

54th MWRM-MEETING AT A GLANCE

Event	Wed PM Oct. 16	Thurs AM Oct.17	Thurs PM Oct.17	Fri AM Oct. 18	Fri PM Oct 18	Sat Oct 19	Location
Plenary Lecture - Sir Fraser Stoddart			4:00-5:00				Kansas Grand Ballroom
Symposium Sessions							
Lab-on-a Chip Technologies for Tackling Biological Challenges		8:00-12:00					Salon A
Nanostructured and Polymeric Materials for Energy Generation and Storage		8:00-12:00					Salon C
Protein Folding, Dynamics Structure Design and Engineering		8:00-12:00	1:00-3:50				Salon D
Nanoporous Materials: Synthesis and Applications		8:00-12:00					Salon 2
Undergraduate Research Symposium		8:00-12:00	1:00-3:50				Arkansas
Graduate Student Awards Symposium			1:00-3:50				Salon A
Natural Resources and the Environment			1:00-3:50				Salon C
Chemical Applications			1:00-3:50				Salon 2
Ultra-Sensitive, High Resolution Fluorescence Spectroscopy				8:00-12:00			Salon A
Organic Chemistry in the 21 st Century				8:00-12:00			Salon B
Chemical Education with a Focus on Online Chemical Education				8:00-12:00			Salon 1
Drug Discovery and Development				8:00-12:00			Salon 2
Energy Conversion with Molecules and Interfaces				8:00-12:00			Salon C
Solvent and Solute Interactions with Macromolecules Organic				8:00-12:00			Sedgwick
Midwest Award Symposium					1:00-3:50		Salon 1
Methods, Molecules & Materials					1:00-3:50		Salon A
Environment & Human Health					1:00-3:50		Salon B
Scorpionate Transition Metal Complexes					1:00-3:50		Salon C
Midwest Award Lecture					4:00-5:00		Salon D
General Sessions							
Inorganic Chemistry		8:00-12:00	1:00-3:50				Salon 1
Inorganic Chemistry				8:00-12:00			Arkansas
Organic Chemistry		8:00-12:00	1:00-3:30				Salon E
Physical Chemistry		8:00-12:00	1:00-3:50				Salon B
Chemical Education		8:00-12:00	1:00-3:50				Sedgwick
Analytical Chemistry				8:00-12:00	1:00-3:50		Salon D
Biochemistry				8:00-12:00	1:00-3:50		Salon E

Event	Wed PM Oct. 16	Thurs AM Oct.17	Thurs PM Oct.17	Fri AM Oct 18	Fri PM Oct 18	Sat Oct 19	Location
Poster Sessions							
SciMix I	7:00-9:00						Salon F
Chemical Education		8:30-10:30					Salon F
Biochemistry		10:30-12:30					Salon F
Analytical Chemistry			1:30-3:30				Salon F
Undergraduate Poster Session			5:00-7:00				Salon F
Undergraduate Poster Session			7:00-9:00				Salon F
Inorganic Chemistry				8:30-10:30			Salon F
Organic Chemistry				10:30-12:30			Salon F
Physical Chemistry					1:30-3:30		Salon F
Plenary Lecture – Sir Francis Stoddart - “Molecular Machines”			4:00-5:00				Kansas Grand Ballroom
Other Events							
Exhibitions	7:00-9:30	9:00-12:00	12:00-9:30	9:00-12:00			Preassembly Area/Atrium
Coffee/Tea/Soda/ Snack Breaks		8:00-12:00	12:00-3:30	8:00-12:00	12:00-3:30		Atrium
YCC/SCC Luncheon			12:00-1:30				Corporate Hills Ballroom
ACS Career Pathways: Finding Yourself				8:00-11:00			Board Room
ACS Career Pathways: Networking				11:00-12:00			Board Room
ACS Career Pathways: Resume Review by Appointment					1:00-5:00		Sedgwick
Vendor - Theater Presentations: Shimadzu, Waters, McGraw Hill					1:00-3:50		Arkansas
Nobel Lecturer Meet & Greet Reception			5:00-6:00				Pool Side
Dinner sponsored by the Watkins Foundation for Sir Fraser Stoddart (RSVP only)			6:30-9:30				Corporate Hills Ballroom
MWRM 2019 Breakfast Board Meeting				8:00-10:00			Fireside Grille
Undergraduate Activities and Program Reception					1:00-5:00		Salon 2
ACS Governance Forum/MWRM Awards Reception					5:00-6:00		Pool Side
MWRM AWARDS BANQUET					6:30-9:30		Corporate Hills Ballroom
High School Teacher Program						9:00-4:00	Salon 1&2
Chemical Waste Management of Undergraduate Chemistry Laboratories						9:00-4:00	Corporate Hills Ballroom

MWRM 2019

D.P. Rillema & A.J. Cruz, *Program Chairs*

WEDNESDAY EVENING

Wichita Marriott
Salon F

Sci-Mix

D. P. Rillema, *Organizer*

7:00 - 9:00

79, 80, 81, 83, 86, 89, 91, 103, 108, 111, 118, 124, 177, 179, 183, 186, 189, 197, 201, 218, 226, 233, 240, 241, 251, 261, 266, 270, 278, 285, 347, 348, 351, 353, 366, 371, 373, 377, 382, 384, 386, 398, 401, 410, 412, 461, 464, 469, 471, 476, 478. See subsequent listings.

THURSDAY MORNING

Wichita Marriott
Sedgwick

Chemical Education

J. R. Oh, *Organizer*
Q. Zhang, *Presiding*

8:00 2. National Science Foundation programs that support undergraduate chemistry education. **T.B. Higgins**

8:20 3. Preferential solvation thermodynamics explored through UV-vis spectrophotometry of Mo(phenanthroline)(CO)₄ in mixed solvents as part of a new integrated upper-level undergraduate chemistry laboratory course. **C.L. Exstrom**, S.A. Darveau

8:40 4. Using complete identification of an inorganic complex as a unifying theme in a multi-technique instrumental boot camp as part of a new integrated advanced undergraduate chemistry laboratory course. **S.A. Darveau**, C.L. Exstrom, K. Kounovsky-Shafer

9:00 5. Addressing student preparation for general chemistry and beyond. **J.S. Overby**

9:20 6. Which learning style suits the most when studying chemistry. **J. Kim**

9:40 Intermission.

