

TECHNICAL PROGRAM

WEDNESDAY EVENING

Fulkerson Center

Sci-Mix

S. L. Hiley, *Organizer*

Sponsored by ThermoFisher Scientific

7:00 - 9:00

27, 30-32, 36-37, 44, 57, 59, 64, 66, 70, 80, 82-85, 88, 91, 93, 95, 99, 102, 105, 138-139, 142, 144-145, 151, 154, 159, 164-165, 169-170, 172-173, 206-207, 210, 215, 218, 229-232, 234, 239, 248.

See subsequent listings.

THURSDAY MORNING

Fulkerson Center, Rochambeau Room 220

Advances in Drug Discovery

S. R. Svojanovsky, *Organizer, Presiding*

Financially supported by the Division of Organic Chemistry

8:00 1. Drug safety: New insights from an old drug: A novel mechanism to explain the mutagenic properties of the antihypertensive agent hydralazine. C. Lewis, D. Melton, M.I. Nejad, N.E. Price, **K.S. Gates**

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**

10:45 6. Exploring bacterial iron metabolism as target for antibiotic development. **M.E. Rivera-Laos**

11:15 7. Identification of genetic sequences recognized by human SC35 protein using artificial neural networks: A deep learning approach. **S.J. Fergione, A.J. Luke, S.R. Svojanovsky**

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**

8:20 9. Development of high-resolution FAIMS/mass spectrometry platform with ETD capability. **A. Bowman,**
G. Anderson, A. Shvartsburg

8:40 10. Identification of in-vivo protein-protein binding partners in *Anopheles gambiae* by immunoaffinity chromatography and mass spectrometry. **K. Sellens,** C.T. Culbertson, K. Michel

9:00 11. Studies of drug binding with alpha₁-acid glycoprotein by using on-line immunoextraction and high performance affinity chromatography. **C. Bi,** R.E. Matsuda, Z. Isingizwe, D.S. Hage

9:20 12. Analysis of drug-protein interactions during diabetes by high-performance affinity chromatography. **Z. Li,** R.E. Matsuda, E. Meza, D.S. Hage

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

10:20 14. Analysis of hormone-protein binding in solution by ultrafast affinity extraction. **X. Zheng,** C. Bi, M. Brooks, D.S. Hage

10:40 15. Role of carnosine in the modulation of nitric oxide production by raw 264.7 macrophages. **G. Caruso,** C.G. Fresta, R.P. de Campos, J.M. Siegel, W.M. Bandara, G. Lazzarino, S.M. Lunte

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

11:20 17. Capillary electrophoresis based separations of opioid peptides using a gold nanoparticles coating capillary. **A.M. Al-Hossaini,** L. Suntornsuk, S.M. Lunte

11:40 18. Spectroscopic single-molecule tracking reveals the one-dimensional diffusion pathways in surfactant-templated mesoporous silica. **R.S. Kumarasinghe,** D.A. Higgins, T. Ito

Blum Union Room 219

Organic Chemistry

S. L. Hiley, S. P. Lorimor, *Organizers*

M. Pattabiraman, *Presiding*

8:00 19. Protease assays for mastitis diagnostics in dairy cattle. **M. Kalubowilage,** T. Samarakoon, H. Wang, R. Ortega, Y. Toledo, L.D. Mendonca, G. Hanzlicek, D.L. Troyer, S.H. Bossmann

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

8:40 21. Synthesis of new amphiphiles for biosensor applications. **A.S. Olson**, A. Zaitouna, R.Y. Lai, P.H. Dussault

9:00 22. Pentafluorosulfanyl (SF₅) substituted *o*-iodoxybenzoic acid (IBX): Making a versatile reagent more user-friendly. **P.P. Thottumkara**, A. Pasupulety, T.K. Vinod

9:20 Intermission.

