron on the directionality of charge separation in photosynthetic reaction centers. **M. A. Harris**, P. D. Laible, L. Kressel, C. Luehr, M. Wander, D. Holten, D. K. Hanson, C. Kirmaier
- 369.** Identification of DNA aptamers for a redox cofactor. **I. Emahi**, A. J. Mason, K. J. Schlund, D. A. Baum
- 370.** *Staphylococcus aureus* and *Enterococcus faecalis* peptidoglycan tertiary structure by rotational-echo double resonance NMR spectroscopy. **H. Yang**, S. Kim, M. Singh, M. Preobrezenskya, J. Schaefer
- 371.** Length requirements of the Hoogsteen bound third strand for the formation of RNA triple helices. **J. A. Holland**, A. Cardozo
- 372.** Immobilization of thylakoids with polyethylenimine-based hydrogel for solar energy conversion. **G. Vellaichamy**, K. H. Sjöholm, M. T. Meredith, S. D. Minter
- 373.** Topology and dynamics of conformational exchange of a small multidrug transporter, EmrE. **S. Dutta**, R. Vafabakhsh, E. A. Morrison, G. T. DeKoster, T. Ha, K. A. Henzler-Wildman
- 374.** Exploring lipid interactions in the *E. coli* mechanosensitive channel of small conductance (MscS). **H. R. Malcolm**, Y. Heo, D. E. Elmore, J. A. Maurer
- 375.** Development of specific inhibitors of JmjC-domain histone demethylases. **B. Gordon**, L. M. Mirica
- 376.** Design, synthesis, and evaluation of inhibitors of norwalk virus 3c protease. **S. Mandadapu**, K. Tiew, G. He, S. Aravapalli, M. R. Gunnam, K. R. Alliston, G. H. Lushington, Y. Kim, K. Chang, W. C. Groutas
- 377.** Cloning and expression of L-fucose metabolizing genes. **T. J. Wiese**, S. C. Rogers, L. Yang, T. J. Wiese
- 378.** Use of chromatography to characterize a substrate binding constant for a His-tag immobilized ascorbate peroxidase. **F. A. Kovacs**, B. White, A. Moser
- 379.** Covalent immobilization of C-terminal hydrazide labeled proteins to ketone-presenting self-assembled monolayers (SAMs). **A. T. Castner**, J. A. Maurer
- 380.** Inactivation of PTP-SHP2 by peroxymonocarbonate. **S. M. Lewis**, D. Seinner, H. Singh, K. Gates
- 381.** Studying neuronal behavior in response to changes in microenvironment: An *in vitro* approach. **D. M. Johnson**, S. M. Spangler, J. P. Abi-Mansour, J. A. Maurer

382. Adenine-4-aminobiphenyl formation by acid hydrolysis of *TP53 exon7* cDNA in the presence of 4-aminobiphenyl as evidenced by LC-ESI-MS/MS. **P. R. Knoll**, J. C. Means
383. Cyclipostins as Inhibitors of Rat Hormone Sensitive Lipase. **E. Vasilieva**, R. K. Malla, S. Dutta, B. Martin, C. M. Dupureur, C. D. Spilling
384. Fluorescent sphingolipid precursors and click chemistry cholesterol analogs for imaging of sphingolipid and cholesterol distribution in the plasma membranes of living cells. **K. Lou**, R. Kim, M. L. Kraft
385. Zinc homeostasis and swarm expansion in *Myxococcus xanthus*. **L. N. Brumley**, F. E. Jacobsen, R. G. Taylor
386. Study of heparin oligosaccharides binding to proteins using affinity capillary electrophoresis. **M. Dinges**, B. Rogers, A. Korir
387. Study of carbon assimilation in plants labeled with stable and radioactive isotopes by solid state NMR and direct positron imaging. **M. Singh**, G. Potter, R. Dirks, L. Sobotka, J. Schaefer
388. Effect of a mutant with altered dynamics on hydride transfers catalyzed by thymidylate synthase. **T. Abeysinghe**, Z. Wang, A. Kohen
389. Halogen bonding interactions in substituted tetraphenylethylenes. **P. P. Kapadia**, D. C. Swenson, F. Pigge
390. Biosynthetic considerations and progress toward a total synthesis of phomopsichalasin/diaporthichalasin. **J. C. Lo**, S. G. Brown, E. P. Sizova, T. R. Hoye
391. Studies of the Bodroux reaction in tetrahydrofuran. **D. C. Hawkinson**, A. Furness
392. Anhydrobase mediated annulation reactions of substituted pyridines. **A. I. Lansakara**, S. G. Parameswarappa, F. Pigge
393. Kinetic resolution of N-acyl- $\beta$ -lactams via non-enzymatic enantioselective alcoholysis. **V. D. Bumbu**, V. B. Birman
394. Kinetic resolution of  $\beta$ -lactams via catalytic, enantioselective N-acylation. **V. D. Bumbu**, X. Yang, V. B. Birman
395. Nucleosome Phase Greatly Affects Deamination rate of a 5-Methylcytosine Containing DNA Photoproduct. **Q. Song**, V. Cannistraro, J. A. Taylor
396. Exploring site-selective oxidative cyclizations on microelectrode arrays. D. Kesselring, **B. H. Nguyen**, K. D. Moeller

- 397.** Development of fluorescent chemosensors for divalent and trivalent cations based on carboxylated ethynylarenes. **A. T. Gallagher**, J. T. Fletcher
- 398.** Unusual secondary kinetic isotope effect behaviors in a hydride transfer reaction in solution. **B. A. Hammann**, Q. Liu, Y. Lu
- 399.** Carboxymethylated 1,2,3-triazole-based bidentate and tridentate chelators: Preparation and amide bond conjugation under solution-phase and solid-phase conditions. **J. T. Fletcher**, B. S. Bruck, H. Ahn, M. G. Keeney
- 400.** New functionalized resin for solid extraction of heavy metal ions in water samples. S. Khazaeli, M. Rabbani, **N. Nezamabadi**

**Thursday, October 20, 2011, 3:00 PM – 6:00 PM**  
**Midwest ACS Award Symposium**  
**Zurich**

Lichang Wang, Patrick Dussault, *Organizers*

*Supported by Division of Computers in Chemistry, St. Louis Section of the American Chemical Society*

- 3:00 401.** Transition metal nanoparticles as catalysts in fuel cell applications. **L. Wang**
- 3:30 402.** DFT optical properties and growth mechanisms of gold nanoparticles. **C. M. Aikens**, B. M. Barngrover, E. B. Guidez
- 4:00 403.** Nanoporous organic structures: Creation and novel properties. **B. Gong**
- 4:30** Break.
- 5:00 404.** Computer-aided nanoscience research: Nanoice, nanoclusters, and superhydrophobicity. **X. Zeng**

The reception for the Midwest/Great Lakes Awards banquet starts at 6:00 pm followed by the banquet at 7:00 pm in Matterhorn.