9:50 7. Comparison of the effects of two different online homework systems on levels of knowledge retention and attitudes of general chemistry students. **L. Nabulsi**, A. Nguyen, O. Odeleye

10:10 8. Teaching spectroscopy with the Wilson open optical platform system. **A.W. Apblett**

10:30 9. Investigating the efficiency of using team based learning (TBL) vs. traditional lecture in teaching undergraduate organic chemistry courses. **A. Arora**

10:50 10. Impact of simulations on student models of acids and bases. **T. Gupta**, S. Chandrasekharan, S. Forte, D. Prasad

11:10 11. Technology-based culturally relevant chemistry education (CRCE). **M.A. Adoma Fosu**, **T. Gupta**

Wichita Marriott
Salon 1

Inorganic Chemistry

D. A. Hanna, *Organizer, Presiding*

8:00 12. Exploring the electrochemistry of calixpyrrole “Pacman” complexes. **P.E. Sues**, A.T. Altamira, E.M. Archer, N.P. Marshall

8:25 13. Phosphorescent three-coordinate copper(I)-NHC complexes: Synthesis, characterization and photoluminescent studies. **K. Ginton**

8:50 14. Enhancing thermoelectric properties of clathrate $\text{Ba}_8\text{Cu}_{14}\text{Ge}_6\text{P}_{26}$ via tuning carrier mobility. **J. Wang**

9:15 15. Electronic structure and reactivity of tetradentate non-innocent ligands with nickel: Changing ligand-centered oxidation with redox-innocent flanking groups. **K.D. Spielvogel**, E.J. Coughlin, H.R. Petras, J.A. Luna, S.K. Shaw, S.C. Bart, J. Shepherd, S.R. Daly

9:40 16. Oxygen-exchange kinetics of the Anderson-type polyoxometalate ion $\text{TeMo}_6\text{O}_{24}^{6-}$ in aqueous solution. **E.M. Villa**

10:05 Intermission.

10:30 17. Synthesis, characterization, and catalytic activity of FeS_2 nanocubes. **M. Adhikari**

10:55 18. Design of *in vivo* sensor to measure cancer-related enzymatic activity. **J. Covarrubias**, M. Kalubowilage, S. Sham, S.H. Bossmann

11:20 19. Withdrawn

11:45 20. Fluorometric detection of metal cations using internal imine derivatives of anthraquinone-18-crown-5. **A. Hussain**, A.G. Sykes

Wichita Marriott
Salon A

Lab-on-a-Chip Technologies for Tackling Biological Challenges

Cosponsored by ANYL
M. Gong, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 21. Nanosensor chips for single-molecule sequencing of DNA and RNA. **S.A. Soper**

8:40 22. Narrow open tubular liquid chromatography for ultra-high-resolution and ultra-fast bioanalysis. **S. Liu**

9:15 23. Flow-gated capillary electrophoresis and technologies for sensitive detection of multiple amino compounds. **M. Gong**

9:50 Intermission.

10:05 24. Mechanisms of sample enrichment with nanofluidic/microfluidic interfaces for proteome analysis. **A.T. Timperman**, D. Chen, T. Fogliatti, K. Suddhapas

10:40 25. Enabling microfluidic technologies for precision cancer medicine. **Y. Zeng**

11:15 26. Rapid analysis of single cells using integrated microfluidic devices. **C.T. Culbertson**, J.R. Sibbitts, A. Kreznor, C. Johnson, K.S. Zuercher

Wichita Marriott
Salon 2

Nanoporous Materials: Synthesis & Applications

T. Gadzikwa, *Organizer, Presiding*

8:00 27. AIM-ing for catalyst synthesis with single-atom precision. **J.T. Hupp**

8:25 28. Two-dimensional polymerization of covalent organic frameworks. **A.M. Evans**, H. Li, I. Castano, M.J. Strauss, J.E. Bredas, W.R. Dichtel, N.C. Gianneschi, L. Parent, E. Vitaku, N. Flanders, R.P. Bisbey, M.S. Kirschner, R. Schaller, L.X. Chen

8:45 29. Stepwise assembly of multi-cluster frameworks from superatomic metalloligands. **C. Bejger**, M.B. Freeman, M. Kocherga, L. Wang

9:10 Intermission.

9:25 30. Point of use hierarchical MoS₂ foam: Application in scavenging heavy metal ions and inactivating bacteria in water. **P.K. Samantaray**, S. Indrakumar, K. Chatterjee, V. Agarwal, S. Bose

9:45 31. Design and synthesis of 3D carbon nanomaterials for solar energy conversion devices. **W. Wei**

10:05 32. Uniform, binary functionalization of a metal-organic framework material. **K. Samarakoon**, C. Satterfield, M. McCoy, D. Pivaral-Urbina, T. Gadzikwa

10:25 33. Synthesis & characterization of a metalated porous organic polymer for the hydrosilylative reduction of CO₂ to formate. **P. McGrier**

Wichita Marriott
Salon C

Nanostructured & Polymeric Materials for Energy Generation & Storage

R. Gupta, *Organizer, Presiding*

8:00 34. Halide perovskites: New class of semiconductors with emergent functional properties. **A.D. Mohite**

8:50 35. Modeling the nanomorphology and electronic properties of hybrid organic-inorganic and polymeric materials for photovoltaic applications. **O. Kobryn**, S. Gusarov, K. Shankar

9:15 36. Photoexcited charge transport and accumulation in anatase TiO₂. **X. Chen**

9:40 Intermission.

