TECHNICAL PROGRAM

WEDNESDAY EVENING

Fulkerson Center

Sci-Mix
S. L. Hiley, Organizer
Sponsored by ThermoFisher Scientific

7:00 - 9:00


THURSDAY MORNING

Fulkerson Center, Rochambeau Room 220

Advances in Drug Discovery
S. R. Svojanovsky, Organizer, Presiding
Financially supported by the Division of Organic Chemistry


8:30 2. New tricks for an enchanted ring: Beta-lactam inhibitors of glutamine synthetase. T.A. Wencewicz

9:00 3. Large-neutral amino acid transporter 1 (LAT-1) for drug delivery to the brain. A.A. Thomas, E. Augustyn, K. Finke, L.M. Hansen, N. Heeren, S. Miller, A.A. Zur, L. Lin, K. Giacomini

9:30 4. From natural products, epigenetics, to diversity orientated synthesis: Where will new therapeutic scaffolds come from? R. Rafferty

10:00 Intermission.

10:15 5. Chemical proteomics to the development of natural glycoconjugates towards novel anticancer agents. W. Shi


**Blum Union Room 218**

**Analytical Chemistry**  
S. L. Hiley, *Organizer*  
G. E. Clapp, *Presiding*  
*Sponsored by Shimadzu*

8:00 8. Detection of adulteration in food using benchtop NMR spectroscopy. **S. Riegel**


9:40 Intermission.

10:00 13. High performance affinity chromatography studies of interactions by dansylamide with human serum albumin. **D. Suresh**, Z. Li, T. Nguyen, D.S. Hage


11:00 16. Two-branch microfluidic switch coupled with capillary electrophoresis for alternate separations. **Q. Zhang**, N. Zhang, M. Gong


**Blum Union Room 219**

**Organic Chemistry**  
S. L. Hiley, S. P. Lorimor, *Organizers*  
M. Pattabiraman, *Presiding*

8:20 20. Fluorescent logic gates as multi-input chemical sensors for neuronal imaging. K.S. Hettie, J.L. Klockow, T.E. Glass


9:20 Intermission.


10:00 24. Tetrapodal molecular tectons for three-dimensional open networks. C. Gunawardana, C.B. Aakerøy, J. Desper

10:20 25. Phosphate tether-mediated, one-pot, sequential protocols for the synthesis of macrolactones and corresponding analogs. S. Javed, M. Bodugam, A. Ganguly, J. Torres, P.R. Hanson

10:40 26. Phosphate tether-mediated, macrocyclic ring-closing metathesis for the formation of P-stereogenic bicyclo[7.3.1]- and bicyclo[8.3.1]phosphates. J.L. Markley, S. Maitra, R. Chegondi, P.R. Hanson

Fulkerson Center

Biochemistry Poster Session
S. L. Hiley, Organizer

8:30 - 10:00

27. Investigation of lithium’s neuroprotective role in Alzheimer’s disease using PC12 pheochromocytoma cells. E. Daniel, L.A. Wetmore


32. Analysis of cellular secretions via conventional nuclear magnetic resonance. S. Herndon, R. Block, R. Gerald, K.H. Woelk
33. The diffusible factors (DF), 3-hydroxybenzioic acid and 4-hydroxybenzoic acid, regulates the expression and production of important secondary metabolites in *Lysobacter enzymogenes* OH11. S.T. Tombosa, Y. Wang, H. Yong, J. Jiang, L. Du, S. Li

34. Functional analysis of the bacteriophage T4 Rad50 Homolog (gp46) coiled-coil domain. T.C. Barfoot, T.J. Herdendorf, B. Behning, B. Stohr, Y. Gao, K. Kreuzer, S.W. Nelson


36. Dopaminergic toxicity of parkinsonian toxin 1-methyl-4-phenylpyridinium (MPP+) is related to its ability to accumulate in the mitochondria: A structure activity study. M. Mapa


38. CRISPR/Cas9 based genetic engineering in *Lysobacter*. W. Su, Y. Zhao, L. Du

39. Myopalladin’s role in cardiac muscle function and disease. V.K. Kadarla, E.W. Wong, M. Bang, M. Beck

40. Split molecular clamp. D. Boamah

41. Effect of the receptor CMG2 on stability changes in domain IV of anthrax toxin protective antigen in comparison to the full-length protein. S. Mamillapalli, J. Bann

42. Investigating the role of palladin Ig34 linker and palladin-ig4 domain in its actin binding and crosslinking activity. R. Vattepu, R. Yadav, M. Beck

43. pH-sensitive conformational changes in anthrax toxin protective antigen prepore monitored by kinetic tryptophan quenching. J. Mayorga, J. Bann

44. Investigating the mechanism of the prepore-pore transition of anthrax toxin protective antigen using circular dichroism spectroscopy. M. Collins, J. Bann

45. Kinetics of folding of the isolated receptor binding domain of anthrax protective antigen. A. Denton, J. Bann

46. Use of a propionate-inducible expression system for production of CS1 pili from Enterotoxigenic *Escherichia coli*. E.T. Salerno, J. Bann

47. HPLC method development assessing the possibly trigger of 6-thiopurine toxicity. C. Weeramange, K. Ferguson, R. Rafferty

316. Characterization of 1,3,5-triazines as potential dihydrofolate reductase inhibitors. A.R. Poffenberger, B.A. Hathaway, T.A. Wencwicz
Materials/Polymer Chemistry
S. L. Hiley, Organizer
R. A. Chavez, Presiding


8:50 49. Band gap engineering in graphene nanoribbon heterojunctions: Tight-binding model. B.O. Tayo


9:50 Intermission.

