

Technical Program

WEDNESDAY MORNING

Bioanalytical Chemistry: Approaches to Biomarker Identification

216 (University Place Conference Center)

Financially supported by Division of Analytical Chemistry

G. Simpson, *Organizer*

R. Whelan, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 1. Right-side and left-side colon cancer follow different pathways to relapse. **K. M. Bauer**, A. B. Hummon, S. Buechler

8:55 2. Integrating proteomics and metabolomics to map bacterial development. **E. E. Carlson**

9:15 3. Multiplexed biomarker analysis using chip-integrated photonic sensor arrays. **R. C. Bailey**

9:35 Coffee Break.

9:50 4. Optical sensing using microelectromagnetic traps. **S. Beeram**, R. Zakeri, J. Basore, L. Baker

10:10 5. Isoelectric focusing in packed capillaries for resolution of protein glycoforms. **M. J. Wirth**

10:30 6. A combined Mass Spectrometry and Nuclear Magnetic Resonance metabolomics approach to detect breast cancer recurrence. **D. M. Raftery**, V. Asiago, L. Alvarado, N. Gowda

Considering the Interface Between Curricular Reform and Measuring Student Learning I

231 (University Place Conference Center)

Financially supported by ACS- Division of Chemical Education Examinations Institute

T. Holme, *Organizer*

R. Pribush, *Organizer, Presiding*

8:30 Introductory Remarks.

8:30 7. Comprehensive safety instruction for an undergraduate chemistry program. **D. C. Finster**

8:55 8. Higher education reform: Reflections on Tuning USA and the Indiana Chemistry Tuning Pilot. **K. S. Anliker**

9:20 Coffee Break.

9:35 9. Measuring student learning in analytical chemistry: content map development and exam item complexity analysis. **M. E. Emenike**, L. Kendhammer, C. F. Bauer, K. Murphy, T. A. Holme

10:00 10. Diagnostic assessment data as a tool for curricular change. **S. M. Villafañe**, J. E. Lewis, J. Loertscher, V. Minderhout

10:25 11. Rethinking Lewis structures: The development and evaluation of a novel instructional scheme. **S. M. Underwood**, C. Z. Hilley, M. M. Cooper, N. P. Grove, M. Klymkowsky

Frontiers of Organometallic and Transition Metal Chemistry

222 (University Place Conference Center)

D. Mindiola, *Organizer*

L. Watson, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 12. Accessing $R^2C=Mo(OR)_3$ complexes via alkyne metathesis of $Mo_2(OR)_6$ complexes. **A. M. Geyer**, R. L. Gdula, M. J. Johnson, J. W. Kampf

8:55 13. Exploring the Rich Electron Transfer Behavior of Mn, Fe, Co, and Ga Complexes with a Redox-Active Bis(phenolate) Phenylenediamine Ligand. **R. L. Lord**, F. D. Lesh, M. M. Allard, H. B. Schlegel, C. N. Verani

9:15 14. Controlled, selective, double C-H bond activation of methane and linear alkanes promoted by a transient titanium alkylidyne. **V. N. Cavaliere**, J. A. Flores, M. G. Crestani, B. Pinter, D. Buck, C. Chen, M. Pink, M. Baik, D. J. Mindiola

9:35 Coffee Break.

9:55 15. On beyond zero: Can we do chemistry with transition metals having less than a d^0 configuration? **S. N. Brown**

10:15 16. Fundamental Organometallic Reactions Mediated by Low-Valent Uranium. **S. C. Bart**, S. J. Kraft, B. A. Schaefer, P. E. Fanwick

10:35 Concluding Remarks.

Natural Products: Isolation, Identification and Synthesis

208 (University Place Conference Center)

Financially supported by Dow AgroSciences

P. Lewer, *Organizer*

J. Gloer, *Organizer, Presiding*

8:30 17. Filamentous fungi as a source of chemical diversity. **N. H. Oberlies**

9:00 18. Tropical Plant Natural Product Diversity – AgroChemical Lead Discovery in Madagascar. **P. R. Graupner**, P. Lewer, D. R. Hahn

9:30 Coffee Break.

9:45 19. Structures and Stereochemical Investigations of the Aflaquinolones: New Bioactive Secondary Metabolites from Fungicolous and Marine *Aspergillus* spp. **S. A. Neff**, J. B. Gloer, H. Oh, J. Baltrusaitis, D. T. Wicklow

10:05 20. Modifications to the 21-butenyl spinosyns via olefin cross metathesis. **J. F. Daeuble**, P. Graupner, P. Johnson, T. Sparks
10:25 21. The chemistry and biology of diocine. **R. W. Fitch**

TB and Malaria Medicine Discovery Initiatives

118 (University Place Conference Center)

Financially supported by Eli Lilly and Company
W. Porter, *Organizer*
M. Miller, *Organizer, Presiding*

8:30 Introductory Remarks.
8:35 22. Modifying old drugs to create new TB therapeutics. **R. Lee**, J. Liu, S. Waidyarachchi, T. Matt, M. Scherman, A. Lenaerts, E. C. Boettger
9:05 23. Evaluation of 2,4-diaminoquinazolines (DAQ) as novel anti-tuberculosis agents. **J. O. Odingo**, T. O. Harris, S. Singh, P. Hipskind, R. Vickers, T. Parish
9:35 Coffee Break.
9:50 24. Dirty by design: a rational approach to the design of new antitubercular nitroimidazoles. **C. E. Barry**
10:20 25. Discovery of antimalarial ozonide drug development candidates OZ277 and OZ439. **J. L. Vennerstrom**

The Crossroads of Research and Practice in Chemistry Education: What Works and How We Know

226 (University Place Conference Center)

L. E. Slocum, *Organizer*
E. J. Yezierski, *Organizer, Presiding*

8:30 26. Will assessment be a signpost or a roadmap at the crossroads of chemistry education? **T. Holme**
8:50 27. Two faces of a screencasting tutorial blog: Balancing research utility while supporting student learning. **N. J. Barrows**, D. Herrington, K. Downey, E. Fought, A. Starr, C. Billman
9:10 28. I thought chemistry was just a math class: Textbook reading comprehension in high school chemistry. A. R. Cutler, **T. M. Owings**, J. R. Wall
9:30 Coffee Break.
9:50 29. Questions lab: An inquiry introduction to a laboratory course in physical chemistry. **D. J. Styers-Barnett**
10:10 30. Enantioselective organocatalytic capstone organic laboratory experiences. K. E. Walsh, **E. O. Wade**

The New Frontier of Combined Quantum Mechanical Molecular Mechanical Methods: Theory and Applications in Chemistry and Biology I

232 (University Place Conference Center)

J. Pu, *Organizer, Presiding*

8:30 31. Dynamical signature of abasic DNA damage: A computational study of coumarin 102 in DNA. **S. Corcelli**
8:55 32. Molecular dynamics simulations of DNA-bound Co(III)-bleomycin. **Y. Fang**, W. M. Southerland, M. M. Georgiadis, E. C. Long
9:20 33. QM/MM methods: recent applications and several remaining challenges. **Q. Cui**
9:45 Coffee Break.
10:00 34. Enhanced Sampling for QM/MM based Molecular Dynamics Simulations. **W. Yang**
10:25 35. Recent developments of efficient semiempirical QM/MM methods for the simulations of complex biomolecular events. **K. Nam**

Nanotechnology from Green Energy to Drug Delivery I

236 (University Place Conference Center)

S. Lieb, *Organizer, Presiding*

9:30 36. Selective attachment of silver nanospheres on the edges of gold nanoplates for raman enhancement. **L. Bao**, Z. Francis
9:50 37. Defining criteria for nanotoxicology. **M. M. Markopoulos**, T. Lockwood, C. Sulentic, I. E. Pavel
10:10 38. Fate and Transport of Silver Nano Particles (AgNPs) in Saturated Porous Media. I. E. Pavel, A. Meyerhoefer, **J. M. Dagher**, M. N. Goltz, J. Flory, S. R. Kanel
10:30 39. Cytotoxicity studies of Creighton colloidal silver nanoparticles in Vero 76 monkey kidney and MLO-Y4 osteocytic bone cells. **N. E. Hunter**, S. A. Paluri, M. M. Markopoulos, J. C. Trefry, A. Chang, Z. S. Arnold, A. J. Meyerhoefer, D. P. Wooley, I. E. Pavel

Welcome and Plenary Lecture I

Auditorium (University Place Conference Center)

Dawn L. Shiang, Associate Director, The Dow Chemical Company

J. Phillips, *Presiding*

11:00 Welcoming Remarks.
11:10 40. Delivering a Sustainable Future Through Innovation. **D. L. Shiang**

WEDNESDAY AFTERNOON

Beverage Flavors

208 (University Place Conference Center)

Financially supported by Dow AgroSciences

P. Lewer, *Organizer*

D. Bolliet, *Organizer, Presiding*

1:30 41. Beverage flavors: untapped growth opportunities. **G. Goel Lal**

1:55 42. Novel application of hop oil fractions for non-beer beverage applications. **S. T. McDonald**, M. Schulze, M. Peltz, D. Bolliet, L. Burroughs

2:20 43. The Misnomer of Beverage Flavors. **C. Moy**

Considering the Interface Between Curricular Reform and Measuring Student Learning II

231 (University Place Conference Center)

Financially supported by ACS- Division of Chemical Education Examinations Institute

L. E. Slocum, *Organizer*

T. Holme, *Organizer, Presiding*

1:30 44. Investigating the relationship between conceptual question complexity and student performance using ACS Exams. **M. L. Grunert**, T. A. Holme

1:55 45. Differential Item Functioning (DIF) on multiple choice general chemistry assessments. **L. Kendhammer**, K. Murphy

2:20 46. Findings from the enzyme-substrate concept inventory. **K. J. Linenberger**, S. Bretz

2:45 Coffee Break.

3:00 47. Development and assessment of ACID I concept inventory. **L. M. McClary**, S. Bretz

3:25 48. Assessing Student Learning Through Reflective Journal Writing. **M. Dianovsky**, D. Wink

Environmental Chemistry - General Papers

226 (University Place Conference Center)

Financially supported by Heritage Environmental Services

K. Weber Stickney, *Organizer, Presiding*

1:30 49. A sustainable future: Role of innovation and chemistry. **S. Selcuk**

2:10 50. Geographic variation in the carbohydrate profile of benthic algal biomass for sustainable biofuel production. **J. G. Thompson**, S. Bertman, K. Hampel, J. B. Miller, C. Strauss

2:30 51. Challenges of qualifying new refrigerants for use in stationary HVAC systems. **J. Majurin**

2:50 Coffee Break.