10:00 37. Self-assemble polystyrene-based block copolymer for highly conductive and stable anion exchange membranes. **S.K. Tuli**, T. Fujiwara, T.A. Zawodzinski

10:25 38. WS₂/activated carbon nanocomposite as efficient counter electrode material for dye-sensitized solar cells. **S. Rashidi**, N. Ghee, W. Wei

10:50 39. Direct comparison of band bending and charge transfer dynamics at ZnPc-MoS₂ interface: Monolayer vs. bulk MoS₂. **T.R. Kafle**, B. Kattel, P. Yao, P. Zereszki, H. Zhao, W. Chan

11:15 40. Microwave assisted synthesis of MoS₂-rGO as a sustainable electrode material for zinc ion batteries. **K. Muthukumar**, J. Li

11:40 41. Microwave assisted synthesis of reduced graphene oxide and vanadium pentoxide hybrid materials for enhanced performance in magnesium ion batteries. **L.A. LeBan**, J. Li

12:05 Concluding Remarks.

Wichita Marriott
Salon E

Organic Chemistry

M. Koralegedara, *Organizer, Presiding*

8:00 42. Transition metal catalyzed synthesis of unsymmetrically substituted triazolium salts. **S. Hutchinson**, J.L. Bolliger

8:20 43. Flexible heteroarotinoid (flex-het) analogs of SHetA2 as potential anti-cancer drugs. **R.A. Bunce**, K.D. Berlin, D.H. Zhou, D.M. Benbrook

8:40 44. Preparation of tricyclic aromatic thiazolium salts. **J.L. Bolliger**

9:00 45. Photocatalytic birch-like arylation via C–F functionalization. **J.D. Weaver**, J. Day, M. Khaled, S. Gratjan, B. Koenig

9:20 46. Alkyl halides via light mediated dehalogenation. **M. Rathnayake**

9:40 Intermission.

9:50 47. Exploration of the regioselectivity of intramolecular silyl nitronate cycloadditions (ISNC) in allylic/propargylic systems in the lab and through computational experiments. **J.L. Duffy-Matzner**, K.G. Stevens, A.L. Schull, E.M. Kaufman, J.C. Stevens, S. Li, K.M. Hassebroek, M.L. Grandbois, A.E. Viste

10:10 48. Synthesis of adamantyl derivatives for biological activity. **R. Neri**, K. Eschliman, S.H. Bossmann

10:30 49. Triple activated halogen bond donors for supramolecular assembly. **A. Huber**, A. Sinha, C.B. Aakeroy

10:50 50. Iodine, the outlier: Significance of the halogen bond in chemistry of the organic solid state. **A. Abeysekera**, V. Day, A. Sinha, C.B. Aakeroy

11:10 51. Hydrodeoxygenation of biomass derived feedstocks: Mechanistic insight from isotopic labeling. K.J. Stephens, **A.M. Allgeier**

Wichita Marriott
Salon B

Physical Chemistry

K. A. Layman, *Organizer, Presiding*

8:00 52. New, scalable Hartree-Fock algorithm for the exascale computing era. **D. Poole**, G. Barca, A. Rendell, M.S. Gordon

8:20 53. Coupled cluster theory with induced-dipole polarizable embedding for ground and excited states. **S. Ren**, F. Lipparini, B. Mennucci, M. Caricato

8:40 54. Correlating plasmon dynamics with nuclear vibration. **G. Kuda Singappulige**, D. Lingerfelt, A. Wildman, X. Li, C.M. Aikens

9:00 55. Efficient modeling of water with pairwise spherical harmonics. **C.J. Fennell**

9:20 Intermission.

9:30 56. Theoretical investigations of plasmonic charge transfer from silver nanowires to small molecules. **O.A. Hull**, C.M. Aikens

9:50 57. Origin of the pH dependence of ferritin reduction in the iron-catalyzed Belousov-Zhabotinsky reaction: Density functional studies of structures of ferroin and ferriin in aggregates with hydrogensulfate and sulfuric acid. **R. Glaser**, **S. McCauley**

10:10 58. Helical chains of diatomic molecules as a model for solid state optical rotation. **T.C. Balduf**, M. Caricato

10:30 59. Molecular docking and molecular dynamic simulation studies of selected pesticides and polycyclic aromatic hydrocarbons binding to human serum albumin. **A. Mishra**, Z. Kee, S. Fakayode

10:50 60. Translocation of soft phyto glycogen nanoparticles through solid-state nanochannels. **W.R. Lenart**, W. Kong, W. Oltjen, M.J. Hore

Wichita Marriott
Salon D

Protein Folding, Dynamics, Structure Design & Engineering

Protein Dynamics & Folding

Financially supported by COBRE Center in Protein Structure and Function (COBRE-PSF) at The University of Kansas

M. R. Beck, *Organizer*

J. Bann, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 61. Probing biomolecular dynamics with 1- μ s resolution. **T. Perkins**

8:50 Discussion.

9:00 62. Role of unfolded proteins in bacterial nanoinjectors. **R.N. De Guzman**

9:30 63. Identification of an intermediate in the pathway of formation of a membrane spanning pore by the anthrax toxin protective antigen. **J. Bann**, H. Scott, W. Huang, S. Gonti, **D. Taylor**

10:00 Intermission.

10:15 64. Kinetic control of proteins by ordered self-assembly *in vivo*. **R. Halfmann**, J. Wu, A. Rodriguez Gama, T. Kandola, S. Venkatesan

10:45 65. Probing sequence constraints associated with the cotranslational folding and misfolding of integral membrane proteins. **F.J. Roushar**, L.M. Chamness, C.P. Kuntz, W.D. Penn, B. Li, H. Woods, B. Jastrzebska, J. Meiler, **J.P. Schlebach**

11:00 66. *In silico* studies in exploring the early stages of aggregation of serum amyloid A. **W. Wang**, P. Khatua, U. Hansmann

Wichita Marriott
Arkansas

Undergraduate Research Symposium

Financially supported by UPG GRANT

M. Ahsan, *Organizer, Presiding*

M. Tran, *Presiding*

8:00 Introductory Remarks.