10:10 52. Tightly-bound polymers: What are they and how do they behave? F.D. Blum

10:30 53. Thermal properties, structures, and interactions of adsorbed poly(vinyl acetate) on silica. H. Mortazavian, C.J. Fennell, F.D. Blum

10:50 54. Dynamics of cetyltrimethylammonium bromide in bulk and on silica by solid-state deuterium NMR spectroscopy. M. Maddumaarachchi, Y.L. Mathota Arachchige, T. Zhang, F.D. Blum

11:10 55. Pyrolysis approach for the large scale synthesis of highly fluorescent carbon dots. M.J. Meziani, M.A. Mottaleb, N. Wu


Fulkerson Center

Organic Chemistry Poster Session
S. L. Hiley, Organizer

8:30 - 10:00

57. Synthesis and characterization of a pteridinedione series as catalysts for proton-coupled electron transfer. H. Nguyen, D.P. Rillema

58. Variable mechanistic reductions of estrogen quinones using dideuterated NADPH. J. Robinson, D.E. Stack

60. P-stereogenic bicyclo[4.3.1]phosphite-boranes: Tunable P-tether systems for the synthesis of complex polyols. J.L. Markley, P.R. Hanson

61. A 'flipped' etherification method: Intramolecular reactions between enolates and dialkyl peroxides. M. Locklear, P.H. Dussault


64. Development of photoacoustic contrast agents: Toward non-invasive deep-tissue imaging. P. Zhang

65. A reaction based approach for detection of H₂S. G. Kim, E. Jang, H. Cao


68. Quinone-promoted formal amine α C–H bond functionalization. X. Liu, M. Leon, J. Phan, M. Clift


70. Synthesis of oxacycles via reaction of stabilized carbanions with peroxides. A. Horn, P.H. Dussault

71. Production of unsaturated cyanohydrins for ISNC reactions. J. Stevens, J.L. Duffy-Matzner

Blum Union Room 222

Advances in Computational Chemistry
J. S. Rhoad, Organizer
J. N. Woodford, Presiding

9:00 73. Golden cage clusters and nanogold catalysis. X.C. Zeng

9:30 74. Peak-shifting in real-time time-dependent density functional theory. M. Provorse, C. Isborn

10:00 75. Computational insights into the reaction mechanisms of the synthesis of B-O functionalized BODIPYs via different experimental methods. P.N. Bobadova-Parvanova

10:30 76. Theoretical consideration of electrochemical reduction of furfural on Cu (111) and Cu (211). N. Shan, B. Liu
11:00 77. A first-principle investigation of hexagonal boron nitride growth on nickel surfaces. S. Liu, B. Liu, J.H. Edgar

**Fulkerson Center**

**Inorganic Chemistry Poster Session**
S. L. Hiley, Organizer

10:00 - 11:30

78. Is the endohedral zintl Pb$_{12}$@Pt$^2$– (Ih) three-dimensionally aromatic? J.R. Dias

79. Reactions of dianionic bis(alkylamido)cyclodiphosph(III)azanes with electrophiles: N versus P electrophilic attack. M. Otang

80. Tandem catalysis by palladium nanoclusters encapsulated in metal–organic frameworks. X. Li, C. Xiao, W. Huang

81. Highly enhanced hydrogen evolution electroactivity of cobalt oxide by hydrogen reduction. X. Yan

82. Optimization of synthesis and annealing for a solvothermally prepared nanocrystalline precursor in forming nanocrystalline WSe$_2$. J.S. Edgar, C.J. Curry, C.L. Exstrom, S.A. Darveau

83. Synthesis of gold nanoparticles using tea extracts and size separation using gel electrophoresis. M.M. Neumann, K. Kounovsky-Shafer, S.A. Darveau, C.L. Exstrom

84. Paramagnetic coordination polymers of cyanoscorpionate ligands. L. Kadel, D.M. Eichhorn

85. Scorpionate and pyrazole complexes of palladium and platinum. A. Oberley, D.M. Eichhorn

**Physical Chemistry Poster Session**
S. L. Hiley, Organizer

10:00 - 11:30

86. Thermodynamics study of absorption of aromatic organic compounds to carbon nanotubes. L.J. Lozenski, M. Watanabe

87. Topological and thermodynamic investigations of molecular interactions in binary mixtures: Molar excess volumes and molar excess enthalpies. A. Sharma

88. 3D printed wall-tube electrochemical cell for complex electrochemical reactions. K.A. Lasseigne, A.S. Munshi, R.S. Martin, I.Z. Kiss
Concentration and ionic strength effects on the formation of cationic H-type dye aggregates in aqueous solutions. Z. Cao, G.L. Indig

Near infrared studies of isotopically mixed water samples: The H/D dependence of the 6000 cm\(^{-1}\) band. H.R. Krueger


The dielectric constant for pure and mixed solvents as a function of electric field. I. Daniels, Z. Wang, B. Laird

Enhanced catalytic performance of graphene-supported catalysts for biomass conversion. C. Xiao, T. Goh, K.T. Brashler, W. Huang