**FRIDAY MORNING SESSIONS**  
**OCTOBER 21, 2011**

**Friday, October 21, 2011, 8:00 AM – 12:00 PM**  
**Analytical Chemistry General Session B**  
**Room: Basel**

- 8:00 405.** Application of twin-chain dithiol amphiphiles in electrochemical DNA sensor fabrication. **S. P. Canete**, T. J. Fisher, P. H. Dussault, R. Y. Lai
- 8:20 406.** Development of a Mitochondria-based Electrochemical Water Quality Sensor for Pesticides. **S. Maltzman**, S. D. Minter
- 8:40 407.** Microdialysis-Microchip Electrophoresis with Electrochemical and Fluorescence Detection. **D. E. Scott**, D. R. McKenzie, R. Grigsby, S. M. Lunte
- 9:00 408.** Demonstration of rapid single cell analysis on simple microfluidic devices: A study nitric oxide production in Jurkat cells. **E. C. Metto**, A. Sharma, A. H. Culbertson, K. Evans, D. B. Gunakesera, C. T. Culbertson, S. M. Lunte
- 9:20 409.** Design and characterization of an imidazole-metal ion self-assembled monolayer amenable to electrochemical biosensing applications. **A. J. Zaitouna**, R. Y. Lai
- 9:40 410.** Graphene oxide based micro-electronic device for detecting norovirus. **A. M. Prior**, D. D. Le, T. D. Nguyen, Y. Kim, K. Chang, W. Li, N. A. Oyler, D. H. Hua
- 10:00** Break.
- 10:20 411.** Electrochemical study of the diffusion of cytochrome c within nanoscale pores derived from cylinder-forming polystyrene-poly(methylmethacrylate) diblock copolymers. **B. Pandey**, K. H. Tran Ba, T. Ito
- 10:40 412.** Finite-element computer simulations on cyclic voltammograms measured at recessed nanodisk-array electrodes derived from Polystyrene-Poly(methylmethacrylate) diblock copolymers . **K. Tran Ba**, B. Pandey, T. Ito
- 11:00 413.** Characterization of Lignin from Prairie Cordgrass and Switchgrass by GC-MS analysis of Cupric Oxide and Nitrobenzene Oxidation products, Pyrolysis-GC-MS and MALDI-TOF-MS. **N. K. Bathula**
- 11:20 414.** Real-time AC voltammetry-based detection of cancerous protease (legumain) using nanoelectrode arrays. **L. Syed**, L. Zhang, A. M. Prior, D. H. Hua, J. Li

**11:40 415.** Identification of peptides from Liver Tissues of 2-Aminoanthracene exposed Fisher-344 Rats. **H. D. Abshiro**, W. E. Gato, E. O. Zargham, J. C. Means

**Friday, October 21, 2011, 8:00 AM – 12:00 PM**

**Inorganic Chemistry General Session A**

**Room: Bern**

- 8:00 416.** B ring methylated flavonols: Effects on hydrogen bonding, Al<sup>3+</sup> chelation and the structures and redox chemistry of ruthenium complexes. **K. V. Peiris**, E. Hughes, B. Spears, J. Browning, S. R. Gwaltney, W. P. Henry
- 8:20 417.** Synthesis and properties of ferrocenyl-containing porphyrins, tetraazaporphyrins, and subphthalocyanines. **V. N. Nemykin**, P. V. Solntsev, G. T. Rohde, J. R. Sabin, S. J. Dammer, K. Spurgin
- 8:40 418.** Phosph(on/in)ate-bridging dimers of vanadium (IV) complexes as potential oxidation catalysts. **C. C. McLauchlan**, A. E. Anderson, X. Riart-Ferrer, M. P. Weberski
- 9:00 419.** Stable mononuclear Pd(III) and Pd(IV) complexes in identical ligand environment: Characterization and direct reactivity comparison. **F. Tang**, J. R. Khusnutdinova, N. P. Rath, L. M. Mirica
- 9:20 420.** Pinpointing the position of an encapsulated fluoride in solution: The utility of multidimensional <sup>1</sup>H and <sup>19</sup>F NMR. **Q. Wang**, V. W. Day, K. Bowman-James
- 9:40 421.** Evaluation of platonic solids as atoms in covalent bonds. **D. Wang**, J. Van Horn
- 10:00** Break.
- 10:20 422.** Novel green light sensitizers for the near-infrared emission of lanthanide ions. **H. He**, Y. Zhong, A. G. Sykes
- 10:40 423.** Use of Ferracarboranes as Electron Transfer Mediators for Glucose Oxidase. **S. S. Graham**, P. A. Jelliss, S. Minter, V. Svoboda
- 11:00 424.** Increasing survival in a murine metastatic pancreatic cancer model, using cell-delivered nanoparticles to cause local hyperthermia. **G. S. Abayaweera**, M. Basel, T. B. Shrestha, H. Wang, O. B. Koper, S. Balivada, S. H. Bossman, D. L. Troyer
- 11:20 425.** Scanning electrochemical microscopy investigation of tribolayer surface corrosion on CoCrMo alloys used in metal-on-metal (MoM) hip joint bearings. **R. J. LeSuer**
- 11:40 426.** Germylenes R<sub>2</sub>Ge: with triplet electronic ground states. **P. P. Gaspar**, A. Solomon, H. Yeon

**Friday, October 21, 2011, 8:00 AM – 12:00 PM**

**Nanoscience General Session C**

**Room: Alpine I**

- 8:00 427.** Sensing drug mimics using size-tunable solution-phase SERS substrates. **J. K. Hedlund**, B. Shrestha, M. Pierre, A. J. Haes
- 8:20 428.** Correlating Molecular Surface Coverage and Solution-Phase Nanoparticle Concentration to SERS Intensities. **M. S. Pierre**, A. J. Haes, P. M. Mackie, M. Roca
- 8:40 429.** Comparison of stability and particle size distribution of gold colloids prepared by the solvated metal atom dispersion method and inverse micelle method. **D. Jose**, K. J. Klabunde
- 9:00 430.** Investigating the proton affinities of pyrogallol versus zinc-seamed C-alkylpyrogallol[4]arene dimeric nanocapsules. **H. Kumari**, C. M. Mayhan, A. E. Kroeger, C. W. Dye, J. L. Atwood, C. A. Deakyne
- 9:20 431.** Capillary electrophoresis promoted personalized chemotherapy. **B. S. Ayres**, A. M. Jones, M. S. Pierre, A. J. Haes
- 9:40** Break.
- 10:00 432.** Using Dielectrophoresis for Reversible Capture and Release of *E. coli* cells at Micropatterned Nanoelectrode Arrays. **L. Syed**, F. R. Madiyar, J. Liu, A. K. Price, Y. Li, C. T. Culbertson, J. Li
- 10:20 433.** Development of electrochemical immunoassay for prostate specific antigen (PSA) and carcinoembryonic antigen (CEA) on nanoporous gold. **B. P. Pandey**, A. V. Demchenko, K. J. Stine
- 10:40 434.** Withdrawn
- 11:00 435.** Toxic material forensic container (TMFC). J. J. Cremer, **A. M. Iseli**, S. Rajagopalan, J. Domino, D. Lickfield, C. W. Cole
- 11:20 436.** Development of antisense agents to detect and suppress iNOS mRNA expression in injured lung. **Y. Shen**, H. Fang, R. Shrestha, K. Wooley, J. Taylor
- 11:40 437.** High aspect ratio hydroxyapatite nanofibers filled dental restorative nanocomposites. **L. Chen**, K. Giddens, Y. Wang, Q. Yu, H. Li