8:05 67. Surfactant-based colloidal systems to promote photoinduced reduction of silver. **W. Halimeh**, D.S. English, S. Shi

8:25 68. Biosensors, biocatalysts, and beyond: Putrescine oxidase immobilization on gold nanostructures via peptide tags. **T.M. Nguyen**, N.J. Kamathewatta, R.T. Lietz, D.O. Deay, S. Seibold, J. Meyer, B. Tomas, B.T. Karaca, T. Hughes, M.L. Richter, C. Tamerler, C.L. Berrie

8:45 69. NaYF₄: Yb,Er upconversion nanoparticles (UCNPs) with an active NaYF₄: Yb,Nd shell for dual-wavelength excitation. **A. Chov**, A. Baride, S. May

9:05 70. Acetate-buffered ozone-mediated synthesis of ceria nanoparticles. **K.E. Derr**, T.J. Fisher, D.J. Stasko, C.L. Cheung

9:25 71. Cyclic voltammetric characterization of lanthanide trifluoromethanesulfonate compounds at a Nafion[®] modified working electrode in an acetonitrile solution. **J. Draghicchio**, K. Idarraga, K.L. Knoche

9:45 72. Upscaling of graphene oxide using a novel fenton oxidation method. **A. Minjarez-Almeida**, J. Covarrubias, S. Eschliman, M. Kalubowilage, S.H. Bossmann

10:05 Intermission.

10:20 73. Novel Fenton oxidation method of detonation-synthesized graphene to graphene oxide. **S. Eschliman**, J. Covarrubias, A. Minjarez-Almeida, A. Nepal, M. Kalubowilage, C.M. Sorensen, S.H. Bossmann

10:40 74. Characterizing [Mn(III)(O₂)(TMC)]⁺ in solution. **E.G. Stewart-Jones**, T.A. Jackson

11:00 75. Ligand-centered reactivity in triaminoborane-bridged diphosphine complexes. **C. Kirkvold**, B. Vlaisavljevich, S.R. Daly, K. Lee

11:20 76. Peeing before the physician bleeds you: Using infrared spectroscopy as an early diabetes mellitus diagnostic tool. H. Newland, **S. Burchett**

11:40 77. Towards the development of a mild phosphorus extrusion reaction for the synthesis of bipyridine and its derivatives. **S.A. Markham**, K. Hillery, S. Smith, Z. Araki, B. Wicker, B.A. Atwater

Wichita Marriott
Salon F

Chemical Education

R. G. Jackson, *Organizer, Presiding*

8:30 - 10:30

78. Reusing a hard drive platter to demonstrate electrocatalysts for hydrogen and oxygen evolution reactions. **R.H. Goncalves**

79. Simple laboratory experiment highlighting multiple chemical principles I: Chemical specificity and selectivity. **A.A. Vartia**, R.S. Black, S.B. Ulapane, M.S. Weerasinghe, M. Maliszewski

80. Learning about protein structure using membrane spanning helices as examples: Simple scoring of membrane spanning protein helices using Excel. **A. Barnes**

- 81.** Comparative analysis of ALEKS and Sapling as a general chemistry course homework system. **A.W. Gachunga**, O. Odeleye
- 82.** Relationship of traditional- and adaptive-responsive online homework systems to student performance in general chemistry: Analyzing extra credit participation. L. Nabulsi, **A. Nguyen**, O. Odeleye
- 83.** Get involved with the ACS Division of Chemical Education. **J.L. Torres Y Torres**
- 84.** Biochemistry learned the write way: Writing as a tool to promote conceptual understanding. **J. Burdelik**, R. Pugh
- 85.** Survey of secondary school chemistry teaching and learning in Kansas. **A.J. Cruz**, E. Legleiter, L.T. Dorn
- 86.** Curriculum mapping and research-based learning in a capstone course: Experimental interplay between chemical synthesis and photoelectrochemistry. **A.J. Cruz**, R. Steinert
- 87.** Integrating service-learning into an organic chemistry laboratory course at a small liberal arts college. **P.P. Pham**, M. Stoops, M. Ramsey
- 88.** Not recyclable: Can Diels-Alder reaction and recycling join hands to solve the problem? **T. Clardy**
- 89.** Using chalcone isomerase to teach spectrophotometry and enzyme kinetics with Vernier sensors. **N. Stevens**
- 90.** Do as I say and as I do: Investigating the role of peer review in writing-to-learn assignments. **M. Schneider**, **F. Tempesta**, **R. Pugh**

Wichita Marriott
Salon F

Biochemistry

J. G. McAfee, I. S. Zegar, *Organizers, Presiding*

10:30 - 12:30

- 91.** EPR reveals the structural dynamics of an unfolded protein in *Yersinia* pathogenesis. **P. Guha Biswas**
- 92.** Exploration of the effect of D-retro-inverso (DRI) peptides on amylin fibril stability. **P. Pandey**, N. Nguyen, U. Hansmann
- 93.** Dependence of proline isomerization on the kinetics of folding of anthrax lethal factor. **W. Halimeh**, J. Bann
- 94.** Understanding the underlying principles behind conformational switch of chemokines. **P. Khatua**, A. Ray, U. Hansmann