9:40 23. Halogen bonding vs hydrogen bonding: Competitiveness and supramolecular system. **J.C. Gamekkanda Gamaethige**, C.B. Aakeroy, J. Desper

10:00 24. Tetrapodal molecular tectons for three-dimensional open networks. **C. Gunawardana**, C.B. Aakeröy, 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

28. Enzymatic hydrolysis of 2,2-diphenylethyl glucosinolate. **C.A. Klingaman**, **M.J. Wagner**, J.R. Mays

29. Observing the kinetic stability of von Willebrand factor triple A domain using a bio-layer interferometry denaturant pulse assay. **A.J. Machen**, A. Tischer, V. Machha, M. Auton, M. Fisher

30. Identification of an allosteric twister ribozyme for use as a synthetic genetic switch. **S. Stoupa**, D. Poston, A. Netzel, S. Lennon, A. Kotula, H. Klem, G. Soukup, J. Strauss Soukup

31. Anti-malaria drug discovery: High-throughput assay to identify inhibitors of the *Plasmodium falciparum* apicoplast DNA polymerase. **M.E. Milton**, E.E. Parrott, R. Singh, S.W. Nelson

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-hydroxybenzoic 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
- 35.** Probing the kinetic stability of tetanus neurotoxin using bilayer interferometry along with a novel denaturant pulse-chaperonin assay with parallel confirmation via transmission electron microscopy. **P. O'Neil**, A.J. Machen, J. Burns, M. Baldwin, M. Fisher
- 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**
- 37.** Development of novel human ATP-binding cassette membrane transporter biosensors for drug discovery and development. **B. Osa-Andrews**, K.W. Tan, S.H. Iram
- 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. Wencewicz

Blum Union Room 223

Materials/Polymer Chemistry

S. L. Hiley, *Organizer*

R. A. Chavez, *Presiding*

8:30 48. The development of blue organic light-emitting diodes based on benzobisoxazole cruciforms. **R.A. Chavez**, M. Cai, B.C. Tlach, R. Shinar, J. Shinar, M. Jeffries-El

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

9:10 50. Development of benzobisoxazole-based conjugated polymers for narrow band gap organic photovoltaic materials. **D.L. Drochner**, J.J. Intemann, A.L. Tomlinson, M. Jeffries-El

9:30 51. Incandescent light: A promising radiation source in photochemistry. **K. Randazzo**, Z. Wang, Z. Wang, Q.R. Chu

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. Mezzani**, M.A. Mottaleb, N. Wu

11:30 56. Single molecule tracking studies of solvent-swollen microdomains in cylinder-forming polystyrene-poly(ethylene oxide) diblock copolymer films. **D.R. Sapkota**, K. Tran-Ba, D.A. Higgins, T. Ito

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

59. Formation of adipaldehyde via hydroformylation of butadiene: Experimental and theoretical studies. **T. Maji**, C.H. Mendis, W. Thompson, J.A. Tunge

- 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
- 62.** Back to the future with 3-hydroxyphenylpyrrolidines: Synthesis and evaluation of D₃ receptor activity. **S. Eslamimehr**, A.M. Crider, W.L. Neumann
- 63.** Synthesis of amide N-H protected amino acids for use in peptide segment condensation reactions. A. Chapman, S. Nastick, S. Black, **J.D. Steinkruger**
- 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**
- 66.** Gold(III)-catalyzed cyclization of propargyl acetates: Theoretical study on the synthesis of bicyclic products. **J.M. Hines**, M.R. Siebert
- 67.** Rotenoid biosynthesis: Computational analysis of competing ionic and radical pathways for cyclization. **A.K. Kirkpatrick**, M.R. Siebert
- 68.** Quinone-promoted formal amine α C–H bond functionalization. **X. Liu**, M. Leon, J. Phan, M. Clift
- 69.** Kinetics of carboxylation of propylene oxide to propylene carbonate in a semi-batch slurry reactor. **P. Bobba**, N. Reding, G. Prasad, **X. Jin**, R.V. Chaudhari
- 70.** Synthesis of oxacycles via reaction of stabilized carbanions with peroxides. **A. Horn**, P.H. Dussault
- 71.** Development of quinone-promoted C-C bond oxidative cleavage. **B. Haugeberg**, J. Phan, T.J. O'Conner, M. Clift
- 72.** 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 $\text{Pb}_{12}@\text{Pt}^{2-}$ (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