**Friday, October 21, 2011, 8:00 AM – 11:40 AM**

**Organic Chemistry General Session D**

**Room: Geneva**

- 8:00 438.** Synthesis and structural analysis of a novel iodinated cyclopentadienone *via* ring-contraction iodination and its application as a substrate for oxygen-free Sonogashira reactions. **X. Chen**, X. Bai, T. C. Sandreczki, J. R. Dias
- 8:20 439.** Monomer-on-Monomer (MoM) Mitsunobu Reactions and ROMP-Derived Oligomeric Phosphates for the Application in Parallel Synthesis. **P. K. Maity**, A. Rolfe, Q. M. Kainz, S. Faisal, T. B. Samarakoon, T. R. Long, R. D. Kurtz, O. Reiser, P. R. Hanson
- 8:40 440.** Novel five-coordinate Ru(II) phosphoramidite complexes and their catalytic activity in the amination of propargylic acetates. A. K. Widaman, **E. B. Bauer**
- 9:00 441.** Metal-assisted photochemical conversion of carboxylic acids to alkanes, alkenes, and halocarbons. **J. M. Carraher**, A. Bakac
- 9:20 442.** Preparation of Benzoxazoles and Benzothiazoles Utilizing a Green Procedure. **M. Ali**, S. Madabhushi
- 9:40** Break.
- 10:00 443.** Deciphering intermolecular communication between 2-aminopyrimidines and carboxylic acids. **A. B. Grommet**, C. B. Aakeroy, J. Desper
- 10:20 444.** Thiophilicity of atomic oxygen in solution. **M. Zhang**, R. McCulla
- 10:40 445.** *cis*-5,6-Dihydro-1,10-phenanthrolines as a new class of ligands: Enzymatic resolution of *cis* and *trans* phenoxy alcohol isomers and assignment of absolute stereochemistry. **E. Schoffers**, L. Kohler, E. Driscoll, M. Zeller, S. Carla
- 11:00 446.** Total synthesis of ( $\pm$ )-*cis*-trikentrin B via intermolecular indole aryne cycloaddition and Stille cross-coupling reaction. **N. Chandrasoma**, N. Brown, A. Brassfield, A. Nerurkar, S. Suarez, K. R. Buszek
- 11:20 447.** Hydrogen-bond mediated catalysis in the organic solid state. **J. Stojakovic**
- 11:40 571.** Modulating supramolecular reactivity using covalent “switches” on a pyrazole platform. **E. P. Hurley**, C. B. Aakeroy, J. Desper

**Friday, October 21, 2011, 8:00 AM – 11:40 AM**

**Physical Chemistry General Session B**



**Room: Zermatt**

- 8:00 448.** Dynamics of networked electrochemical reactions: coupling topology and synchronization. **M. Wickramasinghe**, I. Z. Kiss
- 8:20 449.** Talk moved to Physical Chemistry I, Zermatt, Thursday, 11:40 am.
- 8:40 450.** SAPT calculations: Methods for large system computation. **C. C. Kirkpatrick**, M. Lewis, B. K. Welch, J. N. Coleman, J. Wang, K. Hacke
- 9:00 451.** High level quantum mechanical studies of singlet carbenes HCXH (X=O, S, Se). **J. M. Standard**
- 9:20 452.** Theoretical study of hydrolyzation of B<sub>2</sub>O<sub>3</sub>. T. A. Holme, **C. C. De Silva**
- 9:40** Break.
- 10:00 453.** Obtaining partial molar quantities from computer simulations. **E. A. Ploetz**, P. E. Smith
- 10:20 454.** Application of correlation-gas chromatography to problems in thermochemistry. J. S. Chickos, **Dmitry A. Lipkind**
- 10:40 455.** Solute diffusion in *n*-alkanes and squalane. **B. A. Kowert**, M. B. Watson
- 11:00 456.** Viscosity and thermal conductivity of potassium atoms at high temperatures. **L. Biolsi**
- 11:20 457.** Influence of atom recombination and molecular relaxation on the properties of high-enthalpy flows. S. Doraiswamy, **J. Kelley**, G. V. Candler
- 11:40 458.** Theoretical Investigation of reaction of lactic acid on MgO clusters. **L. B. Pandey**, C. M. Aikens

**Friday, October 21, 2011, 8:15 AM – 11:50 PM**

**NMR-The Next Generation (of Techniques)**

**Room: St. Moritz**

Sophia Hayes, Christopher Jaroniec, Nathan Oyler, *Organizers*

*Supported by Bruker Biospin Corporation, Division of Physical Chemistry*

**8:15** Introductory Remarks.

- 8:20 459.** Protein fold determined by paramagnetic magic-angle spinning solid-state NMR spectroscopy. **C. P. Jaroniec**, P. S. Nadaud, I. Sengupta, J. J. Helmus, C. D. Schwieters
- 9:00 460.** A study of residual solvent in aspirin by variable contact time CRAMPS; shelf lives of drugs. **B. Gerstein**, X. Hsu
- 9:20 461.** Carbon partitioning in leaves under elevated CO<sub>2</sub> conditions using <sup>11</sup>C and <sup>13</sup>C labeling. **J. Schaefer**, R. Dirks, M. Singh, G. S. Potter, L. G. Sobotka
- 10:00** Break.
- 10:20 462.** Is it possible to solve a protein structure with one NMR spectrum? **C. M. Rienstra**, A. E. Nesbitt, M. Tang, M. Brothers, K. Nuzzio, G. C. Comellas, L. J. Sperling
- 11:00 463.** Shifting shapes: Seeing a protein's moves. **A. McDermott**