95. Withdrawn

96. Withdrawn

97. Role of DNA sequence and histone composition on nanoscale nucleosome structure. **T. Stormberg**, M. Stumme-Diers, Y. Lyubchenko
98. Nanoscale characterization of the interaction of PriA helicase with stalled DNA replication forks. **Y. Wang**, Z. Sun, P.R. Bianco, Y. Lyubchenko
99. Interplay between mechanical stress of double stranded and single stranded DNA segments. **K. Zagorski**, T. Stormberg, A. Vologodskii, Y. Lyubchenko
100. Screening for modulators of MRP1: Pivotal pathway to effective combinatorial drug therapy and precision medicine in cancer patients. **V. Osei Poku**, S. Iram
101. Characterization of cucurbitacin-inspired estrone (CIEA) analogues as novel inhibitors of human P-glycoprotein. **J. Kyeremateng**, B. Peterson, M. Mahnashi, F.T. Halaweish, S. Iram
102. Evaluation of anticancer drugs to selectively kill MRP1 overproducing cells. **J. Loecker**
103. Does palladin bind to monomeric actin? **R. Klausmeyer**, K. Young, M.R. Beck
104. Conflicting or collaborating roles for palladin and VASP in the regulation of actin filaments. **S. Albraiki**, M.R. Beck
105. Knockout of a secondary alcohol dehydrogenase gene in *Nocardia cholesterolicum* NRRL 5767 by CRISPR-Cas9 technology. **J. Huang**, K. Samassekou, J. Seiver, S. McClenahan, S. Holt, L. Wen
106. Discovery of a preferred kinetic pathway in the carnitine acetyltransferase reaction. **M. Kratochvil**, M. Moxley
107. Characterization of a *Pseudomonas chlororaphis* mutant strain deficient for the pyrimidine biosynthetic enzyme orotidine 5'-monophosphate decarboxylase. A. Bani Ahmad, Z.L. Solis, **T.P. West**
108. Wheat protein-based bio-scaffold for neural regeneration. **R. Brice**, A. DeBrot, Y. Li, L. Yao
109. Bioscaffold functions as a platform for neural stem cells delivery for neural regeneration. **A. DeBrot**, L. Yao
110. Protein-protein interactions of minor translocon IpaC of the type III secretion system in *Shigella* in presence and absence of micelles. **A. Chakravarty**
111. ¹⁹F-NMR studies to identify pH induced conformational changes in anthrax toxin protective antigen. **S. Gonti**
112. Hormone pretreatment of seeds to build drought stress tolerance and stress memory. **J. Lafferty**, **M. Ward**, **C. Olaciregui**, **R. Pugh**
113. Structural and mechanistic study of *Ostrinia nubilalis* pheromone binding protein 3. **O. Al-Danoon**
114. Production and purification of aromatase for cocrystallization with potent inhibitors AR11 and AR13. **R. Leyva-Montes**, **B.A. Avila**, A. Diproperzio
115. Structural and functional consequences of the cancer-linked mutations in the intrinsically-disordered transactivation domain of p53. **L.G. Schrag**, I. Thevarajan, X. Liu, M. Zolkiewski, O. Prakash, J. Chen

- 116.** Osmolyte flocculation: Simple yet powerful method to isolate extracellular vesicles. **J. Pedersen**
- 117.** Influence of adsorbed proteins on the mechanism of uptake of branched amphiphilic peptide bilayer coated magnetic nanoparticles. **P. Natarajan**, S. Whitaker, S.D. Fleming, J.M. Tomich
- 118.** Construction of molecular surfaces for probing biological interactions. **K. White-Drayton, Y. Zhu**, K.D. Moeller
- 119.** Incorporation of a photo-crosslinking amino acid into evolved SH2 domain for the study of protein tyrosine O-sulfation. **J. Lawrie**, M.I. Kelly, W. Niu, E.D. Dodds, J. Guo
- 120.** Conserved residue Trp37 in the natively unstructured N-terminal region of Ncb5or nucleates formation of an 11-residue α -helix through interaction with the cytochrome b5 domain. **D.R. Benson**, B. Deng, S. Lovell, K.P. Battaile, P. Gao, A. Cooper, H. Zhu
- 121.** Structural and biochemical insights into the dimethylsulfoniopropionate lyase DddL. **M. Razzaghi, A. Brummett**, L. Gakhar, Z. Xu, M. Dey
- 122.** Role of lipid membrane in catalyzing early stages of A β 42 oligomer formation. **S. Banerjee**, M. Hashemi, K. Zagorski, Y. Lyubchenko
- 123.** Using a CURE to design rational mutations to disrupt misfolding. **S. Marella**, J. Varghese, J. Richardson
- 124.** Modulating protein-protein interactions by the presence of excipients. **E. Fazelpour**, C.J. Fennell
- 125.** Exploring the stability of the N-terminal signaling sequence of a heat shock protein DegQ protease, a bacteria analog to pregnancy related serine protease (HtrA3). **N. Mikita**, M. Phillips, K. Constable

THURSDAY AFTERNOON

Wichita Marriott
Corporate Hills Ballroom

YCC-SCC Luncheon

Cosponsored by SCC
A. J. Cruz, *Organizer*
A. Lolinco, *Presiding*

- 12:00 126.** Shifting into second gear: CRISPR gene drive biotechnology and population control. **G. Finnigan**

Wichita Marriott
Arkansas

Undergraduate Research Symposium

Financially supported by UPG GRANT
M. Ahsan, *Organizer, Presiding*
M. Tran, *Presiding*

- 12:30 127.** Methodologies for synthesizing pharmacologically active pyrazole-derivatives. **S. Leonard**, K. Eschliman, A. Delpe Acharige, T. Lewis, F. Al Ibrahim, A. Minjarez-Almeida, S.H. Bossmann

12:50 128. Determination of binding constants of Cu(I) to antibiotics with NNSN motif. **F. Al Ibrahim**, R. Neri, K. Eschliman, A. Delpe Acharige, T. Lewis, A. Tebeje, S.H. Bossmann

1:10 129. Progress towards the development of a green double allylation methodology. **L. Boese**, S. Champagne, J. Placzek, B.A. Atwater

1:30 130. Synthesizing picket porphyrin molecules that bind to the anionic phosphatidylglycerol (PG) head group in the bacterial plasma membrane. **A. Do**, B. Seelam, R. Nguyen, D. Burns

1:50 131. Synthesis of isothiocyanates and aromatic substitution. **T. Lewis**, F. Al Ibrahim, R. Neri, K. Eschliman, S.H. Bossmann

2:10 Intermission.