Facile HMO calculations of series of fullerenes related by rotational symmetry. J.R. Dias

Influence of ligand substitution on electronic properties in bis(diphosphine) nickel catalysts used in hydrogen catalysis. T. Brown, A. Pitts-McCoy, K.L. Mardis

Kirkwood-Buff derived force fields for glycerol and ethylene glycol systems. N. Kariyawasam Manachchige, P.E. Smith

Augmented minimal basis sets with optimized diffuse functions for fast and accurate calculations of optical rotatory dispersion. T. Aharon, M. Caricato

A theoretical study of electron and nuclear dynamics in Au\(_{18}(SH)_{14}\) and Au\(_{25}(SH)_{18}^{-}\) [NH\(_4^+\)] nanoparticles. R. Senanayake, C.M. Aikens

Application of in vivo nuclear magnetic resonance toroid cavity detectors to miniaturize and improve the quality of medical magnetic resonance imaging. R. Block, S. Herndon, R. Gerald, K.H. Woelk


Molecular orbital calculations aid interpretation of \(^{19}\)F NMR chemical shifts. C. Kasireddy, J. Bann, K.R. Mitchell-Koch


One-pot synthesis of GABA amides via the nucleophilic addition of amines to 3,3-disubstituted cyclopropenes. V. Maslivetc, M. Rubina, M.A. Rubin

Computing excited-state Raman activities via numerical differentiation of analytic polarizabilities. M. Barclay, M. Caricato, C.G. Elles

107. Formation, orientation, and packing of linearly functionalized azulenic scaffolds on a gold (111) surface. **M. Okeowo**, M. Hart, B.A. Tappan, M.V. Barybin, C.L. Berrie

108. Multi-scale and multi-state extrapolation of UV-Vis spectra. **S. Ren**, M. Caricato


111. The dative bonding complex F₃B – PH₃ does not exist: The microwave spectrum measured for the "F₃B – PH₃ complex" actually corresponds to F₂B-PH₂. **J. Schell**, W. Yang, R. Glaser

112. Conformational, vibrational studies and ab initio calculations of fluoroacetylchloride. D.K. Sawant, R.E. Brenner, **M. Fernanda De La Torre**, M. McNearney, J.R. Durig


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**THURSDAY AFTERNOON**

**Blum Union Room 218**

**Inorganic Chemistry**

S. L. Hiley, Organizer
S. M. Schmuecker, Presiding
*Financially supported by Rigaku.*

1:00 114. The NIR emission beyond 900 nm from self-assembled 1D polymeric Pt-cyanoximates. **N. Gerasimchuk**, M.Y. Berezin


2:00 117. Activation of dioxygen and nitric oxide by an yttrium-tricopper complex: Different modes of metal-metal cooperativity. **D. Lionetti**, T. Agapie

2:20 Paper number 118 was moved to Materials/Polymer Chemistry on Thursday at 4:10

2:40 Intermission.

3:00 119. Multiple phases of chromium carbide as electrocatalysts for renewable energy. **S.M. Schmuecker**, B.M. Leonard
3:20 120. Electrodeposition of epitaxial materials on silicon with a nanoscale gold buffer layer. J.C. Hill, J.A. Switzer


4:00 122. Heterobimetallic anchoring of the first π-linker featuring mercapto and isocyno junction groups within the same molecule. J. Applegate, N. Erickson, N. Gerasimchuk, M.V. Barybin


Blum Union Room 222

Advances in Computational Chemistry
J. S. Rhoad, Organizer, Presiding

1:30 124. Residue based contributions to the thermodynamic properties of proteins. E.A. Ploetz, P.E. Smith

2:00 125. Structure and dynamics at liquid-solid interfaces. W. Thompson

2:30 126. Modeling excited states of large molecular systems using hybrid QM/QM methods with point charge embedding. A. Biancardi, J.S. Barnes, M. Caricato


3:30 128. Predicting experimental RNA and DNA nearest-neighbor free energy rankings. M.A. Lewis, B. Znosko, E. Jolley

Fulkerson Center, Rochambeau Room 220

Advances in Drug Discovery
S. R. Svojanovsky, Organizer, Presiding

Financially supported by the Division of Organic Chemistry

1:30 129. Rational antibiotic design: From idea to international pharmaceutical company. L.D. Sutton, S. Yu

2:00 130. Hsp90 inhibitors from natural products. B. Blagg

2:30 131. Protecting-group-free synthesis of breitfussin B reveals bromine migration between heterocycles. A.H. Khan, J.S. Chen

3:00 Intermission.
3:15 132. Drug design for Chagas disease by docking and pharmacophore modeling of *T. cruzi* tubulin receptor. C. Ogindo, W.M. Southerland, Y. Fang, O. Bakare

3:45 133. A multifaceted approach towards the identification of novel bacterial caseinolytic protease P activators. A.S. Duerfeldt


**Fulkerson Center**

**Analytical Chemistry Poster Session**
S. L. Hiley, *Organizer*

1:30 - 3:00

135. Analysis of biogenic amines in relation to quality of three fish species commonly consumed in Kuwait. A. Anderson

136. Glycoform analysis of alpha_1_-acid glycoprotein by capillary zone electrophoresis with field enhanced sample injection. C. Zhang, D.S. Hage