**Friday, October 21, 2011, 8:20 AM – 11:00 PM**

**Polymer Chemistry General Session**

**Room: Alpine II**

- 8:20 464.** Numerical analysis of classical free radical addition polymerization: A mathematically stiff system. **A. M. Brown**, H. Iler, G. Peters
- 8:40 465.** Diffusion of Carbon-14 Oxide in Neutron Irradiated Flax Linen. **A. C. Lind**, M. Antonacci, D. Elmore, G. Fanti, J. M. Guthrie
- 9:00 466.** Polymer brush 'nanosponges' for fast protein separation with MALDI mass spectrometry analysis. **C. N. Scott**, B. Mitrovic, S. Eastwood, G. Kinsel, V. Wong, D. Dyer
- 9:20 467.** Fe(II)/MAO catalyzed olefin polymerization: Oxophilicity of cyclic and acyclic aluminoxane ligands in Fe(II) Complexes. **R. Glaser**, X. Sun
- 9:40** Break.
- 10:00 468.** Stepped growth of sp-sp<sup>2</sup> conjugated oligomers and its applications. **X. Chen**, X. Bai, T. C. Sandreczki, J. R. Dias
- 10:20 469.** Physic chemical recycling of tires by modified asphalt formation. **L. S. Cadena**, Z. G. Arroyo, L. C. Valencia, A. R. Uribe
- 10:40 470.** Synthesis, photophysical properties, and photovoltaic applications of non-aggregated hyperbranched phthalocyanine dyes. **Y. Li**, P. Lu, M. Jiang, P. Thapaliya, X. Yan

**Friday, October 21, 2011, 8:25 AM – 11:40 AM**  
**Biomolecular Structure and Function**  
**Room: Zurich**

Dana Baum, Cynthia M. Dupureur, J. Strauss Soukup, *Organizers*

*Supported by Division of Biological Chemistry, Sigma-Aldrich, ChemGenes Corporation, RNA Society, New England Biolabs, Inc., Integrated DNA Technologies, Horiba Scientific, Trilink Biotechnologies*

- 8:25** Introductory Remarks.
- 8:30** **471.** Understanding DNA flexibility *in vitro* and *in vivo*. J. Peters, N. Becker, **J. Maher**
- 9:05** **472.** DNA as a catalyst for covalent modification of biomolecules. **S. K. Silverman**
- 9:40** Break.
- 10:00** **473.** Structure-activity relationships of G-quadruplex interloop photocrosslinking. **J. E. Smith**, J. A. Taylor
- 10:25** **474.** Targeting dynamic ribosomal RNA sites with small molecules. **C. S. Chow**
- 11:00** **475.** Computational Model for Predicting Experimental RNA and DNA Nearest-Neighbor Free Energy Rankings. **C. A. Johnson**, R. J. Bloomingdale, V. E. Ponnusamy, C. A. Tillinghast, B. M. Znosko, M. Lewis

**Friday, October 21, 2011, 8:30 AM – 10:00 AM**  
**General Poster Session V**  
**Versailles Ballroom**

**8:30 - 10:00**

- 476.** Quantum dynamics of a Morse oscillator in real and imaginary time. **C. Hanson**, B. Dey
- 477.** Periodic and complex waveform current oscillations of copper electrodisolution in phosphoric acid in an epoxy-based microchip flow cell. **A. Bi**, Y. Jia, I. Kiss
- 478.** Exploring the quantum dynamics of a multi-particle system. **M. J. Edgington**, B. K. Dey
- 479.** Molecular structural study of thin-film boron carbide. **W. Li**, M. M. Paquette, S. Karki, B. J. Nordell, M. S. Driver, A. N. Caruso, N. A. Oyler

480. Theoretical analysis of surface plasmon resonance of silver and gold nanowires. **E. B. Guidez**, C. M. Aikens
481. Computational investigation of the electronic structures of polymers used in polymer-fullerene composite solar cells. **B. P. Banks**, O. Poluektov, J. Niklas, K. L. Mardis
482. Structures and water dissociation reactions of Mn-doped TiO<sub>2</sub> clusters. **C. Lee**, C. M. Aikens
483. Recovery of carbochemicals from aqueous biomass hydrolyzates using critical fluid carbon dioxide. **J. Phomakay**, S. Mori, J. W. King, K. Srinivas
484. Extensive SAPT and SAPT-DFT energy comparison on small systems: applications towards larger dimers. **B. K. Welch**, C. C. Kirkpatrick, M. Lewis, K. Hacke
485. Fast Marching algorithm for reaction dynamics: A new perspective for Monte Carlo sampling and reaction paths. **N. W. Truex**
486. A computational study of the bonding interaction between chromium, molybdenum, or tungsten carbonyl complexes and cyanoethylenes or fluoroethylenes. **S. L. Johnson**, D. L. Cedeño
487. Comparison of structures of CH<sub>2</sub>ClF...C<sub>2</sub>H<sub>3</sub>F and CH<sub>2</sub>F<sub>2</sub>...C<sub>2</sub>H<sub>3</sub>F as determined by Fourier-transform microwave spectroscopy. **C. L. Christenholz**, D. A. Obenchain, R. A. Peebles, S. A. Peebles
488. Easy as  $\pi$ : Analysis of C-H...  $\pi$  interactions within chlorofluoromethane-acetylene (CH<sub>2</sub>ClF-HCCH). **L. F. Elmuti**, R. A. Peebles, S. A. Peebles, A. L. Steber, J. L. Neill, B. H. Pate
489. Photovoltaic devices based on porphyrin polymeric donor materials: A computational study of linker effects. **Z. L. Dunn**, M. A. Hammer, T. M. Perrine
490. Computational study of substituent effects on the band gap of porphyrin based polymeric systems. **M. A. Hammer**, Z. L. Dunn, T. M. Perrine
491. Quantitative structure-property relationship study of the short-circuit current of thiophene dyes for dye-sensitized solar cells based on neural networks. **S. P. Kamari**, R. LeSuer, K. L. Mardis
492. Computational investigation of the conformational preferences of a cytochrome c<sub>7</sub> dimer. **A. O. Zayed**, D. M. Tiede, K. L. Mardis
494. Convenient approach to composition tunable uncapped semiconducting nanocrystals. **S. Li**, G. Tan, Z. Peng

