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
9:35 Coffee Break.
10:10 5. Isoelectric focusing in packed capillaries for resolution of protein glycoforms. M. J. Wirth

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

Frontiers of Organometallic and Transition Metal Chemistry
222 (University Place Conference Center)

D. Mindiola, Organizer
L. Watson, Organizer, Presiding

8:30 Introductory Remarks.
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 d0 configuration? S. N. Brown
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.

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.
9:35  Coffee Break.
9:50  24. Dirty by design: a rational approach to the design of new antitubercular nitroimidazoles. C. E. Barry

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.
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
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

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.
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

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.
3:30  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.
1:55  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.
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. Photoactivatable riboflavin and phylloquinone as photodynamic antimicrobial chemotherapy agents. J. M. Blain, P. K. Fu
2:35  Coffee Break.
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. 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
2:35 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
2:30 Coffee Break.
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
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

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
2:20 82. Multi-scale simulations by open-boundary QM/MM. S. Pieszeshki, 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
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 commercial carbon containing fuels with regard to CO2 emission. S. A. Studniarz
93. Elemental analysis via energy dispersive X-ray fluorescence of commercial driered, powdered, kelp food supplements for heavy metals. D. M. Garshott, E. MacDonald, M. Murray, E. Roberts-Kirchhoff, M. A. Bervenuto
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
98. Ionic liquid-based solvent extraction systems for improved actinide and fission product separations. S. L. Garvey, M. Dietz
100. Adsorption and desorption of barium to hematite (α-Fe2O3) in artificial seawater. D. S. Lennaerts, S. R. Higgins
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
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

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 Nanoparticles 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 ion solutions. A. Waris
115. Cheluminescence catalyzed by Ag/Au Nanoparticle alloys. S. Abideen
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-pyrenesulphonate immobilized in sol-gel thin film and its evaluation as potential pH sensor. Q. Hu, S. A. Green
121. New direct method for quantifying low molecular weight organic acids in oils. E. Sorensen
122. Withdrawn.
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
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. Z. Zamborini
131. Quantitative determination of common synthetic cannabinoids JWH analogs by thin-layer chromatography. E. Litchfield, G. Lyman, K. Waters, Y. Jhabag, C. C. Debel
132. Modeling of tryptophan on reversed phase liquid chromatography using substituted imidazolium ionic liquids as mobile phase additives. T. J. Ahmad, K. K. Aluguveli, 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. Dophode, M. C. Maurer
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
10:30 146. 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. Coffer
9:15 149. Applications of direct analysis in real time mass spectrometry (DART-MS) to cultural heritage materials. R. Armitage
9:35 Coffee Break.
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 396 (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

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. Heard, Organizer, Presiding

8:30 Introductory Remarks.
8:55 172. Synthesis of aryl organosulfur and organoselenium compounds by AlCl3-catalyzed electrophilic aromatic substitution reactions. X. Sun, D. Haas, K. Sayre
9:35 Coffee Break.
9:50 174. Synthesis of functionalized 1,3-dihydrobenzo[cfuran 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
Teaching and Learning in the Digital Age: Resources Teachers and Students Can Rely On
236 (University Place Conference Center)

L. E. Scocum, 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. Watthen
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. Aniker, Organizer

9:00 - 10:30

186. Thermal behavior of ionic liquid crystalline compounds of transition metals with dimethylhexadecylammonium and hexadecylamine ligands. E. A. Jensen, L. Cichon
187. Fabrication of magnetic mesoporous silica nanocomposite as magnetically recyclable catalyst for reduction of nitroarenes. M. Shokouhinehr
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 thyl radical: Synthesis by chemical oxidants and reactivity studies. R. Chauhan, C. Grapperhaus, M. Mashuta
192. NMR Characterization of Boron-Substituted Poly(pyrazolyl)borate Complexes of Cu(ii). S. M. Greer, D. L. Tierney
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. Altair, 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. Structure and reactivity of uranium(III) alkyl complexes. E. M. Matson, P. E. Fanwick, S. C. Bart
200. Chemistry and spectroscopy of pseudotetrahedral N(u)llarythiolate complexes. T. Deb, J. L. Petersen, V. G. Young, Jr., M. P. Jensen
202. An electrochemical study of hydrogen-generating organometallic compounds. E. S. Donovan, S. E. Froberg, G. A. Felton
204. Photochemistry and photophysics of a polypeptide ligand and corresponding platinum(II) complexes. D. P. Lazaro, D. R. McMillin
205. XANES studies of cobalt containing compounds. J. C. Kaine, D. L. Tierney
211. Interaction of Ru(II)mono-arene Complexes with Serum Proteins. L. Wang, S. Skop, A. Basing

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.
2:40 Coffee Break.