3:10 52. Dissolution kinetics and morphology at calcite-water interfaces: Linking molecular-scale surface properties and macroscopic observables. **M. Xu**, M. E. Smith, M. Mante, K. G. Knauss, S. R. Higgins

3:30 53. H₃PW₁₀Mo₂O₄₀ solution as new liquid redox absorbent for low sulfur containing gas sweetening. **R. Wang**

Inorganic Chemistry - General Papers

222 (University Place Conference Center)

L. Watson, *Organizer*

H. Eppley, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 54. New Class of Trianionic Constrained Geometry Ligands: Synthesis, Characterization, and Representative Complexes. **C. Yeisley**, R. T. Rondo, K. Kirschbaum, M. R. Mason

1:55 55. Alkane C-H activation using a titanium alkylidyne. **C. N. Romer**, M. G. Crestani, V. N. Cavaliere, D. J. Mindiola

2:15 56. Büchner reaction catalyzed by a silver(I) trimer supported by a pyridylpyrrolide ligand. **J. A. Flores**, K. Pal, B. Pinter, K. A. Jonathan, M. Pink, X. Gao, D. J. Mindiola, M. Baik, K. G. Caulton

2:35 Coffee Break.

2:50 57. Graminophosphines: A new class of ionic liquid soluble ligands and their application in C–C coupling reactions. **A. J. Keith**, S. D. Kosik, K. Patel, J. Lopez, L. V. Tillekeratne, M. R. Mason

3:10 58. Metal-containing ionogels: Serendipity and challenges. **H. J. Eppley**

3:30 Concluding Remarks.

Nanotechnology from Green Energy to Drug Delivery II

236 (University Place Conference Center)

S. Lieb, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 59. Lipid membrane editing with peptide cargo linkers in cells and synthetic nanostructures: New approaches to cancer therapy. **S. A. Wickline**

1:55 60. Photoactivated riboflavin and phyloquinone as photodynamic antimicrobial chemotherapeutic agents. **J. M. Blain**, P. K. Fu

2:15 61. Intelligent integrated microfluidics - molecular recognition, catalysis and electrochemistry in single nanopores and nanopore arrays. S. Branagan, N. Contento, **P. W. Bohn**

2:35 Coffee Break.

2:50 62. Probing model membrane compartmentalization using quantum dot-conjugated lipids. **C. A. Naumann**

3:10 63. Nanoencapsulation and controlled release of lipophilic vitamin K into whey protein-biopolymer matrices: effect of pH in Fuzzy clustering and surfaces properties. **G. K. Kouassi**

3:30 64. Ag nanoparticles attached to ITO as an electrocatalyst for oxygen reduction reaction. **R. Masitas**, F. P. Zamborini

Peptides in Therapeutics: From Biological Mechanism to Utility

118 (University Place Conference Center)

Financially supported by Eli Lilly and Company

W. Porter, *Organizer*

L. Parker, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 65. Excitotoxic Neuroprotection and Vulnerability with CaMKII Inhibition. **A. Hudmon**

2:05 66. Genetically Encoded Membrane-Tethered Peptide GPCR Agonists. **M. Nitabach**

2:35 Coffee Break.

2:50 67. Discovery of Potent, Cyclic Calcitonin Gene Related Peptide (CGRP) Receptor Antagonists. **J. P. Mayer**, L. Yan

3:20 68. Biosensors for biomarkers: measuring kinase activity in live cells. **L. Parker**

Spectroscopic Imaging

216 (University Place Conference Center)

G. Simpson, *Organizer*

Z. Schultz, *Organizer, Presiding*

1:30 69. Label-free bond selective imaging. **J. Cheng**

1:50 70. Single-molecule microscopic and spectroscopic study of confined nanocolloids and polymers: when the ensemble average becomes inadequate. **Y. Zhu**

2:10 71. Superresolution Chemical Imaging Microscopy. **J. Spector**, S. J. Stranick, H. Kim

2:30 Coffee Break.

2:50 72. Chemical imaging for histopathology. **R. Bhargava**, M. Walsh, M. Schulmerich, A. Kodali

3:10 73. Fluorescence Measurements of Cell Membrane Receptor Organization and Cellular Factors Affecting Membrane Reorganization. **E. A. Smith**, S. Sander, N. Arora, D. Mainali

3:30 74. Protein-ligand binding investigated by a single nanoparticle-TERS approach. **S. L. Carrier**, Z. D. Schultz

Technology Enabled Organic Synthesis

206 (University Place Conference Center)

Financially supported by Eli Lilly and Company

M. Siegel, *Organizer, Presiding*

1:30 75. Utilizing a technology enabled synthetic approach to discover novel in vivo tool compounds as potential therapeutics for Parkinson's disease. **C. R. Hopkins**

1:55 76. The Virtual MedChem Lab: New Research Paradigms in Drug Discovery. **A. G. Godfrey**

2:20 77. Development of a fully automated strategy for chemical library synthesis. **S. A. Kozmin**

2:45 Coffee Break.

3:00 78. Reflections on 10 Years of High-Throughput Organic Synthesis at Abbott. **D. R. Sauer**

3:25 79. Azides R Us: Rapid generation of versatile molecules using azides in flow. **C. Santini**, J. Aube, J. A. Porco, E. Fenster, T. Painter, P. Thornton, J. L. Poole, D. Vander Velde, J. R. Goodell

The New Frontier of Combined Quantum Mechanical Molecular Mechanical Methods: Theory and Applications in Chemistry and Biology II

232 (University Place Conference Center)

J. Pu, *Organizer, Presiding*

1:30 80. Effective Fragment Potential method: Theory, applications, and benchmarks. **L. Slipchenko**

1:55 81. Structure, dynamics, and spectroscopy of the hydrated electron: The role of solvent polarization. L. D. Jacobson, C. F. Williams, **J. M. Herbert**

2:20 82. Multi-scale simulations by open-boundary QM/MM. S. Pezeshki, **H. Lin**

2:45 Coffee Break.

3:00 83. Towards accurate electronic structure methods for large molecules. **K. Raghavachari**

3:25 84. Combining Constrained QM with MM. **J. Pu**

3:50 85. Methyl transfer reaction mediated by electron transfer in the catalytic cycle of cobalamin-dependent methionine synthase. **N. Kumar**, P. M. Kozlowski

Poster Session: Agricultural and Food Chemistry

132/134/137 (University Place Conference Center)

K. Anliker, *Organizer*

2:00 - 3:30

86. Marine Actinomycetes as a source of novel ovarian cancer drug leads. **S. Carlson**, X. Wei, U. Tanouye, T. Hilliard, J. Burdette, B. Murphy

87. Structural changes in iota-carrageenan induced by urea. **B. K. Patel**, O. H. Campanella, S. Janaswamy

88. Fermentation induced-changes in phenolic profile and antioxidant capacity of cocoa beans. **G. K. Kouassi**, N. K. Kouassi

89. Effect of water activity on the release profile of vitamin A encapsulated into a dual biopolymer system. **G. K. Kouassi**, P. Jagarlamudi, V. Gogineni

Poster Session: Environmental Chemistry

132/134/137 (University Place Conference Center)

K. Anliker, Organizer

2:00 - 3:30

90. Catalytic oxidation of selected VOCs using Zn-doped MnO catalysts: Effect of Zn-dopant and synthesis method on catalytic activity and morphology. **Z. McCoy, M. Krekler, C. Almquist**
91. Energy production of common carbon containing fuels with regard to CO₂ emission. **S. A. Studniarz**
92. Energy dispersive X-ray fluorescence examination of the composition of patent medicines and nostrums archived at the Henry Ford Museum. **D. M. Garshott, E. MacDond, T. Sanday, A. Diefenbch, M. Fahey, M. A. Benvenuto**
93. Elemental analysis via energy dispersive X-ray fluorescence of commercial dried, powdered, kelp food supplements for heavy metals. **D. M. Garshott, E. MacDonald, M. Murray, E. Roberts-Kirchhoff, M. A. Benvenuto**
94. Experimental and theoretical investigations of the gas phase reaction of OH radicals with allyl alcohol. **P. Carey Jr, P. Stevens**
95. Wetland soil analysis: A comparative study of pH, metal concentration and watershed impact. **K. Thut**
96. Clear Creek Watershed Analysis in Bloomington, Indiana. **K. J. Griffith, A. J. Rusch, C. E. Reck, J. A. Karty, K. Lindberg**
97. Elemental characterization of algae grown by Algal Turf Scrubber technology in the eastern United States: assessment of product potential. **K. Hampel**
98. Ionic liquid-based solvent extraction systems for improved actinide and fission product separations. **S. L. Garvey, M. L. Dietz**
99. Temporal study of water quality in the Salt Creek watershed. **L. A. Zook-Gerdau, K. Newman, J. Molden, K. Poland, R. Hentz, S. VanHorn**
100. Adsorption and desorption of barium to hematite (α -Fe₂O₃) in artificial seawater. **D. S. Lennaerts, S. R. Higgins**
101. Influence of water quality on disease rate of Fibropapillomatosis in green turtles in the Indian River Lagoon, Florida. **L. N. Ubadigbo, A. E. McGowin, B. K. Grunden**
102. Aluminum salts as alternative catalysts for preparation of biodiesel from high free fatty acid feedstocks. **S. Simiyu**
103. Electrochemical fabrication of molecule and metal based resistive switching devices: Surface-enhanced raman spectroscopy characterization and molecular electronics applications. **R. Dasari, Z. Francis**

Poster Session: Polymer Chemistry

132/134/137 (University Place Conference Center)

K. Anliker, Organizer

2:00 - 3:30

104. Biofunctional polymer hydrogels based on substituted epoxides. **E. Sokolovskaya, S. Bräse, J. Lahann**
105. Tuning the thermal stimulus response properties of novel gold-hybrid nanoparticles. **N. Chen, A. Tiwari, P. A. Heiden**
106. New routes to multi-block copolymers: Pre-rate-determining selectivity in the terpolymerization of epoxides, cyclic anhydrides and CO₂. **R. C. Jeske, A. M. DiCiccio, J. M. Rowley, G. W. Coates**
107. Kinetic determination in optimization of chain length, hydrophobicity, and chain rigidity of amphiphilic block copolymers by RAFT controlled radical polymerizations. **K. S. Kawchak, D. J. Arnold, G. M. Wilmes**
108. Characterization of the structure and morphology of P3HT:PCBM films by solid-state NMR and microscopy. **J. A. Baughman, C. A. Bailey, M. F. Durstock, M. P. Espe**

Poster Session: Analytical Chemistry

132/134/137 (University Place Conference Center)