495. Self-Regenerative Redox Catalyst: Palladium Oxide Nanoparticles on Cerium Oxide Nanorods. **Y. Zhou**
496. Quenching of coumarin luminescence by CdSe quantum dots. **A. Baride**, S. P. May, D. Engebretson
497. Structural diversity in MgSe nanocrystals. **P. Morrison**, W. E. Buhro
498. Role of Chloride in the growth of Silver nanowires by the polyol synthesis. **W. M. Schuette**, W. E. Buhro
499. Synthesis and isolation of the pure magic-size CdSe nanocluster [(CdSe)<sub>13</sub>(*n*-octylamine)<sub>13</sub>]. **Y. Wang**, Y. Liu, Y. Zhang, F. Wang, H. Rohrs, M. L. Gross, W. E. Buhro
500. Insights into AuSR nanocluster growth via Au(III) chloride. **B. M. Barngrover**, C. M. Aikens
501. Binding of formylxyl radicals to Au<sub>20</sub>: Implications for the growth of gold nanoparticles. **J. M. Hull**, M. R. Provorse, C. M. Aikens
184. Thermo- and pH-stimuli responsive water-soluble copolymers and hydrogels based on acrylate monomers. M. A. Dergunov, **S. A. Dergunov**, E. Pinkhassik, G. A. Mun
503. Towards hybrid nanobiodevice construction: F<sub>1</sub>-ATP synthase adsorption studies. **J. K. Settle**, C. L. Berrie, M. L. Richter
504. Rational design and preparation of polyarginine capped gold nanoparticle for siRNA delivery. **Z. Zhang**, J. A. Taylor
505. Retention of palladium and phosphine ligands using nanoporous polydicyclopentadiene thimbles. **A. Gupta**, N. Bowden
506. Effects of particle size, shape, and temperature on dodecanethiol assisted digestive ripening of Au nanoparticles. **C. Parsons**, D. Jose, K. J. Klabunde
507. Changes in chemical structure, crystallinity and mechanical properties of LDPE and PP composites reinforced by cellulose fibres after exposure to accelerated photoageing. **R. Chollakup**, F. Delor-Jestin, A. Rivaton, S. Thérias, J. Gardette
508. Detection of Sphingolipid Biomarkers in a Murine Model of Niemann-Pick Type C1 (NPC1) Disease. **M. Y. Fan**, H. Fujiwara, R. Sidhu, D. S. Ory
509. Native mass spectrometry of membrane-bound protein-pigment complexes suggests induced pigment dissociation. **L. B. Harrington**, H. Zhang, M. L. Gross, R. E. Blankenship

510. Effects of natural colloids on the adsorption of polycyclic aromatic hydrocarbons (PAHs) by multi-walled carbon nanotubes. **Y. Yang**, W. E. Gato, H. D. Abshiro, J. C. Means
511. Study of Lignin by Pyrolysis GC - MS. **V. R. Sakampally**, R. Douglas
512. Analysis of dissolved methylmercury in environmental samples using Hg-complex ion chromatography: A reoptimized method with increased sensitivity and reduced noise. **A. C. Yerkes**, R. J. Hudson
513. Photo-induced dissolution of metal ions from fly ash particles in a nitric acid media. **N. J. Hamid**, M. A. Kebede, J. Baltrusaitis, J. G. Navea
514. Determination of reactive oxygen species in secondary organic aerosols produced from essential oils. **M. Czerniejewski**, H. Amin, L. Wang, M. McCarroll, K. Huff Hartz
515. Evaluation of the reduction of nitric acid by humic substances. **K. L. Boknevitiz**, J. G. Navea
44. Expression, purification and oligomer formation of amyloid beta(1-42) associated with Alzheimer's disease. **C. Zhang**, N. Oyler
517. Nanoparticles for Mercury Abatement. **S. K. Thanikanti**, P. K. Fu
518. Synthesis of isosorbide diallyl ether in presence of phase transfer catalysts. **M. Sandhu**, M. Ionescu
519. Dynamics of zinc-seamed pyrogallolarene capsules: MD and QM/MM studies. **K. E. Brewer**, D. J. Shaughnessy, J. E. Adams
- Sulforaphane Regulation of Cellular Redox and Growth, C. Lensing, J. Duffy-Matzner.
- In situ* high pressure and temperature NMR analysis of metal carbonate formation from CO<sub>2</sub> with implications for carbon capture, conversion, and sequestration. **J. A. Surface**, P. A. Skemer, S. E. Hayes, M. S. Conradi

**Friday, October 21, 2011, 8:30 AM – 10:00 AM**

**Small Chemical Business Poster Session**

**Versailles Ballroom**

Joseph Sabol, *Organizer*

*Supported by Division of Small Chemical Businesses*

520. Study of the Distribution and Quantity of Iodine in the Brine Waters of Northwestern Oklahoma. J. R. Wickham, **E. C. Pribil**, K. A. Drouhard, D. Mason

522. The future of the chemical enterprise. **J. E. Sabol**

**Friday, October 21, 2011, 9:00 AM – 12:00 PM**

**Chemical Education Research and Practice**

**Room: Davos**

Susan Wiediger, Steven Kinsley, *Organizers*

*Supported by Division of Chemical Education*

**9:00** Introductory Remarks.

**9:05** **523.** Analytical sciences digital library – a unifying force for analytical science education. **T. Spudich**, C. Larive

**9:25** **524.** Medicinal chemistry: Too much to learn in one semester? **H. Zhong**, V. Mashinson, T. A. Woolman

**9:45** **525.** Use of in-situ generated *o*-iodoxybenzoic acid (IBX) for oxidation of alcohols: An introduction of undergraduates to hypervalent iodine reagents, catalytic cycles and green chemistry. M. Bertels, C. LeFever, K. K. Madne, S. R. Pandey, S. V. Saraf, A. Vanoskey, L. Zeman, J. Jin, **T. K. Vinod**

**10:05** **526.** Preparation of divalent Fe, Co, and Ni tosylate salts. H. Nguyen, C. J. Ema, T. H. Ema, **P. J. Janini**, Y. Zhang, N. Rath, S. M. Holmes

**10:25** Break.

**10:40** **527.** Guided inquiry laboratory projects built upon endothermic reaction demonstrations. A. O. Ward, **R. L. Petersen**

**11:00** **528.** Impact of the first-year implementation of process oriented guided inquiry learning in an organic chemistry course on students' attitudes and learning. **T. Chase**, M. Stains

**11:20** **529.** Modifying POGIL to Improve Student Perception of Relevance of Organic Chemistry. **E. Bucholtz**

**11:40** **530.** Development and implementation of streaming online media to enhance pre-lab instruction in first semester organic chemistry laboratory courses. **J. T. Fletcher**

**Friday, October 21, 2011, 10:30 AM – 12:00 PM**

**General Poster Session VI**

## Versailles Ballroom

531. Comparison of phenanthrene and 1,10-phenanthroline derivatives as potential sensors. **J. J. Whitcomb**, L. Kohler, S. Obare, E. Schoffers
532. The Viscosity Lowering of Ionic Liquids. **B. Anderson**, D. E. Raynie
533. The effect of 1-methyl-3-butylimidazolium tetrafluoroborate BMIMBF<sub>4</sub> ionic liquid as mobile phase additive on the peak shapes and resolution of nitroaromatics and nitroanilines on reversed phase liquid chromatography. **B. Redlinski**, T. Ahmad, T. Ahmad, C. Utterback
534. The effect of counter ion of 1-methyl-3-butyl imidazolium ionic liquid as a mobile phase additive on the adsorption behavior of tryptophan on reversed phase liquid chromatography. **T. Ahmad**, B. Redlinski, A. Alalwiat
535. Analysis of Color Degradation in Paper and Artwork Using VISNIR. **J. Cornelius**, B. Kamusinga
536. Determination of phenol concentration in spiked wastewater samples through multivariate regression modeling of UV-visible spectral data. **E. Gripka**, M. Vaughn, J. Ingle
537. Characterization of tannins from *Quercus actissima* leaf extracts by LC-ESI-MS and bioassay directed HPLC fractionation. **L. Rudolf**, C. Zanaboni, K. Severa, C. M. Scholes, J. M. Chapman
538. HDXMS reveals folding of calcineurin upon binding calmodulin. **F. I. Rusinga**, T. Creamer, D. D. Weis
539. Characterization of the chemical constituents of Chinese and Korean Jakyak root and correlation to medicinal activity. I. Fuentes, **N. Frost**, J. M. Chapman
540. Optimization of ETD parameters for top-down proteomics analysis with an ultrahigh-resolution QTOF mass spectrometer. **J. R. Unverferth**, J. B. Sperry, J. A. Carroll
541. Method development for structural characterization of sulfated steroids with mass spectrometry: Applications in animal communication. **Y. Yan**, T. Holy, M. L. Gross
542. Focusing of bacteria and fungi from mixed samples using the isotachopheresis mode of capillary electrophoresis. **J. Bennett**, A. W. Lantz
543. Binding Studies of Dopamine Imprinted Polymers. **A. Goffeney**, D. Goede, G. Mwangi