Fulkerson Center

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

- 89.** Concentration and ionic strength effects on the formation of cationic H-type dye aggregates in aqueous solutions. **Z. Cao**, G.L. Indig
- 90.** Near infrared studies of isotopically mixed water samples: The H/D dependence of the 6000 cm^{-1} band. **H.R. Krueger**
- 91.** Dye-protein investigation with circularly polarized light. **A.B. Braimah**, W.N. Newhart, C.K. Johnson
- 92.** The dielectric constant for pure and mixed solvents as a function of electric field. **I. Daniels**, Z. Wang, B. Laird
- 93.** Enhanced catalytic performance of graphene-supported catalysts for biomass conversion. **C. Xiao**, T. Goh, K.T. Brashler, W. Huang
- 94.** Facile HMO calculations of series of fullerenes related by rotational symmetry. **J.R. Dias**
- 95.** Influence of ligand substitution on electronic properties in bis(diphosphine) nickel catalysts used in hydrogen catalysis. **T. Brown**, A. Pitts-McCoy, K.L. Mardis
- 96.** Kirkwood-Buff derived force fields for glycerol and ethylene glycol systems. **N. Kariyawasam Manachhige**, P.E. Smith
- 97.** Augmented minimal basis sets with optimized diffuse functions for fast and accurate calculations of optical rotatory dispersion. **T. Aharon**, M. Caricato
- 98.** A theoretical study of electron and nuclear dynamics in $\text{Au}_{18}(\text{SH})_{14}$ and $\text{Au}_{25}(\text{SH})_{18}^{-1} [\text{NH}_4^+]$ nanoparticles. **R. Senanayake**, C.M. Aikens
- 99.** 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
- 100.** Analysis of solvent dynamics around *Candida antarctica* lipase B using molecular dynamics simulations. **J.N. Dahanayake**, R. Verma, K.R. Mitchell-Koch
- 101.** Molecular orbital calculations aid interpretation of ^{19}F NMR chemical shifts. **C. Kasireddy**, J. Bann, K.R. Mitchell-Koch
- 102.** Synthesis of C-13 labeled ortho-carborane for solid-state NMR spectroscopy of thin films. **A.S. Alnafisah**, C. Stirling, S.S. Purohit, B. Nordell, T. Nguyen, M. Paquette, N.A. Oyler
- 103.** Influence of facet and oxygen vacancy defects of ceria on the catalytic generation of singlet oxygen from hydrogen peroxide. **C.L. Cheung**, Y. Zhou, T. Fisher, N. Shao, N. Al-Aqtash, K. Tarawneh, R. Sabirianov, W. Mei
- 104.** One-pot synthesis of GABA amides via the nucleophilic addition of amines to 3,3-disubstituted cyclopropenes. **V. Maslivetc**, M. Rubina, M.A. Rubin
- 105.** Computing excited-state Raman activities via numerical differentiation of analytic polarizabilities. **M. Barclay**, M. Caricato, C.G. Elles

- 106.** Tuning graphene's electronic properties with dopants: A fundamental study with Kelvin probe force microscopy. **J. Totleben**, G. Smith, J. Wu, C.L. Berrie
- 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
- 109.** Silver nanowire fabrication using AFM- based patterning of self-assembled monolayers on silicon. **S.B. Ulapane**, C.L. Berrie
- 110.** Geometries of transition metal hydroxides and oxyhydroxides. **D.L. Myers**, N.S. Jacobson
- 111.** The dative bonding complex $F_3B - PH_3$ does not exist: The microwave spectrum measured for the " $F_3B \cdots PH_3$ complex" actually corresponds to F_2B-PH_2 . **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
- 113.** Batch pH oscillations in the acidic periodate-bromide system. **G. Ali**, G.A. Frerichs

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

1:20 115. Investigating crystallohydrates of Ni and Zn cyanoximes coordination compounds. **A.A. Opalade**, N. Gerasimchuk

1:40 116. Iodoalkenes as halogen-bond donors. **M. Perera**, C.B. Aakeroy, J. Desper

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

3:40 121. Fundamental investigation of intermetallic NaAu₂ to help understand catalytic activity. **E. Kwolek**, R. Widmer, O. Gröning, O. Deniz, H. Walen, C. Yuen, W. Huang, D. Schlager, M. Wallingford, P.A. Thiel

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

4:20 123. Direct transformation: A novel approach to convert bulk silver to silver nanoparticles. **A.S. Yapa**, E.J. McLaurin, C.M. Sorensen, S.H. Bossmann