137. Alkyl-methylimidazolium room temperature ionic liquids as mobile phase modifiers in reversed phase HPLC. M.W. Ducey, B.J. Eddy

138. Determination of supercoiled and nicked circular DNA molecule’s mobility in a gel matrix in different ionic strength conditions. R. Flauth, J. Lallman, K. Kounovsky-Shafer

139. Development of 3D printed devices to extract DNA molecules for genome analysis. J. Dophin, M. Moore, K. Kounovsky-Shafer

140. Determination of electroosmotic forces in various ionic strength conditions. J. Lallman, R. Flauth, K. Kounovsky-Shafer

141. Determination of restriction enzyme activity when cutting fluorochrome labeled DNA molecules. A. Maschmann, K. Kounovsky-Shafer


143. Method development and validation for the quantitation of N-α-(1-deoxy-D-fructos-1-yl)-L-arginine (FruArg) using LC-MS/MS. M. Johnson, H. Song, J. Cui, V. Mossine, Z. Gu, C. Greenlief


145. Enhancing spatial resolution in airborne monitoring of volatile organic compounds by passive Fourier transform infrared spectrometry. R. Meredith, G.W. Small
146. Exploration of isotopomer separations by high-resolution differential ion mobility spectrometry (FAIMS). J. Kaszycki, A. Bowman, A. Shvartsburg


148. Optimization of on-column entrapment containing human serum albumin for the study of drug-protein binding by high performance affinity chromatography. S.T. Azaria, J. Vargas

149. Online SCX and reversed-phase extraction method for hydrogen exchange mass spectrometry of samples containing macromolecular crowding agents. F. Rusinga, D.D. Weis

150. Analysis of drug binding with soluble proteins by using ultrafast affinity extraction and alpha1-acid glycoprotein microcolumns. S. Beeram, X. Zheng, C. Bi, D.S. Hage

151. Impedimetric study of carbohydrate and lectin interactions on gold wire. J.K. Bhattarai, A. Alla, V. Mikhaylov, A. Demchenko, K.J. Stine

152. Determination of natural organic matter (NOM) components diffusion coefficients by pulsed field gradient NMR. C. Johnson-Edler, J.A. Rice

153. Determination of the assembly and matrix complexation of humic acid. D. Gibson, J.A. Rice

154. Fabrication of meso-fluidic device for a virus biosensor. A.E. Ripp, J.R. Blum, S.A. Darveau, C.L. Exstrom, K. Kounovsky-Shafer


156. Determination of the illumination profile for a blue light transilluminator. C.L. Exstrom, S.A. Darveau, K. Kounovsky-Shafer, M.K. Breemes


158. Preparation and characterization of nanoporous gold monolith and its application in selective capture of glycoproteins. A. Alla, J.K. Bhattarai, A. Demchenko, K.J. Stine

159. High-throughput microfluidic chip for single cell analysis. D. Ediriweera, C.T. Culbertson, T. Mickleburgh

160. Characterizing the post-translational modifications of peptides by high-resolution FAIMS and electron transfer dissociation. M.A. Baird, A. Shvartsburg


162. Measuring binding interactions between HSA and atrazine metabolites using high performance affinity chromatography. A. Donovan, A. Moser

163. Measuring binding interactions between HSA and atrazine using high performance affinity chromatography. A. Blair, A. Moser
164. Solid state NMR spectroscopic analysis of thermally activated and hydrated Ghanaian clay as a supplementary cementitious material in Portland cement. **S.S. Purohit**, M. Bediako, J. Kevern, N.A. Oyler


166. Monitoring relative concentration changes of volatile organic compounds in red wines after opening. **K. Jones**, A. Caffrey, D. Daszynski, A. Guanzon, D. Dobberpuhl


**Fulkerson Center**

**Chemical Education Poster Session**  
S. L. Hiley, **Organizer**

1:30 - 3:00

168. The teaching of chemistry before and after the periodic table of elements. **J.R. Dias**


170. IUPAC, the game: A fun way to learn organic nomenclature. **P.A. Mazzer**

171. Implementation of a preparatory course to improve student opinion of sophomore organic chemistry. B.D. High, **M.R. Siebert**


173. Using reactions of eugenol and eugenol derivatives to illustrate how natural product pharmaceuticals are derived. M. McAfoos, J. Davis, **D.J. Peitz**

174. Recruitment of high academic ability students to Missouri Western State University through the Dual Credit General Chemistry I Program: New student survey and matriculation data. **E. Hoover**, J.L. Torres Y Torres, M.W. Ducey

175. QSAR and docking analysis of huperzine-derived inhibitors of acetylcholinesterase. **J.A. Morrill**, **J.D. Enders**
Blum Union Junior College Room (Room 234)

Laboratory Safety Training
D. Van Horne, Organizer, Presiding

1:30 176. Introduction to the Laboratory Safety Training Symposium. J.D. Van Horn

1:45 177. Perceptions of safety in the laboratory. S. Galitzer

2:15 178. It all starts at the top. K.P. Fivizzani

2:45 179. Developing laboratory safety training for a diverse campus population. M. Bresnahan

3:15 Panel Discussion.