544. Hydrogen-deuterium exchange mass-spectrometry study of troponin C dynamics and binding within the troponin complex. **R. Huang**, B. J. Summers, H. W. Rohrs, M. L. Gross
545. Characterization of human apolipoprotein E3 and E4 isoforms' interactions with amyloid  $\beta$ 42 by the mass spectrometry-based FPOP protein footprinting method. **B. Gau**, K. Garai, C. Frieden, M. Gross
546. Correlation of Mass Spectrometric Analysis of Heat-Treated Glutaraldehyde Preparations to Their 235 nm/280 nm UV Absorbance Ratio. **A. D. Sen**, R. Dunphy, I. Handley, R. Dieck, L. Rosik
547. Localized Structural Analysis of CBP with Millisecond Timescale Hydrogen Deuterium Exchange MS. **T. R. Keppel**, D. D. Weis
548. UHPLC-MS-MS analysis of pesticides in aqueous environmental samples: An educational outreach program. **M. T. Popko**, R. E. Jackson, B. A. Logue
549. Paper-based microfluidic devices in colorimetric tests. **M. E. Clevenger**, K. Parker, C. Neuville, E. Gross
550. Alternative fragmentation pathways of a model glycopeptide. **V. Kolli**, E. D. Dodds
551. Gas-phase release and sequencing of subunits from non-covalent protein complexes. **D. Rathore**, E. D. Dodds
552. HPLC method to monitor methylcarbonate/acid reaction progress. **E. E. Arens**, S. J. Jamison, D. E. Weisshaar, G. W. Earl
553. Investigation of methylcarbonate/acid reaction as a function of pKa. **K. T. Jacobson**, N. A. Sveiven, D. E. Weisshaar, G. W. Earl
554. MALDI mass spectrometry of membrane proteins in Nanodiscs. **M. T. Marty**, A. Das, S. G. Sligar
555. H/DX-Mass Spectrometry Study of Amyloid beta (Ab 1-42) peptide oligomer. **Y. Zhang**, L. Mirica, M. Gross
556. Investigating insulin oligomers by native spray H/D exchange and top-down mass spectrometry. **Y. Huang**, W. Cui, M. L. Gross
557. Phthalocrowns: New macrocycles for metal binding. **I. Tamgho**, C. J. Ziegler
558. Effect of different oxidants on epoxidation of alpha olefins. **J. Hong**, D. DeGruson, Z. S. Petrovic

- 559.** Utilizing the hydroxyalkylation reaction to prepare bis(benzocrown ethers). **M. E. Zielinski**, A. F. Tracy, D. A. Klumpp\*
- 560.** Fluorinated dienes in the Diels-Alder reaction. **N. Ehterami**, T. Patrick
- 561.** Synthesis of the C(10)-C(17) unit of amphidinolides C, C2, & F, potent cytotoxic macrolides. **S. Roy**, C. D. Spilling
- 562.** Application of 6,7-indolyne aryne cycloaddition and Pd(0)-catalyzed Suzuki-Miyaura and Buchwald-Hartwig cross-coupling reactions for the preparation of annulated indole libraries. P. D. Thornton, N. Brown, D. Hill, B. Neuenswander, G. H. Lushington, C. Santini, **K. R. Buszek**
- 563.** 1,10-Phenanthroline derivatives as potential organophosphate sensors. **M. N. Moses**, L. Kohler, S. Obare, E. Schoffers
- 564.** Synthetic studies of dipyrromethene ligand systems for the discovery of manganese (III)-based peroxyxynitrite decomposition catalysts. **A. Kamadulski**, S. Rausaria, D. Salvemini, W. L. Neumann
- 565.** Preparation, characterization and *Human Carbonyl Reductase* (HCBR) inhibition studies of 2,4-dichlorophenyl-cyanoxime, H(2,4-diCl-PhCO). M. Hilton, **N. N. Gerasimchuk**, H. Charlier
- 566.** Organometallic anticancer compounds: Synthesis and biological activity of a new class of simple alkyne hexacarbonyl dicobalt complexes. **S. L. Debbert**, S. D. Schimler, M. G. Amare
- 567.** Synthesis of several ionic liquid perbromides for the regioselective bromination of polyalkylated aromatic hydrocarbons. **M. L. Miller**, M. J. Kulig, A. Zeiszler
- 568.** Investigation of ruthenium complexes, with the introduction of a novel chiral phosphinoxazoline ligand, to be employed as a catalyst in the Mukaiyama Aldol reaction. **N. Curvey**, A. Widaman, E. Bauer
- 569.** Structure-activity relationship studies of the cyclipostins and their analogs: A means of probing hormone sensitive lipase active site morphology toward the development of new inhibitors. **B. P. Martin**, C. D. Spilling
- 570.** Influence of aromatic amines on the spectroscopic properties of 1,10-phenanthroline. **K. L. Huynh**, S. Obare, E. Schoffers
- 178.** Synthesis of inosamine derivatives to function as nutritional mediators for nitrogen fixation. **J. L. Meloche**, E. Schoffers

- 572.** Antifungal activity of a series of 1,2-Benzisothiazol-3(2H)-one derivatives. **S. Aravapalli**, D. Dou, D. Alex, B. Du, K. Tiew, S. Mandadapu, R. A. Calderone, W. C. Groutas
- 573.** Progress towards the synthesis of a long wavelength fluorescent biosensor for citrate metabolite. **C. Liu**, N. Sattenapally, Q. A. Best, L. Wang, M. McCarroll, C. G. Scott
- 574.** Synthesis and conformational characterization of *N*-alkyl hydroxamic acids. **H. L. Schenck**, R. Zolondek
- 575.** Seeking evidence for electrophilic C-H activation at palladium(IV) centers. **R. Ruffie**
- 576.** Chemical constituents of the Burmese python (*python molurus bivittatus*) sexual attractiveness pheromone. **A. Balloon**, J. Goff, C. Carmichael, S. Snow
- 577.** The total synthesis of (S)-2,4-dihydroxy-1-butyl (4-hydroxyl)benzoate. **S. David**, J. Seagren, A. Radkov
- 578.** Site-selective, cleavable linkers: Quality control and the characterization of small molecules on microelectrode arrays. **B. Bi**, R. Y. Huang, K. Maurer, C. Chen, K. D. Moeller