2:25 132. Synthesis of a chemotherapeutic agent composed of a cell penetrating peptide and doxorubicin. **M. Montes-Gonzalez**, O. Covarrubias-Zambrano, S.H. Bossmann

2:45 133. Development of designer peptides for cancer detection. **V. Hernandez**, O. Covarrubias-Zambrano, S.H. Bossmann

3:05 134. Preparation of a stably labeled mimic of a deuterated protein with ^{15}N to evaluate mass measurement error in a hydrogen exchange mass spectrometry experiment. **A. Grande**, D.D. Weis

3:25 135. Prediction of active genetic human SRp40 sequences by artificial neural network approach. **M. Edlin**, S. Svojanovsky

Wichita Marriott
Salon 2

Chemical Applications

D. P. Rillema, *Organizer*
M. D. Mosher, *Presiding*

1:00 136. Using spectra peak deconvolution to speed method development: EPA method 8330. **J. Mott**

1:40 137. Solid state characterization of 3-(5-methoxy, 2-methyl-1H-indol-3-yl)-1-(4-pyridinyl)-2-propen-1-one (MOMIPP) and its solvates. K. Gwachha, J.G. Sarver, P.W. Erhardt, Y. Kim, **J. Nesamony**

2:10 138. Evaluation of wood aged beer. **M.D. Mosher**, R. Ordonez, E. Theisen, R. Wilson

2:40 139. Converting silanol synthesis from batch production to flow via microfluidics. **C. Pearson**, S. Torres, L. Cummings, T. Robison, N. Pickering, J. Daye, D. Coverdell

Wichita Marriott
Sedgwick

Chemical Education

J. R. Oh, *Organizer*
Q. Zhang, *Presiding*

1:00 140. Data functionalization for gas chromatography in Python. **M. Green**, X. Chen

1:20 141. Transitioning to NGSS approaches with modeling chemistry workshops. **E. Legleiter**

1:40 142. Redox potential of glutathione to determine oxidative stress in asthma and smokers: Interdisciplinary connection of electrochemistry. U. Panse, **V.C. Waghulde**

2:00 143. Inquiry based approach to teaching electrophilic aromatic substitution reaction of monosubstituted benzene. **V.C. Waghulde**, U. Panse

2:20 144. Measuring ethics knowledge among Chinese students in a graduate chemistry seminar. **K. Yang**, **K. Northcut**, A. Krolikowski, C. Guo, **R. Glaser**

2:40 145. Gamification of laboratory safety in college chemistry laboratory. T. Gupta, **C. Sparks**, M.A. Adoma Fosu

Wichita Marriott
Salon A

Graduate Student Awards Symposium

Financially supported by MWR BOARD
S. Donnelly, *Organizer, Presiding*

1:00 146. Platinum anchored vertically aligned carbon nanofibers as a bifunctional electrocatalyst for oxygen reduction and methanol oxidation reaction. **A. Elangovan**, J. Xu, B. Liu, J. Li

1:25 147. Surface chemistry of Au on In₄Se₃ (001). **A. Dhingra**, P.V. Galiy, L. Wang, T.M. Nenchuk, A.J. Yost, W. Mei, P.A. Dowben

1:50 148. Size-dependent mechanical properties of a metal–organic framework: Increase in flexibility of ZIF-8 by crystal downsizing. **A.A. Tiba**, A.V. Tivanski, L. Macgillivray

2:15 149. Pressure-assisted field-amplified sample injection in flow-gated capillary electrophoresis for analysis of high-salt samples. **N. Maddukuri**, M. Gong

Wichita Marriott
Salon 1

Inorganic Chemistry

D. A. Hanna, *Organizer, Presiding*

1:00 150. Hydrodefluorination and Suzuki coupling type C-F activation using dimesityl quinonyl borane based metal complexes. **P. Dhungana**, J.D. Hoefelmeyer

1:25 151. Catalytic Hydrodefluorination of C(sp²-sp³)-F bonds and direct conversion of acyl fluorides to aldehydes by triphenyl germanium hydride (Ph₃GeH). **A. Hayatifar**, C.S. Weinert

1:50 152. Hydrolysis of later 3d transition metal acetates: New process for fabricating thin films of the corresponding oxides. **D. Russel Rahman**, A.W. Apblett

2:15 153. Pushing the boundaries of f-element phosphinodiboranate synthesis via mechanochemical methods. **T.V. Fetrow**, F.D. Eckstorm, R. Bhowmick, B. Vlasisavljevich, S.R. Daly

2:40 154. Transition metal borohydride complexes. A.M. Aboelenen, **M.P. Jensen**

Wichita Marriott
Salon C

Natural Resources & the Environment

H. Ali, *Organizer, Presiding*

1:00 155. New economic treatment method of produced water for dissolved oil and heavy metals. **J. Vilcaez**

1:25 156. Soil analysis of the evacuated naze automobile mechanic village of Imo State, Nigeria. **M.C. Enedoh**

1:50 157. Reclaiming petroleum produced water from two well sites: Larry & Wava. **P.B. Liescheski**, D. Blankennau, M. Metcalf, R. Ganguli, E. Carter, S. Meyer, I.A. Bonyhady

2:15 158. Selenium source in Las Vegas Valley. **S. Ehsani**, D. James, V. Hodge

2:40 159. Self-cleaning fouling-resistant RO membrane for desalination of oily saline wastewater. **B. Shrestha**, M. Ezazi, G. Kwon

3:05 160. Effects of soy proteins on dynamic relaxation of polymer materials toward design and fabrication of functional polymer/plant protein composites. **P. Feikert**, B. Li

Wichita Marriott
Salon E

Organic Chemistry

M. Koralegedara, *Organizer, Presiding*

1:00 161. New photocatalysts with new reactivity: Organic photocatalyst design in organocatalyzed atom transfer radical polymerization for adaptation to new monomers. **B. Buss**

1:25 162. Defusing the bomb in your laboratory. **A.W. Apblett**, N.F. Materer, S. Shaikh, E. Kadossov

1:50 163. Photoredox 1,4-skip dienes: Simultaneous birch-like dearomatization and C–C bond formation, and a path to unnatural cannabinoids. **J. Day**, S. Grotjahn, M. Bani Khaled, B. Koenig, J.D. Weaver

2:15 164. Synthon engineering in carbamate compounds: Versatile hydrogen-bonded system. **K.N. Shunje**, A. Sinha, C.B. Aakeroy

2:40 165. Reactive azolyl intermediates: Their generation via photocatalysis and use within synthesis. **A. Arora**, J.D. Weaver