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

3:00 127. Confronting the complexity of nonlinear systems: Mechanistic insights into the Belousov-Zhabotinsky oscillating chemical reaction. **R. Glaser**, C. Chicone, E.T. Zars, M. Delarosa, M. Lukosi, C. Camasta

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**

4:15 134. Merging ligand- and structure-based drug discovery. **R. Moretti**, J. Meiler

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 alpha₁-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. Flaugh**, 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. Flaugh, **K. Kounovsky-Shafer**

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

142. Development of a microchip electrophoresis with electrochemical detection method to detect nitrite in macrophage cells using a platinum black working electrode. **K.M. Schilly**, J.M. Siegel, M.B. Wijesinghe, S.M. Lunte

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

144. Development and use of a scanning nano-LC system with surface enhanced fluorescence detection. **E.L. Rodriguez**, R.E. Matsuda, J. Vargas, D.S. Hage, Z. Li, M. Stoller, A. Konda, S.A. Morin, S. Gross

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
- 147.** Identification of polyphenols and other compounds in *Sambucus niga* subsp. *candensis* (American elderberry) flowers. **P.H. Bruner**, Z.D. Smith, M. Johnson, A.L. Thomas, C. Greenlief
- 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
- 155.** Immobilization of gold nanoparticles in a meso-fluidic device. **J.R. Blum**, A.E. Ripp, K. Kounovsky-Shafer, S.A. Darveau, C.L. Exstrom
- 156.** Determination of the illumination profile for a blue light transilluminator. C.L. Exstrom, S.A. Darveau, K. Kounovsky-Shafer, **M.K. Breemes**
- 157.** Detection of superoxide in raw 264.7 cells using microchip electrophoresis coupled to laser-induced fluorescence. **C.G. Fresta**, R.P. de Campos, J.M. Siegel, G. Caruso, J.A. Fracassi Da Silva, S.M. Lunte
- 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
- 161.** Detection of gamma-ray emitting radioisotopes using pattern recognition. **B. Dess**, G.W. Small
- 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
- 165.** Electrochemically mediated desalination: Establishing guidelines to form a locally elevated electric field by chloride oxidation. **K.N. Knust**, F.J. Carrillo, M.J. Anderson, R.M. Crooks
- 166.** Monitoring relative concentration changes of volatile organic compounds in red wines after opening. **K. Jones**, A. Caffrey, D. Daszynski, A. Guanzon, D. Dobberpuhl
- 167.** Vibrational assignments and conformer stability determination of cyclobutyldichlorosilane by variable temperature Raman spectra in krypton solution. R.E. Brenner, **C. Tinsley**, B.S. Deodhar, J.R. Durig

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**
- 169.** Using Image and Excel to analyze color spectrum data: Integrating chemistry, mathematics, and technology. **K. Sellens**, F. Ybanez, T. Woods
- 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**
- 172.** Using liquid carbon dioxide as a solvent for undergraduate organic chemistry laboratory procedures. **Z. Reisen**, D.J. Peitz
- 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

1:50 181. Optimization of industrial chemical synthesis via microfluidics. **S.M. Wells**, T. Robison, J. Hendricks

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

2:30 183. Hsp90 inhibitor carrying magnetic nanotheranostics for the treatment of non-small-cell lung cancer. **J. Kallu**, T. Banerjee, S. Sulthana, B. Heckert, N. Gerasimchuk, S. Santra

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**

3:30 185. Effects of microdomain morphology on the electron propagation efficiency of diblock copolymer bearing ferrocene at the side chain. **G. Ghimire**, Y. Yi, M. Derylo, L.A. Baker, T. Ito

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**

4:10 118. Mixed-metal carbonyl clusters as single-source precursors for advanced nanomaterials. **M.W. Hull**, K.H. Whitmire, D.E. Schipper

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**

1:50 188. Synthesis and evaluation of oxadiazole-derived T-type calcium channel inhibitors. **M. Zhang**, B. Zou, M.J. Gunaratna, S. Weerasekara, C. Pascual, C. Lieu, **D.H. Hua**, X. Xie

2:10 189. Synthesis and evaluation of tripeptidyl-derived viral protease inhibitors. **S. Weerasekara**, Y. Kim, M.J. Gunaratna, M. Zhang, A.M. Prior, K. Chang, D.H. Hua

2:30 190. Sequencing alkene hydroacylation and enantioselective α -arylation of indoles and pyrroles. **J.A. Walker**, A. Ghosh, L.M. Stanley

2:50 Intermission.