**FRIDAY AFTERNOON SESSIONS**  
**OCTOBER 21, 2011**

**Friday, October 21, 2011, 1:00 PM – 4:40 PM**

**Analytical Chemistry General Session C**

**Room: Basel**

- 1:00 579.** Metal oxide interferences on lead analysis in tungsten filament atomic absorption spectrometry. **D. Poci**, E. C. Navarre
- 1:20 580.** Kinetic performance comparison of a capillary monolithic and a fused-core column. **T. A. Dioszegi**, D. E. Raynie
- 1:40 581.** Characterization of deep eutectic solvents and comparison with room temperature ionic liquids. **G. Degam**, D. Raynie
- 2:00 582.** Cavity ring-down spectroscopy of liquids using standard cuvettes. **B. J. Culbertson**, S. C. Foster
- 2:20 583.** Determination and quantification of dimethyl methylphosphonate from activated carbon particles. **B. L. Mitchell**, B. A. Logue
- 2:40** Break.
- 3:00 584.** Beeswax processing and refining in supercritical carbon dioxide. **G. N. Gachumi**
- 3:20 585.** Application of 1-ethyl-3-methylimidazolium acetate (EmimAc) in the isolation of lignin and hemicellulose. **V. Essel**, D. Raynie
- 3:40 586.** Synthesis and characterization of 1-ethyl-3-methylimidazolium alkylbenzene sulfonate (EMIM ABS) ionic liquids. **H. Kandala**, D. Raynie
- 4:00 587.** Diffusion-ordered independent component analysis: Separating nuclear magnetic resonance spectra of analytes in a mixture. **J. Zhong**, N. DiDonato, P. G. Hatcher
- 4:20 588.** Top-down fragmentation of protein assemblies: Native electrospray and electron-capture dissociation in FTICR MS. **H. Zhang**, W. Cui, J. Wen, R. E. Blankenship, M. L. Gross

**Friday, October 21, 2011, 1:00 PM – 5:00 PM**

**Chemical Education Research and Practice**

**Room: Davos**

Susan Wiediger, Steve Kinsley, *Organizers*

*Supported by Division of Chemical Education*

*Safety in Chemistry Education:* This invitation-only symposium will focus on how safety can and should be incorporated in the chemistry major curriculum. A closing panel discussion will feature local industry representatives discussing what a graduating senior should know about safety.

**1:00** Introductory Remarks.

**1:05 589.** ACS CHAS: Where chemistry and safety meet. **K. P. Fivizzani**

**1:25 590.** Development, advantages, educational value, challenges, and implementation of a green, microscale organic chemistry laboratory. **T. E. Goodwin**

**2:05 591.** Improving safety education in undergraduate chemistry programs. **D. C. Finster**

**2:45** Break.

**3:00 592.** Laboratory safety and management for teaching assistants. **B. L. Foster**

**3:40** Panel Discussion.

**Friday, October 21, 2011, 1:00 PM – 4:00 PM**

**Environmental Chemistry General Session**

**Room: Alpine II**

**1:00 593.** Developing nanoparticles as mercury eliminating agents. **L. Amarapalli**, P. K. Fu

**1:20 594.** Study of the photochemistry of adsorbed nitrate on different components of mineral dust aerosols. R. M. Welch, E. M. Coddens, **J. G. Navea**

**1:40 595.** Assessment of biogenic secondary organic aerosol in the Kathmandu Valley, Nepal. **E. Stone**, T. Nguyen

**2:00 596.** Effects of biodiesel composition on pollutant emissions from a single cylinder diesel engine. **Y. Zhong**, E. Peltier, M. Mangus, C. Depcik, A. Duncan, S. Williams

**2:20 597.** Speciation and Formation of SOA Generated from Ozonolysis of Realistic Terpene Mixtures. **H. S. Amin**, K. E. Huff Hartz

**2:40** Break.

- 3:00 598.** Determination of Monoamine Neurotransmitters and their Metabolites by Liquid Chromatography - Tandem Mass Spectrometry. **J. F. Gemoules**, J. H. Bisesi, L. E. Sweet, S. J. Klaine, K. A. Johnson
- 3:20 599.** Development of an *in situ* remediation strategy for a metals-contaminated, alkaline groundwater: Initial amendment screening and effect of pH. **A. S. King**, E. Peltier, M. M. Michalsen
- 3:40 600.** Determination of pharmaceuticals and personal care products, endocrine disrupting compounds and metabolites in Illinois groundwater by LC/MS/MS. **M. Salske**, K. A. Johnson

**Friday, October 21, 2011, 1:00 PM – 5:00 PM**

**Inorganic Chemistry General Session B**

**Room: Bern**

- 1:00 601.** “Tensegrity” as an organizing architecture for covalent molecular structure. **J. D. Van Horn**, C. Smith, J. Wade, D. Wang
- 1:20 602.** Enhancing the Thermal Barrier to Reversible Electron Transfer in Cyano-Bridged {Fe<sub>2</sub>Co<sub>2</sub>} Squares. **Y. Zhang**, D. Siretanu, R. Ababei, R. Clérac, C. Mathonière, S. Holmes
- 1:40 603.** Dithiocarbamate ligands bearing amino functionality for polyoxometalate functionalization. **K. Sharma**, J. Karcher, E. A. Maatta, J. Desper
- 2:00 604.** Some novel phosphine complexes of platinum and palladium and their catalytic applications. **S. Acharya**, J. Braddock-Wilking, N. P. Rath
- 2:20 605.** Study of siloles and optical properties related to coordination with metal ions. **J. B. Carroll**, J. Braddock-Wilking
- 2:40 606.** Synthesis and characterization of a series of cyclic germanium compounds for potential use as fluorescent biological probes. **T. Bandrowsky**, J. Braddock-Wilking
- 3:00** Break.
- 3:20 607.** Synthesis, characterization and applications of light-insensitive silver(I) cyanoximates. S. Gross, R. Hougas, **N. N. Gerasimchuk**
- 3:40 608.** Redox chemistry of cationic  $[\eta^5\text{-C}_5\text{H}_5\text{Ru}(\text{PPh}_3)_2]^+$  vinylidene complexes. **M. J. Shaw**, A. Hansen, B. M. Schutte
- 4:00 609.** Non-bridging ligand supported d<sup>8</sup>-d<sup>8</sup> bond in the Pd<sup>II</sup> and Pt<sup>II</sup> complexes. **J. Luo**, N. P. Rath, L. M. Mirica