Wichita Marriott
Salon B

Physical Chemistry

K. A. Layman, *Organizer, Presiding*

1:00 166. Kinetic pathways of CT exciton dissociation at organic semiconductor interfaces with different molecular orientations. **B. Kattel**, S. Shiwanthi Wanigasekara,, T.R. Kafle, W. Chan

1:20 167. Thermodynamic behavior of ionic liquid dilutions revealed by differential scanning calorimetry and variable temperature FTIR. **C.B. Lasar**, J.N. Curry, K.J. Gudenkauf, D.H. Duffy, B.J. Bellott, S.K. Shaw

1:40 168. Investigation into binding of aromatic and non-aromatic ionic liquid cations to active site of cytochrome P-450. **A. Banerjee**, J. Shah

2:00 169. Kinetic doping: Novel, green approach to silica thin film functionalization with promising environmental applications. **J. Jensen**, W.T. Yip

2:20 170. Absorption and analysis of volatile organics using mesoporous silica. **N.F. Materer**, A.W. Apblett, E. Kadossov, D. Dyer

2:40 171. Microwave absorption of aluminum/hydrogen treated titanium dioxide nanoparticles. **M. Green**, X. Chen

Wichita Marriott
Salon D

Protein Folding, Dynamics, Structure Design & Engineering

Protein Design & Engineering

Financially supported by COBRE Center in Protein Structure and Function (COBRE-PSF) at The University of Kansas

J. Bann, *Organizer*

M. R. Beck, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 172. Machine learning for enzyme site detection and enzyme design. R. Feehan, M. Franklin, **J. Slusky**

1:35 173. Unlocking the potential of *Rhodospseudomonas palustris* CGA009 as a biotechnology platform. A. Alsiyabi, C. Immethun, T. Changa, **R. Saha**

2:05 174. Manipulating protein aggregation via chaperone nucleic acids. **S. Horowitz**

2:35 Intermission.

2:50 175. Using light to control therapeutic protein release: Application to insulin therapy. **S.H. Friedman**

3:20 176. Phage-based nanomedicine: From probes to therapeutics. **C. Mao**

Wichita Marriott
Salon F

Analytical Chemistry

J. T. Mitchell Koch, *Organizer, Presiding*

1:30 - 3:30

177. Quantification of L-arginine in dietary supplements using a Sakaguchi colorimetric assay. **B.A. Eley**

178. Variable and sample selection to improve reliability for the classification and authentication of edible oils. **I. Sota-Uba**, M.T. Bamidele, B.K. Lavine

179. Optimization in capillary electrophoresis for fast determination of amino acids. **Q. Zhang**

180. Microfluidic alternating-pull-push active digitization (μ APPAD) strategy for reproducible sample-loss-free digital PCR. **X. Zhou**, G. Ravichandran, P. Zhang, Y. Yang, Y. Zeng

181. Developing a water quality index using sparse principal component analysis for the Tigris River in Iraq. **S. Gamagedara**, S. Ali, T. Cook, S. Ewaid

182. Absolute quantitation of glycated albumin by isotope dilution mass spectrometry. **A. Shin**, K. Kabytaev, R. Little, S. Connolly

183. Determined electroosmotic mobility in microchannels in a dynamic range of low ionic strength solutions. **B. Menke**, **B. Shundoff**, **K. Kounovsky-Shafer**

184. Using 3D printed devices to elute and concentrate lambda and lambda concatemer DNA molecules. **N. Garringer**, **S. Rau**, A. Larsen, C. Masters, J. Dolphin, A. Vonderfecht, **K. Kounovsky-Shafer**

185. Using 3D printed devices to elute and concentrate *Mesoplasma florum* DNA molecules. A. Larsen, K. Christensen, N. Garringer, **K. Kounovsky-Shafer**

186. Fluorescence spectroscopy studies of aldol addition and condensation reactions in the presence of silica-based heterogeneous catalysts. **J. Bautista Gomez**, A. Usman, M. Zhang, R. Rafferty, S.H. Bossmann, K.L. Hohn, D.A. Higgins

187. Rapid quantification of herbicides in water system using field-amplified sample injection in flow-gated capillary electrophoresis. **N. Zhang**, M. Gong

188. Blood protein glycation profile as hyperglycemia biomarker. **Y. Vazmitsel**, S. Connolly, K. Kabytaev

189. pH dependent binding of zinc(II), nickel(II), and cobalt(II) with a series of heptapeptides using ESI-IMMS. **N. Fuentes**, L.A. Angel

190. Development of new cost-effective DNA detection method by using DNA-conjugated carbon dots. **L.F. Owuocha**, K. Yoshimatsu, A. Wanekaya, E. Sanders

191. Development of a paper-based microanalytical device for heavy metal detection using enzyme inhibition. **A.O. Adams**, K. Yoshimatsu

192. Integrated microfluidic system for amplification-free digital detection of EV mRNAs. **G. Ravichandran**, P. Zhang, Y. Zeng

193. Expanding on recent colorimetry methods to include multicomponent systems using vector analysis in the 3D RGB color space. **S. McCauley, J. Schell,** R. Glaser

Wichita Marriott
Kansas Grand Ballroom

Plenary

Financially supported by Watkins Foundation (Endowed at Wichita State University)
D. P. Rillema, *Organizer, Presiding*

4:00 1. Molecular machines. **J.F. Stoddart**

THURSDAY EVENING

Wichita Marriott
Salon F

Undergraduate Poster Session

M. Ahsan, *Organizer, Presiding*

5:00 - 7:00

194. Data for transition metals. **A. Leffel,** K. Basemann, T.L. Windus

195. Determination of the chemical composition of JUUL pods using gas chromatography. **H. Rai,** M. Harris, J. Cox, E. Meister, C. Reid-Tedesco

196. Components & health effects of JUUL. **I. Do Orozco,** M. Harris, T. Charbonneau, J. Fernandes, A. Mudra

197. Analyzing nitric oxide synthase conformations by time-resolved fluorescence decay. **A. Snyder**

198. Disulfide mediated aggregation of γ -crystallins: Can DBF help? **A. Marko, A. Leabo, R. Kern,** C. Dobson

199. Optimization of the electrophoretic separation and electrochemical detection of RNOS protein oxidation products related to Alzheimer's disease. **A. Paige,** K. Schilly, S.M. Lunte