Blum Union Room 223

Materials/Polymer Chemistry
S. L. Hiley, Organizer
M. W. Hull, Presiding

1:30 180. Waterborne non-isocyanate polyurethane adhesives. O. Bilic, I.J. Javni, Z.S. Petrovic


2:10 182. Analysis of the storage properties of polyurea-shell microcapsules containing a free-radical initiator core. B. McFarland, L.R. Haverland, B.J. Pinto


2:50 Intermission.

3:10 184. Development of kinetic and process model for Fisher-Tropsch synthesis on Co-Mo catalyst using experiments and parameter estimation technique. S.A. Gheni


3:50 186. Comparative crystallography of group 12 cation-containing $A_2MTeO_6$ ($A =$ Ca, Sr, Ba) compounds. A. Flores, A. Stiner, T. Mansur, H. Albert, A. Fry, P. Barnes

Blum Union Room 219

Organic Chemistry
S. L. Hiley, Organizer
S. P. Lorimor, Organizer, Presiding

1:30 187. Synthesis of 1,4-substituted piperidines and their inhibition of neuronal T-type calcium currents and mitigation of neuropathic pain in mice. B. Zou, M.J. Gunaratna, C. Pascual, M. Zhang, S. Weerasekara, C. Lieu, X. Xie, D.H. Hua


2:50 Intermission.


3:30 192. Development of a novel method for synthesis of 2-Vinylazaindoles and their chemical and biological applications: Design and synthesis of some carbolines architecture as CDK inhibitors. Y. Mohamed


Spratt Hall Room 101 (Kemper Recital Hall)

Midwest Region Award Symposium
L. C. O'Brien, Organizer
W. E. Buhro, S. E. Hayes, Presiding

3:30 Introductory Remarks.


5:00 197. (Midwest Award Address) Molecular mechanism of action of the cyanobacterial orange carotenoid protein. **R.E. Blankenship, H. Liu, H. Zhang, J. King, D. Niedzwiedzki, M.L. Gross**

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**FRIDAY MORNING**

**Blum Union Room 218**

**Biochemical Structure and Function**
J. Tally, *Organizer*
B. D. Caldwell, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 198. Clarity through resolution: Structural snapshots of APE1 DNA damage processing. **B. Freudenthal**, W. Beard, M. Cuneo, S.H. Wilson


9:35 201. Evolving orthogonal cohesin-dockerin pairs for the assembly of synthetic cellulosome. **X. Song**, W. Niu, J. Guo

10:05 Intermission.


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**Fulkerson Center**

**Materials/Polymer Chemistry Poster Session**
S. L. Hiley, *Organizer*

8:00 - 9:30

205. 3D printed materials characterization using positron techniques. M. Paul, J. Davis, Y. Jean, J.D. Van Horn

206. Graphene nanoribbons for energy storage applications. **N. Aljehany**, R. Gupta

207. Biomass-based polyester prepared from furfural by sunlight polymerization. **Z. Wang**
208. Flexible high performance supercapacitive energy storage devices. J. Candler, P.K. Kahol, R. Gupta


210. Self-reinforcing/self-repair dentin adhesive via visible-light irradiation induced sol-gel polymerization. L. Song, Q. Ye, X. Ge, P. Spencer

211. Water effect on dentin adhesives formulated with a novel co-initiator. X. Ge, Q. Ye, L. Song, A. Misra, P. Spencer

212. Microwave-assisted synthesis of ceria nanocubes with surface modifying agents. T.J. Fisher, Y. Ibrahim, C.L. Cheung


214. New adhesive from isosorbide. C.J. Barnish, M.D. Zenner, J.S. Chen


218. Biosensors derived from copolymers of vinylferrocene with various para substituted phenylmaleimides. N. Alghamdi, C.J. Neef

219. Electrical interactions in copolymers of vinylferrocene and hexylated vinylimidazole. Y. Pashchenko, C.J. Neef

Blum Union Room 219

Organic Chemistry
S. L. Hiley, S. P. Lorimor, Organizers
M. Pattabiraman, Presiding

8:00 220. Palladium-catalyzed decarboxylative synthesis of conjugated allenynes. M.K. Smith, J.A. Tunge

8:20 221. Ligand-controlled regioselective addition to propargylic carbonates to synthesize 1,3-dienes and alkynes. T.M. Locascio, J.A. Tunge

8:40 222. Enantioselective epoxidation catalyzed by manganese-substituted carbonic anhydrase. S.T. Weerasekara, L.M. Stanley

9:00 223. Metal chelating properties of 2-imino-6-(1,2,3-triazol-4-yl)pyridines. M.D. Dillenburg, J.T. Fletcher
9:20 Intermission.

9:40 224. Development of high-load, immobilized Si-ROMP and Co/C magnetic reagents/scavengers and ligands. S. Faisal, P.K. Maity, Q. Zang, P.C. Kearney, D. Stoianova, P.R. Hanson

10:00 225. Carbonyl-directed catalytic asymmetric hydroboration of unsaturated amides. T. Nguyen, G. Hoang, S. Zhang, J.M. Takacs


10:40 227. Transesterification of methanol with propylene carbonate to dimethyl carbonate over CaO catalysts: Pretreatment effects. Z. Song, X. Jin, R.V. Chaudhari, G. Prasad