3:10 191. Catalytic enantioselective synthesis of polycyclic heterocycles through alkene hydroacylation. **K.L. Vickerman**, L.M. Stanley

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**

3:50 193. Design and synthesis of new pyrazolo[3,4-d]4(5H)-one is as sildenafil analogues for treatment of erectile dysfunction. **Y. Mohamed**, A.H. Elsayed, K.M. Omar, M.A. Shaaban, F.T. Halaweish

4:10 194. Design and synthesis of estrone analogs for the treatment of hepatocellular carcinoma. **Y. Mohamed**, M. Mahnashi, A. Oyen, C. McKinley, F.T. Halaweish

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.

3:35 195. Mass spectrometry for characterizing the proteins of photosynthesis. H. Zhang, W. Cui, Y. Lu, H. Liu, R.E. Blankenship, **M.L. Gross**

4:15 196. Tuning the photophysical properties of tetrapyrrole chromophores and incorporating into biohybrid light-harvesting architectures. **D. Holten**, C.R. Kirmaier, P.S. Parkes-Loach, P.A. Loach, D.F. Bocian, J.S. Lindsey

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

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

8:35 199. Lipid headgroups modulate membrane insertion of pHLIP peptide. **V. Vasquez Montes**, A. Kyrychenko, M. Ulmschneider, A. Ladokhin

9:05 200. Structural plasticity in the topology of the membrane-interacting domain of HIV-1 gp41. **A. Kyrychenko**, J. Freites, J. He, D. Tobias, W.C. Wimley, A. Ladokhin

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

10:05 Intermission.

10:20 202. Rheostats and toggle switches for modifying protein function. **L. Swint-Kruse**, S. Meinhardt, M. Manley, D. Parente

10:50 203. Regulation of membrane interactions of anti-apoptotic regulator Bcl-xL by lipids. **M. Vargas-Uribe**, M. Rodnin, V. Vasquez Montes, **A. Ladokhin**

11:20 204. Mechanisms of catalysis of six metallo-carbapenemase-substrate systems. **A.R. Poffenberger**, L.D. Sutton

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
- 209.** Selective synthesis of lactic acid by oxidation of glycerol using bimetallic PtFe/CeO₂ catalysts. **C. Zeng**, **X. Jin**, P. Bobba, M. Zhao, G. Prasad, R.V. Chaudhari
- 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
- 213.** Exploring new physics in photon-photoelectron interactions on micropatterned, orderly branched zinc oxide nanostructures. T. Chism, **G. Torix**, R. Tian
- 214.** New adhesive from isosorbide. **C.J. Barnish**, M.D. Zenner, J.S. Chen
- 215.** New multi-functional nanoceria for the treatment of lung cancer. **S. Sulthana**, T. Banerjee, J. Kallu, B. Heckert, S. Santra
- 216.** Preparation and characterization of naproxen nanosuspensions. **S. Rabel Riley**, N. Chaudhry, H. Jeong, J. Park, S. Minkler, L. Kirkorian
- 217.** Electrical properties and DFT studies of Copolymers from 3-phenyl[5]ferrocenophane-1,5-dimethylene and various para substituted phenylmaleimides. **H.M. Thomas**, B.O. Tayo, C.J. Neef
- 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

10:20 226. Oxime ether-directed catalytic asymmetric hydroboration. **A.J. Bochat**, V. Shoba, 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

229. Computational analysis of proposed tetrafluoromacrolide. **E. Kaufman**, A. Viste, J.L. Duffy-Matzner

230. Synthesis of PDPP2F-2E-T (polydifurodiketopyrrolopyrrole-diethynyl-hexylthiophenes) as low band gap polymers. **G.J. Malmanger**, **A.D. Morales**, D.E. Weisshaar, J.L. Duffy-Matzner

231. Structure-based design of macrocyclic inhibitors of norovirus 3CL protease. **P.M. Weerawarna**, Y. Kim, A. Galasiti Kankanamalage, V. Damlanka, G. Lushington, K. Alliston, N. Mehzabeen, K. Battaile, S. Lovell, K. Chang, W. Groutas