K. Anliker, Organizer

4:00 - 5:30

109. Probing metalloproteins in bacteriophage lambda: an elemental and molecular study using SEC-ICPMS and nanoLC-Chip-ESI-MS. **Y. Zhang, J. Caruso, R. Thompson**
110. Investigations of acetic acid and its quantitative effects on the quasi-liquid layer through ¹H and ¹³C NMR analysis. **J. B. Jones, P. B. Shepson, J. Harwood**
111. Label-free Biosensing Based on Chemically Synthesized Gold Nanoprisms as Sensing Platforms. **G. K. Joshi, P. J. McClory, R. Sardar**
112. Oxidation properties of methionine: As observed by the oxidation of methionine by the strong oxidizing agent, bromate. **H. R. Waterman, E. Chikwana, S. Mordan-McCombs**
113. Development of GC-MS and DART-MS methods for the characterization of carbohydrates in archaeological materials. **B. Dhakal, R. Armitage**
114. Study of the comparison between "impedance resonance" and standard impedance spectroscopy using interdigitated electrode arrays in metal ions solutions. **A. Waris**
115. Chemiluminescence catalyzed by Ag/Au Nanoparticle alloys. **S. Abideen**
116. Non-destructive and non-invasive analysis of historical inks using Raman scattering spectroscopy. **J. L. Tharp, E. H. Witlicki, W. E. Hooper, W. R. Newman, A. H. Flood**
117. Correlation of in vitro and in silico kinome selectivity data with inhibitor affinity capture-MS results from cell lysate. **M. J. Patterson, M. S. Duggan, D. B. Ready, S. M. McLoughlin, S. E. Warder, V. L. Marin, P. L. Richardson, P. J. Merta, L. L. Kifle, M. D. Kurnick, J. T. Metz, R. W. Johnson, S. G. Spanton**
118. Use of residual gas analyzer mass spectrometer for the analysis of solutions. **C. Bowers, M. Hammer**
119. Spectroscopic behavior of 8-hydroxy-1, 3, 6-pyrenetrisulphonate immobilized in sol-gel thin film and its evaluation as potential pH sensor. **Q. Hu, S. A. Green**
120. Degradation of Environmentally Harmful Materials in a Flow-Through Electrochemical Reactor. **K. J. Griffith**
121. New direct method for quantifying low molecular weight organic acids in oils. **E. Sorenson**
122. *Withdrawn.*
123. Serum Uric Acid Quantitation by Liquid Chromatography Tandem Mass Spectrometry: A Potential Alternative to the Uricase/Peroxidase Enzymatic Method. **M. L. Copeland, A. S. Ptolemy**
124. Characterizing Archaeological Residues by Direct Analysis in Real Time Mass Spectrometry. **D. Fraser, R. Armitage**
125. Simultaneous detection of protein crystals by UV-SHG and TPE-UVF. **J. T. Madden, G. J. Simpson**
126. Annealing of non-porous silica to reduce the concentration of isolated silanols and peak tailing in RPLC. **J. J. Newby, M. A. Legg, B. Rogers, M. J. Wirth**
127. In vitro detection of 2D membrane protein crystals. **E. DeWalt, G. J. Simpson**
128. Autonomous nanocargo transport system using actin bundle-myosin bionanomotor. **H. Takatsuki, K. Rice, S. Nalabotu, M. Kolli, K. Kohama, P. Famouri, M. Norton, E. Blough**
129. Functionalization of films of Au monolayer protected clusters via vapor phase thiol-place exchange reactions and its chemiresistive sensing applications. **Y. Yang**
130. Electrochemical Deposition of Silver Nanorods and Nanowires Directly on Indium tin oxide and Microgap Electrodes. **N. Shah, F. P. Zamborini**
131. Quantitative determination of common synthetic cannabinoids JWH analogs by thin-layer chromatography. **E. Litchfield, G. Lyman, K. Waters, Y. Jaghab, C. C. Deibel**

- 132.** Modeling of tryptophan on reversed phase liquid chromatography using substituted imidazolium ionic liquids as mobile phase additives. **T. J. Ahmad**, K. K. Aluguvelli, A. Alalwiat, T. Z. Ahmad
- 133.** New cell design for spectroelectrochemical studies. **C. A. Schroll**, S. Chatterjee, W. R. Heineman, S. A. Bryan
- 134.** Practical Comparison of Commercial HPLC columns Packed with Different Superficially Porous Particles for Separation of Small Molecules and Medium Size Natural Products. **P. Yang**

Poster Session: Small Chemical Businesses

132/134/137 (University Place Conference Center)

K. Anliker, *Organizer*

4:00 - 5:30

- 135.** Lessons in transforming an antiquated R&D sample management system into an efficient yet flexible R&D production system. **A. Latham**, P. Scherer
- 136.** Where all the elements come together for a successful chemical business. **J. E. Sabol**, K. E. Leach

THURSDAY MORNING

MEDI/PHYS Computer-Aided Drug Design I

118 (University Place Conference Center)

S. Meroueh, *Organizer, Presiding*

- 8:15 137.** Computational design of small molecule inhibitors disabling IL-6/IL-6R/GP130 functional hexamer for cancer therapy. **C. Li**
- 8:50 138.** Mimicry of protein-protein interactions: An effort to design interferon mimetics. **L. P. Kotra**
- 9:25** Coffee Break.
- 9:40 139.** Relating molecular properties and in vitro ADME/tox surrogate assay results to in vivo outcomes. **J. Sutherland**
- 10:15 140.** Computational Design of Small Molecules that Target Protein Interactions of the Urokinase Receptor. **S. Meroueh**

Biochemistry - General Papers I

226 (University Place Conference Center)

B. Blacklock, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35 141.** Kinetic and solution NMR approaches for evaluating the interactions of Factor XIII AP V34X and Fibrinopeptide B with Thrombin. **M. A. Jadhav**, W. N. Goldsberry, M. C. Maurer
- 8:55 142.** Investigating Factor XIII Specificity for Glutamine Containing Substrates by MALDI-TOF MS. **P. G. Doiphode**, M. C. Maurer
- 9:15 143.** Sighting-in on a new antibiotic target. **E. M. Koehn**, T. Mishanina, S. A. Lesley, I. I. Mathews, A. Kohen
- 9:35** Coffee Break.
- 9:50 144.** Investigating the collective contributions to catalysis of a non catalytic active site leucine in a thiamin diphosphate-dependent enzyme. **F. H. Andrews**, M. J. McLeish
- 10:10 145.** Probing allosteric pathways in yeast and bacterial pyruvate decarboxylases. **R. Stan**, M. J. McLeish
- 10:30 146.** Dihydrofolate reductase: A correlation between the donor-acceptor distance and its fluctuation to the catalyzed hydride transfer. **V. Stojkovic**, L. L. Perissinoti, S. J. Benkovic, A. Kohen

Chemistry of Art

216 (University Place Conference Center)

P. Lang, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35 147.** The chemical analysis of a painted medieval wooden sculpture. **P. L. Lang**, S. Leary, A. Klein, R. Short, R. Carey, R. Hamilton, M. Coffey
- 8:55 148.** The Archaic Mark Codex: Case Study of a Collaborative Analysis. **J. G. Barabe**, M. M. Mitchell, A. Quandt
- 9:15 149.** Applications of direct analysis in real time mass spectrometry (DART-MS) to cultural heritage materials. **R. Armitage**
- 9:35** Coffee Break.
- 9:55 150.** Synchrotron techniques for the study of Chinese bronzes and altered pigments. **F. Casadio**, M. L. Young, J. Almer, D. R. Haeflner, L. Zanella, J. Gaillard, S. Schnepp, I. Fiedler, K. A. Gray, R. Warta, Q. Ma
- 10:15 151.** Lasers used in the study and treatment of pigment degradation on artwork. **G. D. Smith**, S. Maleki

Computational Chemistry - General Papers

232 (University Place Conference Center)

J. Pu, *Organizer, Presiding*

- 8:30 152.** Investigation of inhibitory potency of BHQ derivatives as SERCA inhibitors: Binding free energy computation using MD/FEP. **M. Jayasinghe**, S. Paula
- 8:50 153.** Computational investigations on Organophosphorus Hydrolase, a potential therapeutic for chemical warfare agents - PHS 398 (Rev. 6/09). **H. A. Taha**, C. M. Hadad
- 9:10 154.** DFT studies of the hydrated carbohydrate, glucose: Optimization and DFTMD simulations of ten explicit waters superimposed with an implicit solvation method, COSMO. **F. A. Momany**, U. Schnupf

9:30 Coffee Break.

9:50 155. Intramolecular interactions in oxidized beta structures. **M. C. Green**, J. S. Francisco

10:10 156. Computational studies of Chloroquine binding to Plasmodium falciparum Glyceraldehyde-3-phosphate dehydrogenase. **V. F. Waingeh**, J. A. Eberle, A. T. Groves

10:30 157. *Withdrawn*

Details of Dissemination

231 (University Place Conference Center)

Financially supported by Division of Chemical Education

L. E. Slocum, *Organizer*

A. Cutler, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 158. The Journal of Chemical Education: Print journalism in a digital age. **N. J. Pienta**

9:05 159. ACS and C&EN. **M. Jacobs**

9:35 Coffee Break.

9:50 160. Nuts and bolts of publication. **A. Teter**

10:20 161. Path to first decision: Realities of the editorial process. **A. R. Cutler**

Foods and Nutrition I

208 (University Place Conference Center)

Financially supported by Dow AgroSciences

P. Lewer, J. Phillips, *Organizers*

C. Weaver, *Organizer, Presiding*

8:30 162. Metabolism of prebiotic sugars by gut bacteria. **R. Hutkins**

9:00 163. Designer carbohydrates to deliver functional compounds to targeted areas of the gastrointestinal tract. **D. Rose**

9:20 164. Designer carbohydrates and glucose control. **B. R. Hamaker**

9:40 Coffee Break.

9:55 165. Prebiotics and mineral absorption. **C. Weaver**

10:15 166. Product development with fibers for calorie reduction. **J. R. Daniel**

10:35 Discussion.

Forensic Chemistry and Microchemistry

223 (University Place Conference Center)

J. Goodpaster, *Organizer*

J. Siegel, *Organizer, Presiding*

8:30 167. Identification of diesel and biodiesel blends as arson accelerants through burn pattern analysis. S. R. Dugan, **Z. Prugar**, C. Cordell, F. Jessmon, J. Milie, D. Schauer

8:55 168. Identification of diesel and biodiesel blends by IR spectroscopy. **J. Milie**, F. Jessmon, C. Cordell, Z. Prugar, S. Dugan, D. Schauer

9:20 Coffee Break.

9:40 169. Odor availability of nitromethane. **K. M. Kitts**, J. V. Goodpaster

10:05 170. Nicotine quantification of dissolvable tobacco products using solid phase micro-extraction (SPME) GC/MS. **C. Rainey**, P. Conder, J. Goodpaster

Organic Chemistry - General Papers I

206 (University Place Conference Center)

Financially supported by Eli Lilly and Company

D. Hoard, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 171. Synthesis of aromatic derivatives of benzothienopyrimidines showing anti-cancer activity. **M. Kumar**, B. Xu, A. J. Vaisberg, G. B. Hammond

8:55 172. Synthesis of aryl organosulfur and organoselenium compounds by AlCl₃-catalyzed electrophilic aromatic substitution reactions. **X. Sun**, D. Haas, K. Sayre

9:15 173. Non-linear Hammett correlation for the hydroxide-dependent breakdown of aromatic substituted N-(hydroxybenzyl)acetamides. **R. W. Nagorski**

9:35 Coffee Break.