**4:20 610.** Halogen bonding or close packing? Examining the structural landscape in a series of Cu(II)-acac complexes. **A. S. Sinha**, P. D. Chopade, C. B. Aakeroy, J. Desper

**4:40 611.** New iPrN4 Pd complexes. **F. Qu**, L. Mirica

**Friday, October 21, 2011, 1:00 PM – 5:00 PM**

**NMR: The Next Generation (of Techniques)**

**Room: St. Moritz**

Chris Jaroniec, Nathan Oyler, Sophia Hayes, *Organizers*

*Supported by Bruker Biospin Corporation, Division of Physical Chemistry*

**1:00 612.** Direct measurement of exchange rate of hydrogen and deuterium between gas and hydride phases. **M. S. Conradi**, R. L. Corey

**1:40 613.** Local physical structure in hydrogenated boron carbide materials. **N. A. Oyler**, W. Li, M. Paquette, A. Caruso

**2:20 614.** *In situ* high pressure and temperature NMR analysis of metal carbonate formation from CO<sub>2</sub> with implications for carbon capture, conversion, and sequestration. **J. A. Surface**, P. A. Skemer, S. E. Hayes, M. S. Conradi

**2:40** Break.

**3:00 615.** Studies of atomic and molecular interactions of laser-polarized xenon and parahydrogen for magnetic resonance applications. **B. M. Goodson**, N. Whiting, P. He, P. Nikolaou, L. Walkup, A. Coffey, K. Groome, H. Newton, B. Gust, K. Ranta, A. Hunter, N. Eschmann, M. J. Barlow, E. Chekmenev

**3:40 616.** Dynamic nuclear polarization for enhanced sensitivity in solid-state NMR experiments. **M. Rosay**, S. Pawsey, R. J. Temkin, R. G. Griffin, W. E. Maas

**4:20 617.** Chemical and biochemical reactions investigated by dynamic nuclear polarization. **C. Hilty**

**Friday, October 21, 2011, 1:00 PM – 4:40 PM**

**Organic Chemistry General Session E**

**Room: Geneva**

**1:00 618.** Co-Crystals of Photochromic Compounds. **B. A. DeHaven**, C. B. Aakeroy, S. Panikkattu, J. Desper

- 1:20 619.** Balancing hydrogen and halogen bonding in co-crystal assembly. **S. K. Dembowski**, C. B. Aakeröy, P. D. Chopade, J. Desper
- 1:40 620.** An exacting test of whether activation energy controls regioselectivity of competitive nucleophilic aromatic substitutions from an excited state. **G. G. Wubbels**, R. Tamura, E. J. Gannon
- 2:00 621.** New iron pyridyl amine complexes and their catalytic activity in oxidation reactions. **M. Lenze**, E. Bauer
- 2:20 622.** Synthesis and characterization of Iron(II) complexes of  $\alpha$ -Imino pyridine and their catalytic application in oxidation of activated methylene group and secondary alcohols. **P. Shejwalkar**, E. Bauer
- 2:40 623.** Efforts toward the synthesis of high oxidation state iridium complexes. **S. Whitemore**, J. Stambuli
- 3:00** Break.
- 3:20 624.** Measuring Energy Transfer Processes among Cyanine Dyes. **C. Robinson**, D. Udukala, M. Kalita, H. Wang, D. L. Troyer, S. H. Bossmann
- 3:40 625.** Iodine bonding stabilizes methyl iodide in Midas pesticide. **K. Prugger**, R. Glaser
- 4:00 626.** Protease assays for the detection of cancer. **D. N. Udukala**, H. Wang, S. H. Bossmann, D. Troyer, O. Koper, F. Kroh, G. Abayaweera, L. Bossmann, C. Robinson
- 4:20 627.** Long Wavelength Fluorophores for the Generation of Singlet State Oxygen. **Q. A. Best**, C. Scott, M. McCarroll

**Friday, October 21, 2011, 1:20 PM – 5:10 PM**  
**Sigma-Aldrich Symposium on Nanomaterials**  
**Room: Alpine I**

Shashi Jasty, Angel Thompson, *Organizers*

*Supported by Sigma-Aldrich*

- 1:20** Introductory Remarks.
- 1:25 628.** Chemically directed assembly of charge-transferring hybrid nanostructures. **R. J. Hamers**
- 2:05 629.** Synthetic pathway to and optical properties of CdSe quantum belts. **W. E. Buhro**



- 2:45 630.** Controlled assembly of nanoparticles to superlattice crystals. D. Jose, J. Matthiesen, C. Parsons, Y. Sun, C. Sorensen, **K. Klabunde**
- 3:25** Break.
- 3:45 631.** Wrapping up nanorods. **C. J. Murphy**
- 4:25 632.** Plasmonic nanomaterials for disease diagnostics. **A. J. Haes**, M. S. Pierre, B. Shrestha, A. Volkert
- 5:05** Concluding Remarks.

**Friday, October 21, 2011, 1:30 PM – 4:50 PM**  
**Biomolecular Structure and Function**  
**Room: Zurich**

Cynthia M. Dupureur, Dana Baum, J. Strauss Soukup, *Organizers*

*Supported by Division of Biological Chemistry, Sigma-Aldrich, ChemGenes Corporation, RNA Society, New England Biolabs, Inc., Integrated DNA Technologies, Horiba Scientific, Trilink Biotechnologies*

- 1:30** Introductory Remarks.
- 1:35 633.** Direct observation of conformational exchange in the small multidrug resistance transporter EmrE. E. A. Morrison, G. T. DeKoster, S. Dutta, M. Clarkson, R. Vafabakhsh, D. Kern, T. Ha, **K. A. Henzler-Wildman**
- 2:10 634.** Structural and biophysical studies of proline catabolic enzymes. **J. J. Tanner**
- 2:45 635.** DNA binding properties of a large antiviral polyamide. **G. He**, K. J. Koeller, C. M. Dupureur, J. K. Bashkin
- 3:05** Break.
- 3:25 636.** Chasing fluorescence lifetimes in complex biological systems. What can fluorescence lifetime imaging microscopy (FLIM) tell us? **R. M. Clegg**, Y. Chen, J. Eichorst, K. Teng, Govindjee, S. Matsubara
- 4:00 637.** Mass spectral studies of intrinsically disordered proteins. **D. D. Weis**
- 4:25 638.** Tryptophan substitutions as fluorescent probes of amyloid- $\beta$  structure. **M. R. Nichols**, J. C. Touchette, L. L. Williams, D. Ajit, F. Gallazzi, R. T. McDonough, G. Paranjape

**SATURDAY MORNING SESSIONS**  
**OCTOBER 21, 2011**

**Workshop on Peer-Led Team Learning**  
**Alpine II**

Susan Wiediger, Steve Kinsley, *Organizers*

**9:00 639.** Incorporating peer-led team learning (PLTL) into lower-level chemistry courses: implementation and insights. **R. F. Frey**