11:00 228. A titanium promoted modular synthesis of conjugated amides. R. Rahaim

Fulkerson Center

Organic Chemistry Poster Session
S. L. Hiley, Organizer

8:00 - 9:30


232. Design and synthesis of novel estrone analogues as inhibitors of pancreatic cancer. M. Alluhaibi

233. Synthesis of potential inhibitors of GGTase II. R.A. Matthiesen, D.F. Wiemer


235. Comparison of OpenEye and Autodock scoring functions in refining molecular binding affinity of ormeloxifene analogs to EGFR kinase pathway proteins. A. Moy, J. Apraku, S. Chauhan, F.T. Halaweish

236. Synthesis of structurally diverse, P-stereogenic bicyclic phosphonamidates. J. Torres, S. Javed, P.R. Hanson


238. Five-membered ring closure via intramolecular nucleophilic attack by nitrogen ylides on C-C bond of cyclopropenes. C. Barrett, M.A. Rubin
239. Microwave synthesis of quinabactin analogs. **G.P. Nora**


243. HPLC-ELSD study of soybean oil equilibration by interesterification. **D. Radojcic**, M. Ionescu, Z.S. Petrovic

244. Ferrocenium hexafluorophosphate as catalyst for etherification of propargylic alcohols. **M.J. Queensen**, J. Rabus, E. Bauer

245. A practical, multi-gram synthesis of (±)-herbindole A, (±)-herbindole B, and (±)-herbindole C from a common intermediate via 6,7-indole aryne cycloaddition and Pd(0)-catalyzed cross-coupling reactions. **K.R. Buszek**, N.L. Chandrasoma, S. Pathmanathan

246. Phosphate tether-mediated studies towards the syntheses of Sch-725674 and 13-demethyllyngbyaloside B. **M. Bodugam, A. Ganguly**, S. Javed, P.R. Hanson

247. Tribromoindoles as versatile synthetic intermediates for regioselective metal-halogen exchange, indole aryne formation, and further reactions: Synthesis and reactions of 4,5,6- and 4,5,7-tribromoindoles. **A. Nerurkar**, K.R. Buszek

248. Novel ruthenium catalyst to facilitate propargyl rearrangement. M.J. Stark, M.J. Shaw, **E.B. Bauer**

249. Design and a novel synthesis of 2-vinylazaindoles and carbolines architecture as CDK inhibitors. **Y. Mohamed**, F.T. Halaweish

250. Efforts towards the total synthesis and final structural elucidation of lagunamide C. **C. Weese**, Y. Zhang, S. Valdez, A. Elkiwan, R. Rafferty

**Fulkerson Center Rochambeau Room 220**

**Advances in Drug Delivery**  
S. H. Bossmann, *Organizer, Presiding*


10:00 Intermission.


10:45 255. Protein nanocarriers for drug delivery applications. **O. Perumal**

11:15 256. Development of therapeutics to treat autoimmune diseases and autoimmune associated inflammation in the eye. **J. Sestak**

**Blum Union Room 222**

**Chemical Education**
S. L. Hiley, *Organizer*
S. Burchett, *Presiding*

8:30 257. Student success in face-to-face, blended, and online chemistry courses: Analysis and discussion of the modalities as applied by a research university and a community college. **S. Burchett**, J.L. Hayes, K.H. Woelk

9:00 258. Fischer esterification: A diverse flavor for laboratory portfolios. **J.L. Hayes, S. Burchett**

9:30 259. Incorporation of benchtop NMR spectroscopy into undergraduate laboratories: An active-learning approach. **S. Riegel**

10:00 Intermission.


11:20 262. Using written assignments in organic chemistry to guide students to better study habits. **J.S. Rhoad**

**Blum Union Room 223**

**Physical Chemistry**
S. L. Hiley, J. N. Woodford, *Organizers*
J. R. Dias, *Presiding*

8:30 263. Ligand exchange mechanism on thiolate monolayer-protected Au_{25}(SR)_{18}/Au_{38}(SR)_{24} nanocluster. **A. Fernando**, C.M. Aikens

8:50 264. A tractable model of charged nanoparticle aggregation behavior. **G.S. Blaustein**

9:10 265. Location and orientation of a fluorescent solute in mesoporous silica. **J. Harvey**, W. Thompson
9:30 266. Simulations of the infrared, Raman, and 2D-IR photon echo spectra of water in nanoscale silica pores. P. Burris, D. Laage, W. Thompson

9:50 Intermission.

10:10 267. Reorientation of isomeric butanols: The multiple effects of steric bulk arrangement on hydrogen-bond dynamics. O. Mesele, W. Thompson, D. Laage

10:30 268. Strong tunable visible absorption predicted for polysilo-acenes using TDDFT calculations. K.M. Weerawardene, C.M. Aikens

10:50 269. Polarization of core orbitals and computation of nuclear quadrupole coupling constants using Gaussian basis sets. G.S. Harbison

Fulkerson Center

Undergraduate Research Poster Session
S. P. Lorimor, Organizer
Financially supported by the Office of Undergraduate Programs

9:30 - 11:30


271. Bioavailability and quantification of trace heavy metals in edible fish of lakes and local supermarkets by inductively coupled plasma–optical emission spectrometry (ICP-OES). D.R. Johnson, M.A. Mottaleb, K. Nagel, M.A. Mottaleb


273. Implementing and assessing diverse avenues of student support: The CSU S-STEM Program. C. Moore, M. Sabella, K. Mardis


276. Effect of charge state and conformational structure on spin delocalization of PCDTBT and similar polymers used in bulk heterojunction solar cells. N. Perez, K. Mardis