9:50 174. Synthesis of functionalized 1,3-dihydrobenzo[c]furan systems through a one-pot tandem Henry-Michael reaction. **O. E. Okoromoba**, F. A. Luzzio

10:10 175. Hydrogenation and isomerization of allyl alcohol in the presence of Pd and PdAg monolayer protected clusters. **M. A. Moreno**, F. P. Zamborini, L. N. Kissell

10:30 176. Odorless addition of thiol moiety through diacyl disulfide cleavage. **M. Ozols**

True Stories of Success from Chemical Entrepreneurs

222 (University Place Conference Center)

Financially supported by Division of Small Chemical Business

K. Leach, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 177. Starting and running a chemical business: the ABCs. **J. E. Sabol**

9:00 178. BASi: 1974 to the present. **A. C. Myers**

9:25 Coffee Break.

9:55 179. Being a consultant: from before when the phone rings to when the check clears. **J. E. Sabol**

10:20 180. The chemist's dilemma: Do I optimize or explore? Organizing experimentation to increase success in the U.S. Patent Office. **M. E. McKee**, C. S. Andrzejak
10:45 Concluding Remarks.

Teaching and Learning in the Digital Age: Resources Teachers and Students Can Rely On

236 (University Place Conference Center)

L. E. Slocum, *Organizer*

L. Fanis, *Organizer, Presiding*

8:35 Introductory Remarks.

8:40 181. Using technology to move beyond traditional teaching and learning aims. **T. M. Clark**

9:00 182. Using digital identifiers for chemical informatics. **S. P. Wathen**

9:20 Coffee Break.

9:35 183. Reliable resources from the ChemEd DL. **L. N. Fanis**

Poster Session: Inorganic Chemistry

132/134/137 (University Place Conference Center)

K. Anliker, *Organizer*

9:00 - 10:30

184. Novel microwave assisted synthesis of high-aspect ratio Iron Oxide nanoparticles. **C. J. Flynn**, M. J. O'Malley, T. F. Ekiert, M. D. Alexander

185. Microwave assisted synthesis of γ -Fe₂O₃ and CoFe₂O₄ via solvothermal decomposition. **M. M. Lyle**, C. J. Flynn, M. J. O'Malley, T. F. Ekiert, M. D. Alexander

186. Thermal behavior of ionic liquid crystalline compounds of transition metals with dimethyldihexadecylammonium and hexadecylamine ligands. **E. A. Jensen**, L. Cichon

187. Fabrication of magnetic mesoporous silica nanocomposite as magnetically recyclable catalyst for reduction of nitroarenes. **M. Shokouhimehr**

188. Layered and core/shell growth of Fe₃O₄ and CoFe₂O₄ nanoparticles via solvothermal decomposition. **J. A. Lippold**, B. J. Yocum, D. W. Mirre, M. J. O'Malley, T. Ekiert, M. D. Alexander

189. Theoretical Study of the Protonation of [Pt₃(μ -L)₃(L')₃] (L = CO, SO₂, CNH; L' = PH₃, CNH). **F. Mendizabal**

190. Effects of metal coordination and ring expansion on the reduction of an alloxazine derivative in aprotic solvents and in the presence of H-bonding and H+-donating solvents. **R. Cunningham**, M. E. McGuire

191. Alkene addition to a Ru-coordinated thiyl radical: Synthesis by chemical oxidants and reactivity studies. **R. Chauhan**, C. Grapperhaus, M. Mashuta

192. NMR Characterization of Boron-Substituted Polypyrazolylborate Complexes of Co(II). **S. M. Greer**, D. L. Tierney

193. Synthesis and reactivity of rhenium based cluster complexes. **J. N. Tirado**, L. F. Szczepura*

194. Synthesis and characterization of rhenium cluster complexes containing azido and triazolato ligands. **J. L. Durham**, S. A. Knott, L. F. Szczepura*

195. Recent developments in the synthesis of a series of podand ligands utilizing diethylenetriamine (N₃), triethylenetetraamine (N₄), or spermine (sp-N₄). **C. N. Kashat**, L. Gschwender, M. A. Benvenuto

196. Synthesis and characterization of a series of multi-dentate ligands incorporating 1,3-diaminobenzene or 2,6-diaminotoluene, and metal complexes thereof. **A. M. Koglin**, M. Altaii, B. Korfel, S. Padi, M. A. Benvenuto

197. Formation of metal carboxylates using benzoic acid-derived ligands. S. E. Clark, M. S. Lewandowski, D. N. Mikesell, B. J. Stillman, **E. K. Haub**

198. Synthesis and reactivity of uranium(III) alkyl complexes. **E. M. Matson**, P. E. Fanwick, S. C. Bart

199. Tetrazines: Coordination complexes and molecular switches. **C. R. Benson**, K. Parimal, J. A. Thomas, C. Chen, A. H. Flood

200. Chemistry and spectroscopy of pseudotetrahedral Ni(II) arylthiolate complexes. **T. Deb**, J. L. Petersen, V. G. Young, Jr., M. P. Jensen

201. Synthesis, computational and electrochemical investigations of di- μ -oxo dimetal systems: Toward water oxidation catalysts. **A. R. Stahl**, E. S. Donovan, G. A. Felton

202. An electrochemical study of hydrogen-generating organometallic compounds. E. S. Donovan, **S. E. Froberg**, G. A. Felton

203. Synthesis and Photophysical Studies of Platinum(II) Expanded Framework Terpyridines. **L. M. Hight**, D. R. McMillin

204. Photochemistry and photophysics of a polyimine ligand and corresponding platinum(II) complexes. **D. P. Lazzaro**, D. R. McMillin

205. XANES studies of cobalt containing compounds. **J. C. Kaine**, D. L. Tierney

206. Multiplexed Magnetic Resonance Probes for the Tracking of Cells In Vivo. **D. J. Mastarone**, E. K. Kohlmeir, V. S. Harrison, A. L. Eckermann, G. Parigi, C. Luchinat, T. J. Meade

207. Carbonic Anhydrase as a Model for Matrix Metalloproteinase Inhibition. **T. Woodruff**, N. Wagle, E. Swigart, M. Graham, T. Brophy, W. K. Myers, D. L. Tierney

208. Horseradish Peroxidase and Metalloporphyrin Catalyzed Oxidation of Sulfonated Azo Dyes. **M. Dörner**, H. Hadac, A. Gengenbach

209. Metalloporphyrin catalyzed oxidation of dibenzothiophenes. **8C. Thurber**, D. Swedien, E. Stuckert, A. Gengenbach

210. Sterically friendly copper(II) porphyrins with unimolecular quadruplex DNA. **A. J. Gaier**, R. McGuire, D. R. McMillin

211. Interaction of Ru(II) mono-arene Complexes with Serum Proteins. **L. Wang**, S. Skop, A. Basing

212. VIPER: Virtual Inorganic Pedagogical Electronic Resource. **L. A. Watson**, H. J. Eppley, J. L. Stewart, B. A. Reisner, M. J. Geselbracht, E. R. Jamieson, A. R. Johnson, S. R. Smith, B. S. Williams

Plenary Lecture II

Auditorium (University Place Conference Center)

11:00 . John C. Lechleiter, Chairman, CEO, Eli Lilly and Company

A. Debaille, *Presiding*

THURSDAY AFTERNOON

Best Practices for Entrepreneurs - Panel Discussion

236 (University Place Conference Center)

Financially supported by Division of Small Chemical Business

J. Sabol, *Organizer*

K. Leach, *Presiding*

1:30 Introductory Remarks.

1:35 213. Best practices for entrepreneurs: Introductory statements from panelists. **P. T. Kissinger**, W. F. Carroll, J. E. Sabol

1:55 Panel Discussion.

2:55 Concluding Remarks.

Case Studies in Neuroscience Drug Discovery

118 (University Place Conference Center)

Financially supported by Eli Lilly and Company

W. Porter, *Organizer*

M. Kort, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 214. Synthesis and structure-activity studies of pyrazinecarboxamides and pyridinecarboxamides as $\alpha\beta 2$ nicotinic acetylcholine receptor ligands. **M. J. Scanio**, L. Shi, W. H. Bunnelle, D. J. Anderson, C. Lee, M. Gopalakrishnan

2:05 215. Novel asymmetric pyran derivatives as triple monoamine uptake inhibitors: New generation antidepressants with broad-spectrum activity. **A. Dutta**

2:40 Coffee Break.

2:50 216. Central inhibition of Alzheimer's β -secretase in humans: proof of concept with LY2811376. **D. J. Mergott**, P. C. May, R. A. Dean, S. L. Lowe, F. Martenyi, S. M. Sheehan, L. N. Boggs, B. M. Mathes, B. M. Watson, S. L. Stout, D. E. Timm, E. Smith LaBell, C. R. Gonzales, M. Nakano, S. S. Jhee, M. Yen, L. Ereshefsky, T. D. Lindstrom, D. D. Calligaro, P. J. Cocke, D. G. Hall, S. Friedrich, M. Citron, J. E. Audia

3:20 217. Novel opioid peptides with drug-like properties as potential analgesics. **J. V. Aldrich**, S. S. Kulkarni, S. N. Senadheera, N. C. Ross, K. J. Reilley, S. O. Eans, M. L. Ganno, J. P. McLaughlin

Fluorescent and Plasmonic Probes in Chemical Systems

216 (University Place Conference Center)

G. Simpson, *Organizer*

N. Fang, *Organizer, Presiding*

1:30 218. Sensing applications for photon upconverting nanoparticles. **P. Zhang**

1:55 219. Scanning Angle Total Internal Reflection Raman Microscopy of Thin, Smooth and Rough Noble Metal Films. **E. A. Smith**, K. McKee, M. Meyer

2:20 220. Novel nonlinear optical characterizations of nanowires and nanowire heterostructures. **C. Yang**

2:45 Coffee Break.

3:05 221. Deciphering Rotational Motions Generated by Protein Machinery in Live Cells. **G. Wang**, W. Sun, N. Fang

3:30 222. Novel "non-blinking" quantum dots used in 3D high-resolution molecular tracking. **K. Marchuk**

Foods and Nutrition II

208 (University Place Conference Center)

Financially supported by Dow AgroSciences

P. Lewer, J. Phillips, *Organizers*

M. Ferruzzi, *Organizer, Presiding*

1:30 223. Spices and energy balance. **R. D. Mattes**

1:55 224. Does the food matrix matter to delivery of bioactive polyphenols? **M. G. Ferruzzi**

2:20 225. Carbohydrate nanoparticle-mediated colloidal assembly for the protection and delivery of bioactive compounds. **Y. Yao**

2:45 Coffee Break.