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

234. Synthesis of ormeloxifene analogs: Potential protein kinase inhibitor. **J. Apraku**, A. Moy, S. Chauhan, F.T. Halaweish

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 phosphoramidates. **J. Torres**, S. Javed, P.R. Hanson

237. Novel sultam analogs of tetramic acid *via* intramolecular Dieckmann condensation. **J. Jun**, M.Y. Hur, T.R. Atkinson, 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**
- 240.** Synthesis of vinyl sultams via Pd-catalyzed intramolecular C-vinylation of triazoles. **A. Cassity**, J.H. Jun, N.M. Windmon, N. Asad, A.J. Diepenbrock, P.R. Hanson
- 241.** Optimizing the preparation of 4(5)-benzyl-L-histidine methyl ester, an intermediate in the preparation of protected derivatives of 4(5)-benzyl-L-histidine for peptide synthesis. D.D. Smith, **P.A. Lievens**, M.R. Hulce
- 242.** Synthesis and reactions of 3-hydroxymethylphthalimides. **D.C. Hawkinson**, A.J. Barmore
- 243.** HPLC-ELSD study of soybean oil equilibration by interesterification. **D. Radojic**, 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 (\pm)-herbindole A, (\pm)-herbindole B, and (\pm)-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-demethyllyngbyalose 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 carboline 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*

8:30 251. Cell-based drug delivery. **S.H. Bossmann**, H. Wang, A.P. Malalasekera, M.T. Basel, T.B. Shrestha, D.L. Troyer

9:00 252. Loading white blood cells with drug delivery agents. **S.O. Wendel**, S. Menon, H. Alshetaiwi, T.B. Shrestha, S. Narayanan, D.L. Troyer, S.H. Bossmann

9:30 253. Fabricating streptavidin coated CpG loaded polymeric particles to surface functionalize tumor cells. **K.K. Ahmed**, S.M. Geary, A.K. Salem

10:00 Intermission.

10:15 254. Peptide nanovesicles as protease responsive drug delivery vehicles. **H. Wang**, T.B. Shrestha, M.T. Basel, P. Maynez, S.O. Wendel, H. Huang, J. Yu, A.S. Yapa, T. Samarakoon, H. Manawadu, P. Thapa, S. Sun, D.L. Troyer, S.H. Bossmann

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.

10:20 260. A renovation in pre-labs: A new hands-on approach. **A.E. Neybert**, **B.M. Jack**, P.K. Morehouse, D. Colombo

10:50 261. Teaching scientific writing and scientific peer review in the United States and China. **R. Glaser**, K. Yang, C. Guo, Y. Guo

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 Au₂₅(SR)₁₈/Au₃₈(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

270. The Soap Project: An undergraduate service-research project. **K.N. Weber**, **A.J. Arampatzis**, H. Ford, A. Vincent, B. Melroe Lehrman, P.A. Mazzer

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**

272. Synthesis and characterization of neutral and ionic forms of ortho- and para-hydroxyphenyl benzimidazoles. **M. Laurich**, E. LaCoursiere, B. Tradewell, V. Mukku, T. Dudley, E. Peterson, W.J. Boyko, N.A. Piro, W.S. Kassel, J.J. Paul

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

274. Exceptionally thin porous nanosheets of NiCo₂O₄/Graphene for malleable electronics. **A. Jimenez**, P.K. Kahol, R. Gupta

275. Substituted amino acids as LAT-1 substrates for use in drug delivery. **K. Finke**, L.M. Hansen, E. Augustyn, A.A. Zur, L. Lin, K. Giacomini, A.A. Thomas

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**
- 279.** Synthesis and activity of amino acid bioisosteres as LAT-1 substrates. **E. Augustyn**, N. Heeren, S. Miller, A.A. Zur, L. Lin, K. Giacomini, A.A. Thomas
- 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*-quereduction 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
- 287.** Evaluation of the electrochemical behavior of a novel dye, N3-CAA, for dye-sensitized solar cells. **T.Z. Crawford**, A. Kudire, B.A. Logue
- 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 (PPAR γ) 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 Ph₃P-Au-SR (R = azulenyl) scaffold. **B.A. Tappan**, A.D. Spaeth, O. Torres-Textidor, N. Gerasimchuk, M.V. Barybin
- 299.** The study of nitrate removal from water using Ti₂O₇ reactive electrochemical membrane. **A. Pitts-McCoy**, A. Paula Castro, L. Guo, B.P. Chaplin
- 300.** Identification of genetic sequences recognized by human SC35 protein using artificial neural networks: A deep learning approach. **S.J. Fergione**, **A.J. Luke**, S.R. Svojanovsky
- 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
- 304.** Molecularly imprinted polymers for dopamine analysis. **E. Isaac**, **J. Springer**, G. Mwangi
- 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 Ti₄O₇. **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. Dvogan**, 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. Meziari**, M. Bellamy