277. Understanding the effect of excess charge on the electronic structure of polymers used in polymer composite solar cells. C. Mallares, K.L. Mardis
278. Direct mercury analysis: Comparison of catalytic core composition, morphology, and performance. R.C. Richter, M. Noboa


280. A fluorescence-based assay on actin to investigate myosin binding. R. Wynia, M. Moutsoglou

281. Preparation of fatty acid analogs incorporating reactive peroxides. S.A. Chambers, A.S. Olson, P.H. Dussault

282. Facile method for increasing hydrophilicity of 3D-printed microfluidic devices. T.A. Myers, A. Hodges, M. He

283. Layer-by-layer assembly of polyelectrolyte multilayer films for drug delivery applications. R.C. Johnson, S. Chattopadhyay

284. Regioselectivity of estrogen o-quireduction promoted by NADPH. J. Robinson, D.E. Stack

285. The effects of structure on amino acid aerosol hygroscopic properties: A comparison between glycine and alanine. S. Gottuso, J.P. Darr

286. Synthesis and coordination chemistry of 1,2,3-triazole-substituted quinolines and isoquinolines. M.D. Dillenburg, J.T. Fletcher


288. Synthesis of CdSe/ZnS nanocrystals and their bioconjugation to DNA. L. Mohror, C. Hanson, B. Eichler

289. Analysis of tryptophan as a non-toxic ink for covert pharmaceutical security features. S. Altena, B.A. Logue

290. Mixed Ru(II) complexes of 1,2,3-triazole-containing tridentate chelators. J.R. Jagannathan, J.T. Fletcher

291. Investigating the parameters of 4-imino-1,2,3-triazole L’abbé rearrangements. A.L. Cheek, J.T. Fletcher

292. Kinetic evaluation of a novel inhibitor of acetate kinase from methicillin–resistant Staphylococcus aureus MU 50 strain. W. Lawrence, C. Wu

293. A computational study of heparin and heparan sulfate oligosaccharides binding to chemokine CXCL14. S. Morrison, C. Deligkaris

294. Physical binding of the ultimate carcinogen of aristolochic acid to the human tumor suppressor gene TP53: Implications for DNA damage. T. Hufham, C. Deligkaris

295. Poisson-Boltzmann electrostatic potential calculations of chemokine molecular surfaces: Implications for binding to glycosaminoglycans. C. Martin, C. Deligkaris

296. Impact of palmitic acid and α-linolenic acid on the β-catenin pathway with inhibition of the peroxisome proliferator-activated receptor γ (PPARγ) in HCT116 colon cancer cells. M. Myers, L.A. Wetmore
297. Virtual space truncation for frozen natural orbital coupled cluster. A. Schile, D. Sherrill, J. Gonthier

298. Tuning luminescence profile of the Ph$_3$P-Au-SR (R = azulenyl) scaffold. B.A. Tappan, A.D. Spaeth, O. Torres-Texidor, N. Gerasimchuk, M.V. Barybin

299. The study of nitrate removal from water using Ti$_2$O$_7$ reactive electrochemical membrane. A. Pitts-McCoy, A. Paula Castro, L. Guo, B.P. Chaplin


301. New synthetic routes to 6-oxocatechol estrogens. R. Eastman, D.E. Stack

302. Progress towards a selective fluorescent Li$^+$ probe. E.J. Geddes

303. The synthesis of 9-bromo-10-diarylaminoanthracene for use in triarylamino dyes for solar cells. K. Dolge, B. Eichler


305. Analysis of factors affecting helicity in peptoid design. M. Finley, H. Straley, A. Hodges, J. Mantha

306. Algal separation from water through the reactive electrochemical membrane Ti$_4$O$_7$. J.N. Webb, J. Spataro, Y. Jing, B. Chaplin

307. Progress in exploring the essentiality of acetate kinase from methicillin/multiple resistant *Staphylococcus aureus*. J. Tice, K. Schmidt, C. Wu

308. NMR analysis of the estrogen *o*-quito estrogen *o*-quimethide equilibrium. J.R. Granstrom, D.E. Stack

309. Investigating the isomerization of estrogen catechol *o*-quinones. J.R. Granstrom, D.E. Stack

310. Front propagation of electrochemical reactions on star and tree networks. R. Varghese, M.L. Sebek, I.Z. Kiss

311. Recent advances in lanthanide phosphites via solvothermal synthesis. S.H. Byer, E.M. Villa

312. Hydrothermal synthesis of lanthanide sulfites and sulfates. J.T. Dovgan, E.M. Villa

313. Equilibrium studies of the iron exchange reaction of ferrioxamine B with 8-hydroxyquinoline-5-sulfonate. K. Glover, E.G. Olmstead

314. Thermal degradation of an aged Nafion® membrane. D. Agoumba

315. A computational investigation of solvent effects on geometries and intramolecular hydrogen bonding of carbazolopyridinophane and diphenylaminopyridinophane. A. Mendenhall, D. Bretey, G.S. Blaustein

316. *Paper 316 has been moved to the Biochemistry Poster Session on Thursday morning at 8:30.*

317. Perchlorate detection at low concentrations by silver-resin nanocomposites using surface-enhanced Raman scattering. D.A. Beery, I. Pires Miranda, M.A. Mottaleb, M.J. Meziani, M. Bellamy