3:00 226. Food based interventions – Metabolites as markers of intake and bioavailability. **S. J. Schwartz**

3:30 227. Water-solid interactions and implications for the stability of bioactive compounds. **L. J. Mauer**, N. Li, R. Lipasek, M. West, L. S. Taylor

Frontiers in Materials and Bioinorganic Chemistry

222 (University Place Conference Center)

L. Watson, *Organizer*

S. Collins, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 228. Alcohol dependent production of Fe₃O₄ and CoFe₂O₄ nanoparticles. **B. J. Yocum**, M. J. O'Malley, T. F. Ekiert, M. D. Alexander

1:55 229. Hydrothermal production and characterization of Yttrium doped Fe₃O₄ nanoneedles. **A. Griner**, M. O'Malley, T. Ekiert, M. Alexander

2:15 230. Biologically-inspired alpha-hydroxy acid-containing chelates for light-responsive, reductive release of iron. **M. J. Baldwin**

2:35 Coffee Break.

2:50 231. Metalloregulatory proteins: Metal selectivity and allosteric switching. **D. P. Giedroc**

3:10 232. Metal-based therapeutics for cancer treatment: Gold (III) and ruthenium (II) polypyridyl complexes. **S. N. Collins**, J. D. West, S. Chatterjee, J. A. Krause, W. B. Connick, Y. Sun, C. Turro

3:30 Concluding Remarks.

Modeling Instructions in High School Chemistry

231 (University Place Conference Center)

L. E. Slocum, *Organizer*

K. Harper, *Organizer, Presiding*

- 1:30 233. Modeling Instruction in high school chemistry: A robust and research-based curriculum framework. **K. A. Harper**, T. M. Clark
1:55 234. Energy changes and connections to the student's world. **L. E. Slocum**, W. R. Thornburgh
2:15 235. Under pressure: Investigating the gas laws using modeling chemistry. **J. Cervenec**, B. Kovach
2:35 Coffee Break.
2:50 236. Organizing stoichiometry: Using BCA charts for conceptual understanding in the modeling classroom. B. Buehler, **K. Kennedy**
3:10 237. Another benefit of professional development workshops: Adopting modeling practices in undergraduate chemistry courses. **T. M. Clark**
3:45 Discussion.

Organic Chemistry - General Papers II

206 (University Place Conference Center)

Financially supported by Eli Lilly and Company

M. Hansen, *Organizer*

D. Mitchell, *Presiding*

- 1:30 Introductory Remarks.
1:35 238. N-O Chemistry for antibiotics: New N-alkyl-N-(pyridin-2-yl)hydroxylamine antibacterial scaffolds generated from nitroso ene chemistry. **T. A. Wencewicz**, B. Yang, J. R. Rudloff, M. J. Miller
1:55 239. Formation of 1,1-disubstituted allenes by regioselective Stille cross-coupling reactions and applications in the Pauson-Khand reaction. D. R. Williams, **A. A. Shah**
2:15 240. Gold catalyzed intramolecular oxygen transfer reactions of 2-alkynyl-1,5-diketones: a novel [4+2] cycloaddition revealed. **D. Malhotra**, L. Liu, G. Hammond
2:35 Coffee Break.
2:50 241. Analytical study of quinone methide generation for re-activation of aged Acetylcholinesterase: Treatment against nerve agent exposure. **S. Vyas**, J. D. Brown, R. J. Yoder, C. S. Reid, J. M. Beck, C. S. Callam, C. M. Hadad
3:10 242. Employment of a Dithiopin-based framework in the synthesis of cages and carcerands. **E. O. Wade**
3:30 243. Isoindolinone inhibitors of MDM2-p53 through arylation/selective oxidation of N-alkylhydroxylactams. **R. K. Dempster**, L. B. Hutcherson, F. A. Luzzio

PHYS/MEDI Computer-Aided Drug Design II

232 (University Place Conference Center)

S. Meroueh, *Organizer, Presiding*

- 1:30 244. Targeting epigenetic diseases. **G. L. Estiu**, O. G. Wiest, J. Bradner
2:05 245. Protein flexibility and dynamics in protein-ligand docking. **M. Lill**
2:40 Coffee Break.
2:55 246. Multipole Electrostatics Required to Reproduce Experimental Data. **G. R. Marshall**
3:40 247. Structure-based design of small-molecule anticancer drugs to target protein-protein interactions. **S. Wang**

Poster Session: Colloid and Surface Chemistry

132/134/137 (University Place Conference Center)

K. Anliker, *Organizer*

2:00 - 3:30

248. Shape control of iron oxide nanoparticle formation. **F. Kidwai**, J. E. Atkinson, A. G. Malyutin, B. D. Stein, L. M. Bronstein
249. Controlling the Architecture of Au/Pd Nanocrystals for Optical and Electrocatalytic Applications. **C. J. DeSantis**, S. E. Skrabalak
250. Real Time Monitoring of the in situ Growth of Silver Nanoparticles Under Mild Reduction Conditions. **J. C. Newton**, N. W. Dennis, R. Sardar
251. A facile approach to dendritic nanoparticle formation. **N. Ortiz**, S. E. Skrabalak
252. Designing advanced photocatalysts: Controlling crystal shape using innovative precursors with ultrasonic spray pyrolysis. **A. K. Mann**, S. E. Skrabalak
253. Quarternary Architecture of a Bacterial Red-Light Photoreceptor as Revealed by Scanning Tunneling Microscopy. **M. S. Goldmeier**, A. C. Sakols, H. Le, A. Gawedzka, K. T. Nicholson, S. Tsonchev, E. A. Stojkovic
254. Investigating the reactive landscape of porous materials. **E. A. Opsitnick**, H. Lee, X. Jiang, D. Lee
255. Evaluation of poly(butylcyanoacrylate) nanoparticle toxicity: A correlation between in vivo and in vitro models of the blood-brain barrier. **J. Squeri**, A. Gottula, R. Spaulding, M. Caroway, K. L. Haik, H. A. Bullen
256. Spectroscopic evaluation of the role of enterobactin in Escherichia coli adsorption to metal oxide surfaces. **A. Yarawsky**, H. A. Bullen
257. Periodic trends in structure function relationship of organic heteroacene semiconductors. **M. A. Loth**, S. R. Parkin, J. E. Anthony
258. Wet chemical functionalization of gallium-based III-V semiconductors. **S. L. Peczonczyk**, J. Mukherjee, S. Maldonado
259. Metal-responsive gelators built with linked-bipyridine ligands. **B. Park**, X. Jiang, H. Lee, D. Lee
260. Experimental studies of optical force on gold nanoparticle solution. **E. Koh**, A. Dabir, B. Dragnea
261. Switchable plasmon-chromophore coupling and surface-enhanced Raman scattered light: Applications in molecular detection, motion and logic. **C. W. Marlatt**, E. H. Witlicki, S. W. Hansen, D. W. Silverstein, V. J. Bottomley, J. O. Jeppesen, E. W. Wong, L. Jensen, A. H. Flood
262. Electronic energy relaxation in graphenes. **M. Mueller**, L. Li, X. Yan, J. McGuire
263. Synthesis of MoS₂ nanoparticles and nanorods from MoO₃ precursors of different morphology. **R. Combs**, T. Zubkov
264. One-Pot Synthesis of Gold-Coated Silver Nanoparticles at Room Temperature. **B. W. Boote**, G. Venam, B. W. Lavin, J. Kim

265. Photothermally-enhanced catalytic activities of anisotropic gold nanoparticles. **J. Kim**, J. A. Pham, B. W. Lavin, B. W. Boote
 266. Probing Adsorption Surface Sites on MoS₂ and WS₂: Comparison Between Nanoparticles and Bulk Materials. **J. B. LeRoy**, T. Zubkov
 267. Templated Growth of Metal Clusters on Colloidal Graphene Quantum Dots. **X. Yan**, Q. Li, L. Li
 268. Evaluation of creaming and sedimentation for nutritional beverages via analytical centrifuge, particle size analysis and rheology. **Y. Heo**

Poster Session: Physical Chemistry

132/134/137 (University Place Conference Center)

K. Anliker, *Organizer*

2:00 - 3:30

269. Lifetime dependence of total luminescence yields from 3 nm Alq₃ films deposited on plasmonic silver substrates. **S. T. Paquette**, L. J. Rothberg
 270. Synthesis and characterization of nitrogen-doped TiO₂/SnO₂ composite photocatalysts with high visible light activity. **L. Xu**, E. Steinmiller, S. Skrabalak
 271. Central importance of water and associated hydrogen bonding interactions in the determination of acetaminophen's conformation in the crystal lattice. **R. Burnette**
 272. Fluorescence Quenching Study of Gold and Silver Alloy Nanoparticles. **T. Brewer**, S. Chalasani
 273. Computational studies of chloroquine binding to Plasmodium falciparum lactate dehydrogenase and glyceraldehyde-3-phosphate dehydrogenase. V. F. Waingeh, **A. T. Groves**
 274. Novel application of ONIOM to elucidate structural information obtained from high resolution NMR investigations. **S. G. Lieb**
 275. Hydrogen atom isotope dynamics and hyperfine interactions in analogues of all-silicon zeolite cages: Density functional theory studies. **R. M. Macrae**
 276. Infrared spectral investigations of alcohol association in a variety of solvents including an ionic liquid. **J. L. Kirsch**
 277. Biacore X Surface Plasmon Resonance for anti-Amyloid Beta antibody detection. **A. L. Yokom**, J. C. Humes, J. M. Finke
 278. Characterization of Disintegration Profiles of Pharmaceutical Drugs Using Thermomechanical Analysis. **N. Idippily**, V. Rao, J. Moran, A. Riga
 279. *Withdrawn*.
 280. Spectroscopic, gravimetric, and EDAX characterization of the photoproducts of β -carotene generated in CCl₄ solvent. **T. C. Sack**, Y. Zhao, D. W. Johnson, M. B. Masthay
 460. Computational Modeling of Rhodopsin Protein Mimics. **M. R. Huntress**, M. Olivucci

Poster Session: Medicinal Chemistry

132/134/137 (University Place Conference Center)