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. Matas
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

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
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
Modeling Instructions in High School Chemistry
231 (University Place Conference Center)

L. E. Slocum, Organizer
K. Harper, Organizer, Presiding

1:55 234. Energy changes and connections to the student's world. L. E. Slocum, W. R. Thornburgh
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.
1:55 239. Formation of 1,1-disubstituted alenes by regioselective Stille cross-coupling reactions and applications in the Pauson-Khand reaction. D. R. Williams, A. A. Shah
2:35 Coffee Break.
3:10 242. Employment of a Dithiepin-based framework in the synthesis of cages and carcerands. E. O. Wade

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. West, J. Bradner
2:05 245. Protein flexibility and dynamics in protein-ligand docking. M. Lill
2:40 Coffee Break.
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
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
256. Spectroscopic evaluation of the role of enterobactin in Escherichia coli adsorption to metal oxide surfaces. A. Yarawsky, H. A. Bullen
258. Wet chemical functionalization of gallium-based III-V semiconductors. S. L. Peczczonczyk, J. Mukherjee, S. Maldonado
259. Metal-responsive gelators built with linked-bipyridine ligands. B. Park, X. Jiang, H. Lee, D. Lee
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 Au3 films deposited on plasmonic silver substrates. S. T. Paquette, L. J. Rothberg
270. Synthesis and characterization of nitrogen-doped TiQ2/SnO2 composite photocatalysts with high visible light activity. L. Xu, E. Steinmiller, S. Skrabalka
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. Wainghe, A. T. Groves
274. Novel application of ONIOM to elucidate structural information obtained from high resolution NMR investigations. S. G. Lieb
276. Infrared spectral investigations of alcohol association in a variety of solvents including an ionic liquid. J. L. Kirsch
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
281. 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

283. Unusual conformational property of 2-aminoo-4-thiazolyl-methoxyimino polymers exhibiting activity against HIV-1 reverse transcriptase. V. K. Naganaboina, K. L. Chandra, J. Desper, S. Rayat
286. Xanthine oxidase inhibition by coumarins. J. Hand, R. Medlock, R. Patel, M. Jayasinghe, S. Paula
287. Inhibition of the sarcoplasmic 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. Khanh, J. Jo, F. Wang, N. M. Ashpole, A. Hudson, S. O. Mercuem
291. Support vector machine scoring of multiple receptor-ligand conformations in virtual screening. B. Wang, S. Mercoue
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. Biteit

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 antiydaoiditalols from commodity carbohydrates. C. Yuan, R. Hollingsworth
297. Iodo derivatives of advanced carbohydrate intermediates. C. Yuan, R. Hollingsworth
300. Chemoisselective 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
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
305. Masking reactive carbonyl groups in situ form nucleophiles. F. J. Barrios, X. Zhang, D. A. Colby
307. Synthesis and Structural Characterization of Terphenyl Scaffolding 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


311. N-(Hydroxybenzyl)benzamides: pH-Profile profiles and Zn2+ catalysis of their breakdown in H2O. P. Siena, T. Koyanagi, R. W. Nagorski


313. Asymmetric, Tandem Wittig/Aldol and Wittig/Mannich Reactions. N. C. Giampietro, J. P. Wolfe

314. Use of Combinatorial Chemistry to Support Lead Generation Approaches. Z. Benko, L. K. Lawler, B. Lorsbach, 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 αvβ3-targeted radiotracers: from discovery chemistry to clinical practice. S. Liu

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 Ditheipin-based host. J. J. Kawa, E. O. Wade
8:35  321. Indirect amperometric detection of inulin using a biocatalytic system. J. Pollock, N. J. Ronkainen
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

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
9:35  Coffee Break.
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)
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
9:30 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

Physical Chemistry - General Papers
232 (University Place Conference Center)
J. Pu, Organizer
M. Nguyen, Presiding
8:50 351. CoI+ ion-induced H-Bond tunes the redox potential of a thermodynamically challenging cob(I)alamin/cob(I)alamin reduction: Potential mechanistic implications with regard to Methyltransferases and Adenosyltransferases. M. Kumar
9:30 Coffee Break.

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.
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)
226 (University Place Conference Center)

L. E. Slocum, Organizer
K. Thompson, Organizer, Presiding

1:30 Introductory Remarks
1:35 451. 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.

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. Krivokhzizhina, 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.
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.
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
2:50 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
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.
2:05 430. Triazole-based NK-1 receptor antagonists: Selected C4- and C5-position SAR. K. M. Gardinier
2:35 Coffee Break.

Young Investigator Symposium
206 (University Place Conference Center)

M. Van Nieuwenhze, Organizer, Presiding

1:30 Chemoselective Enrichment for Natural Products Discovery. E. E. Carlson, D. J. Trader, A. Y. Odendaal
2:00 Harnessing Masked Electrophilicity: Alternative Strategies for Selective Carbonyl Functionalization. B. L. Ashfeld
2:30 Coffee Break.
2:50 Oxidant-Controlled Stereoselectivity in the Pd-Catalyzed Allylic Oxidation of cis-Vinylsilanes. J. Stambuli
3:20 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. Klopokalo
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. Crumpacker, 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
445. Isolation of a biologically active compound from the leaf gel of Aloe cameronii. C. D. Rodriguez, M. R. Lee, R. L. Bretz
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. Feeken, 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


452. Studies on catalytic activities of carbamic acids. S. Adhikari, K. Yamamoto

453. Oxidative Amide Bond Formation. H. Yao, K. Yamamoto


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 cyanacetamide containing isoxazoles and isoxazolines. L. C. Moores, R. E. Sammelson