318. Potential drugs for human African trypanosomiasis (sleeping sickness). **A. Mitra**, J.P. Hagen

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.

2:40 325. TILE: Transform, interact, learn, and engage for success in STEM education. **R.S. Cole**, S. Van Horne, J. Emberger

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**

1:20 330. Methods for qNMR: Spin counting in NMR coil volume. **M. Huang**, L. Chi, R.E. Gerald, K.H. Woelk

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

2:00 332. New electronic transitions of NiCl: A comparison of theoretical and experimental studies. **J. Harms**, E.M. Grames, S. Han, L.C. O'Brien, J.J. O'Brien

2:20 Intermission.

2:40 333. Preferential solvation in solution mixtures: A new approach based on local volume fractions. **G.N. Pallewela**, P. Smith

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

3:40 336. Gas-phase infrared spectrum of toluene: Conformation dependence of vibrational anharmonicities of a free methyl rotor. **R. Glaser**, X. Yang, A. Li, J. Zhong

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. Weerasekera, E. Carlson, J. Comer, D.H. Hua

2:30 339. Design, synthesis and biological evaluation of copper activated drugs. **A.P. Malalasekera**, O. Kutsch, F. Wolschendorf, K. Janik, D.L. Troyer, S.H. Bossmann

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

3:45 341. Genetically engineered neuronal stem cells for treatment of glioblastoma tumor in a mouse model. **T.B. Shrestha**, M.T. Basel, D. Lu, M. Pyle, S.H. Bossmann, D.L. Troyer

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-Uribe, A. McCluskey, J.C. Flores-Canales, M. Kurnikova, A. Ladokhin

1:55 344. In vitro activity of D-K6L9 peptide derivatives. **J. Yu**, T.B. Shrestha, H. Wang, D.L. Troyer, S.H. Bossmann

2:15 345. Evolution of SH2 domain to recognize sulfonylated 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**

2:55 347. Protease detection through nanoparticles for cancer diagnosis and prognosis. **R. Ortega**, H. Wang, A.P. Malalasekera, S. Wendel, M. Kalubowilage, A.S. Yapa, G. Zhu, D.L. Troyer, S.H. Bossmann

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**

3:50 349. Analysis of protease assays for early cancer detection. **S.O. Wendel**, H. Wang, D. Udukala, A.P. Malalasekera, A.S. Yapa, G. Zhu, D.L. Troyer, S.H. Bossmann

4:10 350. Post-translational diagnostic sensor for arginase detection. **A.P. Malalasekera**, H. Wang, S. Dai, P.E. Smith, D.L. Troyer, S.H. Bossmann

4:30 351. Imaging of multiple myeloma in mice using Il2pa-based optical molecular probes. **H. Zhou**, D. Hathi, W. Akers, M. Shokeen

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**

2:30 355. Tuning selectivity in cavitand-mediated [2+2] photocycloaddition: Role of intermolecular interactions in the photochemistry of alkyl cinnamates. **N. Nguyen**, M.K. Breemes, A.R. Clements, J. Hoffert, M. Pattabiraman

2:50 Intermission.

3:10 356. Determination of thermodynamic parameters of tripodal nitrogen hetero cycles with multitopic acids and benzoic acid derivatives in the aqueous phase. **S. Andree**, C.B. Aakeroy

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 stereochemical outcome of 3-alkynyl- and 3-alkenyl-2-cycloalkedouble hydride reductions. M.A. Gubbels, R.W. Huang, E.M. Villa, **M.R. Hulce**

4:10 359. Greener solvents for artists: A collaboration across different fields. **K. Janik**, H. Wang, J. Covarrubias, B. Neuman, A.P. Malalasekera, J. Scuille, S.H. Bossmann