K. Anliker, *Organizer*

4:00 - 5:30

281. Synthesis of Benzothiophene Carboxamide Derivatives and Their Pharmacological Evaluation as Potent Antihypertriglyceridemic Agents in Rats. **T. Al-Qirim**, G. Shattat, G. Abu Sheikhaa, Y. Al-Hiari
 282. Bioactivity of synthetic 2-halo-3-aryl-4(3H)-quinazolininium halides in L1210 leukemic and SK-BR-3 mammary tumor cells in vitro. **J. H. Perchellet**, A. M. Waters, E. M. Perchellet, V. K. Naganaboina, K. L. Chandra, J. Desper, S. Rayat
 283. Unusual conformational property of 2-amino-4-thiazolyl-methoxyimino polymers exhibiting activity against HIV-1 reverse transcriptase. **K. A. Kill**, D. B. Boyd
 284. Potentially Increasing the Metabolic Stability of Drug Candidates via Computational Site of Metabolism Prediction by CYP2C9: The Utility of Incorporating Protein Flexibility via an Ensemble of Structures. **M. Danielson**, M. Lill
 285. Significant enhancement of docking sensitivity using implicit ligand sampling. **M. Xu**, M. Lill
 286. Xanthine oxidase inhibition by coumarins. **J. Hand**, R. Medlock, R. Patel, M. Jayasinghe, S. Paula
 287. Inhibition of the sarco/endoplasmic reticulum calcium ATPase by bisphenols. **M. Woeste**, J. Steller, R. Patel, M. Jayasinghe, S. Paula
 288. Probe-based explorations of the ATP-binding sites of histidine kinases. **S. Francis**
 289. Molecular dynamics studies of the cholesterol and its fluorescent analog with the binding sites of NPC1 and NPC2 proteins. **N. A. Khatri**, G. L. Estiu, O. Wiest
 290. Target-specific support vector machine scoring in structure-based virtual screening: Computational validation, in vitro testing in kinases, and effects on lung cancer cell proliferation. **L. Li**, M. Khanna, I. Jo, F. Wang, N. M. Ashpole, A. Hudmon, S. O. Meroueh
 291. Support vector machine scoring of multiple receptor-ligand conformations in virtual screening. **B. Wang**, S. Meroueh
 292. Investigation of the electrostatic potential of inhibitors of β -amyloid cleaving enzyme-1 (BACE1). **A. F. Nastase**, M. J. Ketterer, D. B. Boyd
 293. Live-cell single-molecule fluorescence studies of the pathogenic pathway in Vibrio cholerae. **B. L. Haas**, J. S. Matson, V. J. DiRita, J. S. Biteen

Poster Session: Organic Chemistry I

132/134/137 (University Place Conference Center)

K. Anliker, *Organizer*

4:00 - 5:30

294. Relative rates of bond rotation and ring closure in the photocycloaddition intermediates from fullerene-C60 and the isomeric 2,4-hexadienes - a reinterpretation of reported data. **W. L. Dilling**
 295. Pterocarpenes and coumestans via an unusual 6-endo Heck cyclization. **G. W. Morrow**, K. J. Fowler, J. L. Ellis
 296. Preparation of anhydroalditols from commodity carbohydrates. **C. Yuan**, R. Hollingsworth
 297. Iodo derivatives of advanced carbohydrate intermediates. **C. Yuan**, R. Hollingsworth
 298. Furan derivatives: Utilization of biomass byproducts as renewable building blocks. **N. C. Tice**, A. Z. Preston, J. R. Armstrong, R. S. Estes, C. A. Snyder
 299. Synthesis and mechanistic investigation of new Benzyloxypyridinium Salt Derivatives. **C. T. Hubley**, P. A. Albinak
 300. Chemoselective Decarboxylative ortho-Acylation of Aryl Carboxylic Acids with α -Oxocarboxylic Acids via Palladium-Catalyzed sp² C-H Bond Activation. **J. Miao**, H. Ge
 301. New methods for the synthesis of selenoglycosides. **K. E. Walsh**
 302. Electron reduction and trimerization of aromatic substituted isocyanates. **M. E. Kassabaum**, S. J. Peters, N. C. Smart
 303. Manipulating the electronic properties of organic structures via transition metal coordination: Generation of conjugated, bidentate ligands for Pd(II) and Ag(I). **N. Bowling**, D. Hamm, K. Ness, A. Burazin, C. Biebel, A. Gauthier
 304. Olefinations by trifluoroacetate release. **M. V. Rioski**, J. P. John, M. M. Zheng, J. Kirshner, D. A. Colby
 305. Masking reactive carbonyl groups in situ form nucleophiles. **F. J. Barrios**, X. Zhang, D. A. Colby
 306. Computational study of the intramolecular [4+3] cycloaddition reaction intermediates using density functional theory. **R. C. Conyers**, B. Gung

- 307.** Synthesis and Structural Characterization of Terphenyl Scaffolded S-C-S Palladium Pincer Complexes and Studies of their Catalytic Activity in the Suzuki Coupling Reaction. J. D. Protasiewicz, **P. R. Challen**, M. D. Kwan, D. J. Barlett, N. Deligonul
- 308.** Synthesis of chiral N-Heterocyclic carbene based Au(I) catalyst with a dynamic ligand. **M. R. Holmes**, B. Gung
- 309.** Combined experimental and computational evidence for an sp²-hybridized N atom stacking interaction with a phenyl ring: pi-pi interactions in carbamate-benzene complexes. **B. U. Emenike**, B. W. Gung
- 310.** Intramolecular phosphate catalysis in the Maillard reaction of ribose 5-phosphate and amines. **R. K. Sandwick**, J. A. Colianni, M. S. Hirsch
- 311.** N-(Hydroxybenzyl)benzamides: pH-Rate profiles and Zn²⁺ catalysis of their breakdown in H₂O. **P. Siena**, T. Koyanagi, R. W. Nagorski
- 312.** Synthesis and biological activity of the aminosulfones. **A. M. Buysse**, L. C. William, I. Morrison, J. R. Phillips, B. Rieder, M. T. Sullenberger
- 313.** Aryl isocyanate anion radicals: Formation of PAHs via a reductive elimination. S. J. Peters*, **J. R. McGee**, M. E. Kassabaum
- 314.** Asymmetric, Tandem Wittig/Aldol and Wittig/Mannich Reactions. **N. C. Giampietro**, J. P. Wolfe
- 315.** Use of Combinatorial Chemistry to Support Lead Generation Approaches. Z. Benko, **L. K. Lawler**, B. Lorschbach, M. Parker, J. Ruiz, J. Webster

FRIDAY MORNING

Molecular Imaging and Drug Discovery

118 (University Place Conference Center)

Financially supported by Eli Lilly and Company

W. Porter, *Organizer*

B. Smith, *Organizer, Presiding*

8:15 316. The Utility of Molecular Imaging. **V. N. Barth**

8:50 317. Discovery and development LY2959530, a potent and selective NOP-1A radioligand for positron Emission Tomography. **Z. Chen**

9:25 Coffee Break.

9:40 318. Integrin α V β 3-targeted radiotracers: from discovery chemistry to clinical practice. **S. Liu**

10:15 319. Optical Imaging Strategies for the Development of Drugs and Novel Molecular Probes. **W. M. Leevy**

Multidisciplinary Undergraduate Research Symposium (M.U.R.S.)

226 (University Place Conference Center)

Financially supported by Division of Chemical Education

L. E. Slocum, *Organizer*

J. Giessler, *Organizer, Presiding*

8:15 320. Toward the caging of C60 using a Dithienyl-based host. **J. J. Kawa**, E. O. Wade

8:35 321. Indirect amperometric detection of inulin using a bienzyme system. **J. Pollock**, N. J. Ronkainen

8:55 322. Analysis of biofilm decontamination as a function of short wavelength LED intensity. **S. O'Neil**, E. Benjamin, D. Province, A. Tufts, S. Brand, S. D. Allen

9:15 323. Sweet medicine: Expression, purification, and characterization of a sugar nucleotidyltransferase for use in the glycosylation of drug candidates. **J. D. Vail**, G. J. Howell, L. N. Mitchell, S. C. Timmons

9:35 Coffee Break.

9:50 324. Characterization of esterase activity from the bacteria, *Francisella tularensis*, the causative agent of tularemia. **L. A. Weston**, R. Johnson

10:10 325. Isolation of a biologically active compound from the leaf gel of *Aloe striata*. **R. L. Schloss**, G. A. Wada, M. R. Lee, R. L. Bretz

10:30 326. Synthesis of novel Lavendamycin analogs. **J. Giessler**, R. E. Sammlson

Environmental Analysis and Sensing

216 (University Place Conference Center)

Financially supported by Heritage Environmental Services

G. Simpson, *Organizer*

D. Go, *Organizer, Presiding*

8:30 327. Analysis of iodinated acetic acids in drinking water. **Y. Li**

8:55 328. Colorimetric analysis for chromium (VI) in Lafayette, Indiana drinking water. J. L. Berman, **S. M. Gates**, D. J. Schauer

9:15 329. Determination of Chromium Contamination in Lafayette, Indiana by Atomic Absorption Spectrophotometry. **J. Covarrubias**, R. Duane, D. J. Schauer

9:35 Coffee Break.

9:55 330. Measuring the elusive hydroxyl radical in the atmosphere. S. Griffith, S. Dusanter, **P. S. Stevens**

10:20 331. Multiple isotope analysis in nitrate: Probing nitrogen pollution and remediation. **G. Michalski**

Functional Nanoscale Materials: Synthesis, Characterization, and Applications

236 (University Place Conference Center)

D. Lee, L. Li, S. Skrabalak, S. Tait, *Organizers*
A. Flood, L. Bronstein, *Organizers, Presiding*

- 8:30 332. Composition tuning of Fe- and W-based binary and ternary oxide photoanodes for use in the photoelectrolysis of water. K. J. McDonald, J. C. Hill, R. L. Spray, **K. Choi**
8:50 333. Synthesis of multifunctional Au/Pd nanocrystals. **S. E. Skrabalak**
9:10 334. Recent advances in the characterization of colloidal semiconductor nanowires. **M. Kuno**
9:30 Coffee Break.
9:50 335. Colloidal Graphene Quantum Dots and Their Application in Energy Conversion. **L. Li**
10:10 336. Electron-accepting low bandgap conjugated polymers based on azadipyrromethene. **G. Sauve**, L. Gao
10:30 337. Molecule design for organic electronics. **J. E. Anthony**

New Advances in Polymer Materials

222 (University Place Conference Center)

Z. Xiao, *Organizer, Presiding*

- 8:30 338. Polymer/inorganic nanocomposites: Tailoring the hierarchical structure to enhance performance. **E. Manias**
8:50 339. Characterization of interface of Polymer-Nanoparticle composites. **B. Lama**, M. P. Espe
9:10 340. Irradiated polyimide composites for nuclear batteries. **K. Bower**, S. Yousaf, M. Sychoy, A. Kavetskiy, G. Yakubova
9:30 Coffee Break.
9:50 341. Novel nanomaterials for improving conductivity in solid polymer electrolytes for rechargeable lithium-ion batteries. **S. K. Fullerton Shirey**
10:10 342. Impact of nanoparticle size and shape on the segregation of deuterated polystyrene to the air surface in polymer nanocomposites. **M. Mutz**, M. Dadmun
10:30 343. Activity and biocompatibility of PEGylated quaternary antimicrobial copolymers. **J. P. Youngblood**, B. M. Applegate, J. L. Rickus, T. R. Stratton, B. Allison

Organic Chemistry - General Papers III

206 (University Place Conference Center)