319. Antimicrobial light-curable polymeric composites of Silver(I) cyanoximates for indwelling medical devices. S. Popis

320. Synthetics efforts towards the cyclic peptide natural product reniochalistatin E and analogs, and biological evaluation. M. Small, G. Baca, R. Rafferty

321. Synthesis of Compounds to Treat Human African Trypanosomiasis. G. Darner, J.P. Hagen

FRIDAY AFTERNOON

Blum Union Room 222

NSF Programs that Support Undergraduate Education
C. A. Burkhardt, Organizer
R. K. Boggess, Organizer, Presiding

1:00 322. National Science Foundation programs that support undergraduate education. R.K. Boggess

1:30 323. Transforming undergraduate physical chemistry education: Development of context rich materials to teach kinetics, quantum mechanics, and spectroscopy. E.M. Marzluff, M. Crawford

2:00 324. VESTA: A national collaboration addressing the workforce needs of the grape and wine industry. M. Norgren, W. Alter III

2:30 Intermission.


3:10 326. Transforming STEM instructional practices and culture around STEM teaching at a research-intensive institution: Descriptions and results of the implementation of two National Science Foundation projects at the University of Nebraska-Lincoln. M.N. Stains

3:40 Intermission.

3:50 327. Hendrix Noyce-STEM Teacher Education in the Arkansas Delta (N-STEAD). D.B. Jackson

4:20 328. STEP and SPECTRA scholars: Increasing student success with a pre-college bridge program and an interdisciplinary introduction to the sciences. B.K. Kramer, T.D. Walston

Blum Union Room 223

Physical Chemistry
S. L. Hiley, Organizer
J. N. Woodford, Organizer, Presiding
1:00 329. Gas phase infrared, NMR, and computational investigation of the conformers of diacetone diperoxide (DADP). C. Guo, J. Persons, J.N. Woodford, G.S. Harbison


1:40 331. Rapid, broadband spectroscopic temperature measurement of carbon dioxide using VIPA spectroscopy. A. Klose, G. Ycas, F. Cruz, D. Maser, S. Diddams


2:20 Intermission.


3:00 334. A plasmon-enhanced bio-solar cell to study the plasmonic effect on photovoltaic properties of light harvest complexes. Y. Yang, J. Li, R. Jankowiak

3:20 335. Synchrony transitions due to dynamical quorum sensing in single-cathode multi-anode nickel dissolution system. M.J. Hankins, I.Z. Kiss


Fulkerson Center Rochambeau Room 220

Advances in Drug Delivery
S. H. Bossmann, Organizer, Presiding

1:30 337. Designing a cleavable, cell surface protein that will bind and deliver biotin-containing moieties. M.T. Basel, T.B. Shrestha, M. Pyle, S.H. Bossmann, S. Aryal, D.L. Troyer

2:00 338. Chitosan copolymer nanocarriers for the delivery of small molecules and siRNA. B. Hao, S. Weerasekara, E. Carlson, J. Comer, D.H. Hua


3:00 Intermission.

3:15 340. C5aR targeted biodegradable nanoparticles for mucosal delivery of immunogens. S. Tallapaka, B. Karuturi, P. Yeapuri, S. Sanderson, J. Vetro


4:15 342. Synthesizing dendrimers for the delivery of prodrugs to solid tumors and metastases. Y. Toledo
Blum Union Room 218

Biochemistry
B. D. Caldwell, Organizer
J. Tally, Organizer, Presiding

1:30 Introductory Remarks.

1:35 343. Role of acidic residues in helices TH8-TH9 in membrane interactions of the diphtheria toxin T domain. M. Rodnin, C. Ghatak, M. Vargas-Urbe, A. McCluskey, J.C. Flores-Canales, M. Kurnikova, A. Ladokhin


2:15 345. Evolution of SH2 domain to recognize sulforylated tyrosine. T. Ju

2:35 346. Simple cyanines are transporter independent in vitro dopaminergic toxins with specificity of toxicity similar to MPP+. C.C. Kadigamuwa


3:15 Intermission.

3:30 348. The effects of simulated microgravity on the microbial physiology of Ralstonia pickettii isolates from the International Space Station. S.J. Fergione


Blum Union Room 219

Organic Chemistry
S. L. Hiley, S. P. Lorimor, Organizers
D. K. Howell, Presiding

1:30 352. Dual catalytic decarboxylative allylation of α-amino acids and their divergent mechanisms. S.B. Lang, K. O'Nele, J.A. Tunge
1:50 353. Establishing supramolecular control over solid state architectures. **B. Sandhu**, C.B. Aakeroy, J. Desper

2:10 354. Lawesson’s reagent mediated formation of molecular electronics: Theoretical investigations into the cycloaddition chemistry used to produce substituted-9,9’-bifluorenylidenes. M. Nothnagel, **M.R. Siebert**


2:50 Intermission.


3:30 357. What accounts for the regioselectivity of thermal and photochemical aromatic substitutions? The strange case of the missing Bell-Evans-Polanyi Principle. **G.G. Wubbels**

3:50 358. Determining the sterechemical outcome of 3-alkynyl- and 3-alkenyl-2-cycloalkedouble hydride reductions. M.A. Gubbels, R.W. Huang, E.M. Villa, **M.R. Hulce**