Financially supported by Eli Lilly and Company
M. Hansen, *Organizer, Presiding*

- 8:30 Introductory Remarks.
8:35 344. Development of a green method for amide synthesis. **M. R. Darragh**, A. M. Wilson
8:55 345. Charge-transfer complexes vs transition states electrostatics in the Diels-Alder reactions of o-chloranil and styrenes. **S. Rosokha**
9:15 346. An improved c-3 reductive alkylation of indoles. **J. R. Rizzo**, T. Y. Zhang, C. A. Alt
9:35 Coffee Break.
9:50 347. Pharmacophore based design: The synthesis of novel neonicotinic insecticides. **Z. L. Benko**, D. A. Demeter, C. V. DeAmicis, R. Erickson, G. B. Watson
10:10 348. Microwave assisted Cope and Claisen Rearrangements: Adaptations to greener pathways. **A. M. Wilson**, O. Wenrich, M. Slack, C. Hon
10:30 349. Discovery and synthesis of Penoxsulam, a new rice herbicide. **M. A. Pobanz**, T. C. Johnson, R. K. Mann, T. P. Martin

Physical Chemistry - General Papers

232 (University Place Conference Center)

J. Pu, *Organizer*
M. Nguyen, *Presiding*

- 8:30 350. Characterizing Bacterial Red-Light Photoreceptors by Scanning Probe Microscopy. A. C. Sakols, S. M. Vorpahl, M. S. Goldmeier, A. Gawedzka, E. A. Stojkovic, S. Tsonchev, **K. T. Nicholson**
8:50 351. Co¹⁺ ion-induced H-Bond tunes the redox potential of a thermodynamically challenging cob(II)alamin/cob(I)alamin reduction: Potential mechanistic implications with regard to Methyltransferases and Adenosyltransferases. **M. Kumar**
9:10 352. Estimating the SERS-based sensing capabilities of colloidal silver nanoparticles: A novel physical chemistry and nanotechnology laboratory experiment. **J. D. Baker**, K. S. Alnajjar, J. L. Monahan, A. C. Stahler, N. E. Hunter, K. M. Weaver, A. J. Meyerhoefer, D. A. Dolson, I. E. Pavel
9:30 Coffee Break.
9:50 353. Improved Photovoltaic performance of Dye-sensitized Solar Cells by Using 3-Aminopropyltriethoxysilane and Gold Nanoparticles. **T. Luitel**, F. P. Zamborini
10:10 354. Self-Assembly of Nanorods into Designer Superstructures: the Role of Templating, Capillary Forces, Adhesion and Polymer Hydration. **S. Tsonchev**, J. W. Ciszek, L. Huang, Y. Wang, K. Shull, M. Ratner, G. Schatz, C. Mirkin

Student Assisted Teaching in Chemistry

231 (University Place Conference Center)

P. Varma-Nelson, G. Ammerman, *Organizers, Presiding*

- 8:30 355. Student Assisted Teaching in Chemistry: Theory, Research, and Practice. **M. S. Cracolice**
9:15 356. Peer-led tutorial videos as a tool to promote student learning. **H. Zhao**, F. Timm
9:35 Coffee Break.
9:50 357. Cyber peer-led team learning in general chemistry. P. Varma-Nelson, L. Zhu, **J. Sours**, K. Mauser
10:10 358. Reinforcing organic chemistry learning through facilitated problem-solving discussions. **S. B. Wilson**, R. Denton, P. Varma-Nelson, R. Minto
10:30 359. Comparison of face-to-face and online peer lead teamed learning general chemistry workshops. **G. Ammerman**, J. V. Banks, P. Varma-Nelson

Systems Biology

208 (University Place Conference Center)

Financially supported by Dow AgroSciences
P. Lewer, *Organizer*
J. A. Morgan, D. McCaskill, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 360. Metabolomics provides fundamental insights to understanding *Medicago* secondary metabolism. **Z. Lei**, M. A. Farag, C. D. Broeckling, D. V. Huhman, E. Ubanczyk-Wochniak, W. Li, M. Bedair, B. S. Watson, M. Naoumkina, B. Deavours, R. A. Dixon, L. W. Sumner

9:05 361. Metabolic flux analysis in plants and microbes. **Y. Shachar-Hill**, W. Chen

9:35 Coffee Break.

9:50 362. Identification of unknown and highly conserved genes in the bacterium *Rhodobacter sphaeroides*. **A. T. Setterdahl**, S. Strom, A. Green, K. Lett

10:10 363. Biosynthesis of alkalimides by *Echinacea purpurea*. **R. E. Minto**, M. R. Shepard, A. S. Ransdell, H. W. Scott, B. J. Nikolau

10:30 364. Proteomic and metabolic flux analysis of recombinant CHO cell cultures. **J. A. Morgan**, M. Zhang, N. Sengupta

Poster Session: Biological Chemistry

132/134/137 (University Place Conference Center)

K. Anliker, *Organizer*

9:00 - 10:30

365. Effect of osteopontin on erythrocyte calcium levels. **B. Oliver**, C. Myers, K. Giger, A. Wickrema, P. Low

366. Stimulation of a PriA helicase by PriB reveals species-specific adaptations in DNA replication restart primosome proteins. C. Feng, M. E. Greenwood, **M. E. Lopper**

367. Founding an alkalimide biosynthesis model for *Echinacea*. **M. R. Shepard**, H. W. Scott, J. R. Lage, R. E. Minto

368. Identifying new haplotypes and potential cryptic species for marine leeches (*Ozobranchus* spp.) from Hawaiian and Florida sea turtles based on molecular data. **T. M. Truong**, A. E. McGowin, P. Lavretsky, J. L. Peters

369. Lipidomic profiling of *Dictyostelium discoideum*. **G. L. Birch**, R. E. Minto, B. J. Blacklock

370. Withdrawn.

371. Analysis of the DNA binding site-selectivity of bleomycin using fluorescent intercalator displacement. **S. A. Henkes**, R. MacKay, M. A. Lewis, E. C. Long

372. Services and expertise provided by the IUPUI/IUSCC Chemical Synthesis & Organic Drug Lead Development Core. **T. M. Georgiadis**, E. C. Long

373. Design, synthesis, and study of DNA-targeted benzimidazole-amino acid conjugates. **M. L. Garner**, J. B. Li, E. C. Long

374. Domain structure of the minor allergen Ovomuroid by solution NMR. N. E. Stenzoski, **B. D. Ray**, G. W. Gebriel, H. I. Petrache

375. Improvement in cell viability and migration of Glioma cells in vitro using hemoglobin-based oxygen carriers (HBOCs). **A. D. Roth**, J. Elmer, T. Nelson, J. De Jesus, P. Agudelo-Garcia, J. J. Lannutti, M. S. Viapiano, A. F. Palmer

376. Exploring the spore photoproduct formation using d3thymidine. **D. M. Ames**, G. Lin, L. Li

377. Chemoselective Isolation for Carboxylic Acid-Containing Natural Products. **D. J. Trader**, E. E. Carlson

378. Characterization of *Rhodobacter sphaeroides* gene RSP1463. **S. L. Strom**, A. T. Setterdahl

379. Identification and characterization of unknown gene function in *Rhodobacter sphaeroides*. **A. J. Green**, A. T. Setterdahl

380. Cloning, purification, and enzymatic characterization of lipases from *Mycobacterium tuberculosis*. **A. Gehring**, R. Johnson

381. Chemical and physical modification of the immunofluorescent staining technique to enhance identification of Polycystin 1 in human kidney tissue. **T. T. Dick**, S. V. Bell, D. J. Pedley, A. M. Shouse

382. Expression, characterization and mutagenesis of the ARO10 gene product, a phenylpyruvate decarboxylase, from *Saccharomyces cerevisiae*. **M. M. Kneen**, R. Stan, A. Yep, R. P. Tyler, M. J. McLeish

383. Purification and characterization of a putative essential esterase from *Francisella tularensis*. **A. M. Farberg**

384. Is a tetramer required for benzoylformate decarboxylase activity? **F. H. Andrews**, M. J. McLeish

385. Biochemical characterization of a fatty acid elongase condensing enzyme. **S. Hernandez-Buquer**, B. J. Blacklock

386. Increasing the expression of alkaline phytase in *Pichia pastoris*: effect of gene optimization and gene dosage on expression levels. **M. Yang**, S. C. Johnson, T. E. Johnson, P. P. Murthy

387. Synthesis and characterization of ester derivatives of antibiotics via a novel method. **N. H. Clarke**, R. J. Johnson

388. Chemical probes for global histidine kinase profiling. **K. E. Wilke**, E. E. Carlson

389. Hydrophobic packing is a key component in the allosteric switching mechanism for *Staphylococcus aureus* CsrA. **G. C. Campanello**, D. P. Giedroc

390. Chemoselective enrichment for the discovery of novel natural products from *Streptomyces*. **A. M. Sidebottom**, E. E. Carlson

391. Characterization of a trisulfide-like selenium bridge in the *Staphylococcus aureus* transcriptional repressor CstR. **J. L. Luebke**, D. P. Giedroc

392. Characterization of *Mycobacterium tuberculosis* lipases. **E. E. Ellis**

393. Comparative Analysis of Various Extracts of Seeds *Trachyspermum Copticum* and *Nigella Satvia* on 15-Lipoxygenase. D. P. Brown, B. W. Noffke, **S. Buddha**

394. Chemical probing of the Cu(I)-sensing repressor B. subtilis CsoR in various allosteric states. **F. Chang**, M. Lauber, J. P. Reilly, D. P. Giedroc

395. Biochemical and structural characterization of the putative copper chaperon and the metal binding domain of copper exporting P-type ATPase in *Streptococcus pneumoniae*. **Y. Fu**, D. Giedroc

396. Understanding manganese and zinc homeostatic interplay in *Streptococcus pneumoniae*. **J. P. Lisher**, D. Giedroc

397. Enzymatic Characterization of ybfF, a thioesterase of *Vibrio cholerae*. **N. Galovska**, R. Johnson

398. Ni(II)/Co(II) Metalloregulator NmtR: Structure, Metal Binding Site, and Allosteric Regulation. **C. Lee**, H. R. Caballero, D. P. Giedroc

Plenary Lecture III

Auditorium (University Place Conference Center)

11:00 . Michael A. Evans, President and CEO, AIT Laboratories

J. Siegel, *Presiding*

FRIDAY AFTERNOON

ACS Hach High School Chemistry Grants: Supporting Innovative Ideas in the High School Chemistry Classroom

226 (University Place Conference Center)

L. E. Slocum, *Organizer*

K. Thompson, *Organizer, Presiding*

1:30 Introductory Remarks

1:35 461. Exploring Forensic Chemistry with the ACS-Hach High School Chemistry Grant. **R. Thomas**

2:00 400. Expanding Student Boundaries with the ACS-Hach High School Chemistry Grant. **M. Janek**

2:25 399. Foundry in a Box: Casting a New Approach to Chemistry Education with the ACS-Hach High School Chemistry Grant. **E. Escudero**

2:45 Coffee Break

3:00 401. Write Your Way to Success: Grant Writing Strategies for You and Your Chemistry Students. **K. Thompson**

Advances in Mass Spectrometry: New Method Development and Instrumentation

216 (University Place Conference Center)

G. Simpson, *Organizer*

H. Chen, *Organizer, Presiding*

1:30 402. Single cell level, high spatial resolution mass spectrometry imaging for plant metabolites. **Y. Lee**

2:00 403. Comparison of CID, ETD, and metastable atom-activated dissociation (MAD) of phosphorylated tau peptides. **G. P. Jackson**

2:30 Coffee Break.

2:50 404. Applications of covalent footprinting and top down mass spectrometry in structural biology. **H. W. Rohrs**, H. Zhang, W. Cui, M. L. Gross

3:20 405. Advances in DESI Mass Spectrometry: Tissue Imaging, TLC Plates and SPME. **J. M. Wiseman**

Biochemistry - General Papers II

208 (University Place Conference Center)

B. Blacklock, *Organizer*

R. Johnson, *Presiding*

1:30 Introductory Remarks.

1:35 406. Cardiolipin as a proton trap: Investigation by solid state NMR. **T. V. Krivokhizhina**, R. J. Wittebort

1:55 407. Liposome encapsulated hemoglobins as red blood cell substitutes. **S. Rameez**, A. F. Palmer

2:15 408. Characterizing the Substrate Specificity of Bacterial Esterases Using Latent Fluorophores. **R. Johnson**, M. Hedge, L. Weston

2:35 Coffee Break.

2:50 409. Towards the structure and function of *S. pneumoniae* AdcR: A novel MarR-family transcriptional regulator. **A. J. Guerra**, H. Reyes-Caballero, F. E. Jacobsen, U. K. Koppolu, R. A. Scott, K. M. Kazmierczak, M. E. Winkler, D. P. Giedroc

3:10 410. Isoelectric focusing of proteins in capillaries and planar substrates. **B. M. Koshel**, R. E. Birdsall, Y. Hua, M. J. Wirth

3:30 411. Micro-Raman imaging of the bone development in chick embryos exposed to 1.0 ppm sublethal doses of platinum group metals. **A. Stahler**, I. Pavel, Z. Gagnon, M. Markopoulos, J. Monahan, J. Dagher, J. Baker, T. Lam

CHEM TALK: A Symposium for AP Chemistry Teachers

231 (University Place Conference Center)

L. E. Slocum, *Organizer*

L. Ford, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 412. An inquiry activity to explore inter vs intra molecular forces. **E. C. Kentrup**

1:55 413. Chemical Equilibrium - An Experimental Model Utilizing Large Pop Beads. **E. Escudero**

2:15 414. Eclectic internet resources to aid AP Chemistry teachers. **M. Geyer**

2:35 Coffee Break.

2:50 415. Keeping the students engaged after the AP exam. **L. Slocum**

3:10 416. POGILing in AP Chemistry. **L. Ford**

Chemometrics with Forensic Applications

236 (University Place Conference Center)

J. Siegel, *Organizer*

J. Goodpaster, *Organizer, Presiding*

1:30 417. Monitoring and characterizing microbial degradation of gasoline on different soil types. **D. A. Turner**, A. Flores, J. V. Goodpaster

1:50 418. Using multivariate statistical procedures to identify ignitable liquid residues in the presence of interferences. **K. Prather**, V. L. McGuffin, R. Waddell Smith

2:10 419. Lipid profiling of decomposed tissue by nano-electrospray ionization tandem mass spectrometry for postmortem interval determination. **J. W. McIlroy**, G. Reid, R. Waddell Smith

2:30 Coffee Break.

2:50 420. Discrimination of *Salvia divinorum* from related *Salvia* species using chromatographic techniques and chemometric procedures. **M. L. Bugeja**, M. Bodnar Willard, V. L. McGuffin, R. Waddell Smith

3:10 421. Inter-laboratory study with red cotton fibers based on microspectrophotometry. **C. Szkudlarek**, J. Goodpaster

3:30 422. Instrumental and chemometric analysis of automotive clear coat paints by micro laser Raman. **A. N. Mendlein**, J. A. Siegel, J. V. Goodpaster

Dynamics of Lipid Membranes and Proteins

232 (University Place Conference Center)

K. Seu, Organizer, Presiding

1:30 Introductory Remarks.

1:35 423. Structure of E. coli membranes as determined by single molecule mobility studies. **K. Ritchie**

2:00 424. Erythrocyte membrane-cytoskeletal interactions monitored with single molecule diffusion. **K. Giger**, K. Ritchie, P. Low

2:25 425. Utilizing Electron Spin Echo Envelope Modulation (ESEEM) Spectroscopy to Probe the Structure of Membrane Proteins. **D. J. Mayo**, G. A. Lorigan

2:50 Coffee Break.

3:05 426. Using replica exchange molecular dynamics to study lipid protein interactions. **S. E. Feller**

3:30 427. Effect of native ligands on integrin oligomerization state and raft recruitment processes studied in cholesterol containing polymer-tethered lipid bilayer systems. **A. P. Siegel**,

A. C. Kimble-Hill, R. Jordan, C. A. Naumann

3:55 428. Cholesterol induced buckling in physisorbed polymer-tethered lipid membranes. **N. F. Hussain**, M. A. Johnson, A. P. Siegel, C. A. Naumann

4:20 Concluding Remarks.

Open Medicinal Chemistry Session

118 (University Place Conference Center)

Financially supported by Eli Lilly and Company

W. Porter, Organizer, Presiding

1:30 Introductory Remarks.

1:35 429. Pyrazolone containing small molecules exhibit activity in a G93A-SOD1 mouse model of Amyotrophic Lateral Sclerosis. **P. C. Trippier**, T. Chen, R. Benmohammed, D. R.

Kirsch, R. J. Ferrante, R. I. Morimoto, R. B. Silverman

2:05 430. Triazole-based NK-1 receptor antagonists: Selected C4- and C5-position SAR. **K. M. Gardinier**

2:35 Coffee Break.

2:50 431. Nanoencapsulated Drug-Carrying Systems for Photodynamic Antimicrobial Chemotherapy (PACT). **G. K. Kalapala**, P. K. Fu

3:20 432. Design, synthesis, and biological evaluation of selective inhibitors of protein kinase D. **K. Bravo-Altamirano**, K. M. George, M. Frantz, C. R. LaValle, M. Tandon, E. R.

Sharlow, J. S. Lazo, Q. Wang, P. Wipf

Young Investigator Symposium

206 (University Place Conference Center)

M. Van Nieuwenhze, Organizer, Presiding

1:30 433. Chemoselective Enrichment for Natural Products Discovery. **E. E. Carlson**, D. J. Trader, A. Y. Odendaal

2:00 434. Harnessing Masked Electrophilicity: Alternative Strategies for Selective Carbonyl Functionalization. **B. L. Ashfeld**

2:30 Coffee Break.

2:50 435. Oxidant-Controlled Stereoselectivity in the Pd-Catalyzed Allylic Oxidation of cis-Vinylsilanes. **J. Stambuli**

3:20 436. Tandem catalysis: Advancing the scope of enolate chemistry. **S. Cook**

Poster Session: Chemical Education

Slate Hallway (University Place Conference Center)

K. Anliker, Organizer

2:00 - 3:30

437. Performance of U.S. High School Students in IChO and PISA. **L. H. Kolopajlo**

438. Green Hydrogenation Reactions for the Undergraduate Organic Lab: The Solvent-less Hydrogenation of Unsaturated Esters. **K. J. O'Connor**, D. K. Fry

439. 2011 Midland Section ACS election of executive committee members – problems in multiple instant run-off elections with small numbers of voters and comparison of alternate voting procedures. **W. L. Dilling**

440. Electronic data collection in the biochemistry teaching laboratory: Updating an enzyme kinetics experiment. **S. M. Tremain**

441. Development of an online knowledge base for the first semester organic chemistry lecture. **T. Crumacker**, M. Collins, R. Denton

442. Estimating the analytical and surface enhancement factors in SERS: A novel physical chemistry and nanotechnology laboratory experiment. **A. J. Meyerhoefer**

443. Gender differences in high school chemistry students' confidence in lab and content knowledge: Investigating the impact of an authentic science curriculum. **K. S. Kingery**, G. C. Weaver

444. Comparative cytotoxicological study of ionic silver and silver nanoparticles using an MTT bioassay. **Z. S. Arnold**, A. Chang, A. J. Meyerhoefer, N. E. Hunter, M. M. Markopoulos, S. A. Paluri, J. C. Trefry, D. P. Wooley, I. E. Pavel

445. Isolation of a biologically active compound from the leaf gel of Aloe cameronii. **C. D. Rodriguez**, M. R. Lee, R. L. Bretz

446. Integrating webinar and blogging technologies into chemistry seminar. **D. W. Randall**, D. H. Murray, D. Hamstra, J. N. Kemsley

447. Modeling chemical behavior with QSAR. **S. P. Wathen**

Poster Session: Organic Chemistry II

Slate Hallway (University Place Conference Center)

2:00 - 3:30

448. Synthesis of highly substituted A-ring Vitamin D3 analogs and CD ring system from diene sulfone. **V. Sikervar**
449. α -Hydroxyhippuric acid derivatives: pH-Dependent aqueous kinetics and buffer catalysis. **K. Feken**, R. W. Nagorski
450. Synthesis of N-(α -alkoxybenzyl)amide derivatives and initial pH-dependent rate studies in H₂O. **S. C. Stewart**, R. W. Nagorski
451. Condensation investigation: An acid-catalyzed, microwave assisted approach. **T. L. Friebe**, W. Joesten, T. Faust, A. Sinha
452. Studies on catalytic activities of carbamic acids. **S. Adhikari**, K. Yamamoto
453. Oxidative Amide Bond Formation. **H. Yao**, K. Yamamoto
454. 5-(4-Alkoxyphenyl)thieno[3,2-b]thiophene-2-carboxylate esters: Synthesis and liquid crystal properties. **J. I. Tietz**, J. R. Mastriana, P. Sampson, A. J. Seed
455. Carbazole-based , color-tuned, fluorescent organic nanoparticles. **K. N. Upamali**, D. C. Neckers
456. Stereoselective Synthesis of the C28–C33 Subunit of Aplyronine A. **D. Gunasekera**
457. Synthesis of malononitrile and cyanoacetamide containing isoxazoles and isoxazolines . **L. C. Moores**, R. E. Sammelson
458. Synthesis and Biological Activity of Formyl Hydrazones. **B. Nugent**, K. Meyer, J. Babcock, Y. Adelfinskaya, G. Crouse, G. DeBoer, G. Watson
459. Catalytic transfer hydrogenation of multi-functional chalcones with ammonium formate. **T. Nguyen**, T. Rickard, D. Hartley, T. Iqbal, R. Denton