200. Exploring the synthesis of the furanone side-chain in anisucoumaramide. **A. Selkow,** R.J. Felix

201. Attachment of copper(I)-dependent antibacterial drugs to peptide nanosponges. **A. Tebeje,** K. Eschliman, M. Payne, R. Neri, S.H. Bossmann

202. Development of a separation-based sensor for monitoring neurotransmitters. **A. Barybin,** G. Bulgakova, S. Gunawardhana, S.M. Lunte

- 203.** Single step selective polyfluoroarylation of amides. **B.J. Keen**, M. Hamilton, A.M. Noel, D. Jespersen, J. Day, J.D. Weaver
- 204.** Developing a truncated version of human thyroid peroxidase for X-ray crystallography. **C. Kjetland**, N.M. Devore
- 205.** Toward a cyclic supramolecular square using [Pt(mnt)(4,4'-bpy)₂] building blocks. **C.E. Welton**, B.W. Smucker
- 206.** Synthesis of novel surfactants for enhanced drug delivery and against gram-positive bacteria. **D. Hassen**, L. Chlebanowski, R. Neri, S.H. Bossmann
- 207.** Green one-step, one-pot route to cyclic carbonates for the synthesis of polyurethanes. T. Hinkle, **E.A. Nalley**, E. Grau
- 208.** Green chemistry synthesis of heterocyclic imides used in medicinal chemistry. S.T. Myers, **E.A. Nalley**, R. Paris
- 209.** Green synthesis of heterocyclics using microwave and ultrasonic energy and their use in drug design. **E.A. Nalley**, R. Paris, S.T. Myers
- 210.** Analyses of polycyclic aromatic hydrocarbons in whole milk, apple juice, orange juice and grape juice by FTIR spectroscopy and multivariate regression analysis. **E. Blitz**, B. Fakayode, S. Fakayode
- 211.** Fabrication and characterization of PVDF electrospun nanofibers. **E. Schnetzer**, S. Yang, C. Jiang
- 212.** Development of lanthanide enhanced methanol dehydrogenase electrodes for improved bioelectrocatalysis applications. **G.D. Schwoerer**, L.W. Dawson, K. Kemper, K.L. Knoche
- 213.** Alternative synthesis of dithioisonicotinate and its coordination to 2+ metals. **H.C. Neal**, B.W. Smucker
- 214.** Construction of a chirped-pulse Fourier transform microwave spectrometer. **I. Blackall**, **M. Corry**, L.N. Zack
- 215.** Examining the effect of steric bulk on electrocatalytic CO₂ reduction in [Mn(CO)₃] diimine complexes. **J.P. Stiel**, W. Henke, J.D. Blakemore
- 216.** Synthesis and characterization of (1,2-dicyanoethene-1,2-dithiolato)(dithiooxamide)platinum(II). **J. Boring**, B.W. Smucker
- 217.** Antimicrobial effects and extraction efficiency of thymol from plants native to Kansas. **K. Wilson**, K. Varney, J.T. Mitchell Koch, K.A. Layman
- 218.** Synthesis of pyridyl substituted phosphonium species for use as novel cationic ligands and other applications. **K. Hillery**, **S. Smith**, S.A. Markham, B. Wicker, B.A. Atwater
- 219.** Understanding the mechanism of disulfide bond rearrangement by DBF. **K. Peterson**, **A. Tipler**, **M. Butler**, **R. Poland**, C. Dobson
- 220.** Design of MRI: Sensors for *in vivo* detection of caspase activity. **L. Soto**, J. Covarrubias, S.H. Bossmann

221. Design of a linear 6,6'-biazulenenic π -linker terminated with mercapto junctions. **L. Feden**, J. Applegate, M.V. Barybin
222. Metabolic flux-driven sialylation labels secreted cancer-associated glycoproteins for analysis. **L. Ha**, C. Agatemor, V. Dharharma, A. Osman, K. Muthiah, M. Jukes, B. Robertson, H. Li, C. Saeui, J. Song, R. Ariss, M. Buettner, H.E. Katz, Q. Le Thi, K.J. Yarema
223. Determination of human iodine levels as a measure of population health. **M. Meier**, **L. Tran**, J.T. Mitchell Koch
224. Selectivity studies of phosphatidylinositol 3-kinases (PI3Ks) by docking and free-energy calculation methods. **M. Al Hasan**, S. Almahmoud, H.A. Zhong
225. Examination of the effect of glycylglycine on the hygroscopic properties of NaCl aerosols. **M. Alfarra**, J.P. Darr, W.J. Zamora
226. Testing APEH enzyme activity as a biomarker of stress in a mouse model of e-cigarettes. **N. Twogood**, K. Tyler, G. Mayer, S. Honeycutt, T.M. Covey, T. Hillhouse
227. Analysis of structural and thermal properties of GlyGlu. **N. Piccirillo**, A. Hoff, T. Kuraan, A. Callow, K. Benner, J. Lisko, **A. Ferrucci**, M. Zeller, R. Moser, G. Balendiran
228. Computational modeling of ethyl, ethenyl, and ethynyl-linked BODIPY dimers. M. Brauninger, D. Barbosa, **P.N. Bobadova-Parvanova**
229. Computational modeling of linker-free BODIPY-glycine conjugates substituted at the boron atom. L. Odom, D. Barbosa, M. Wang, G. Zhang, M. Vicente, **P.N. Bobadova-Parvanova**
230. Uniform distribution of covalently linked transparent immiscible phase in epoxy. **R. Francis**, S. K. R.
231. Attempting the synthesis of the coumarin derivative in anisoucoumaramide. **S. Haque**, **R.J. Felix**
232. Synthesis and coordination chemistry of N-butylglycine derivatives as a model for an undergraduate lab course. **S. Konur**, S.A. Costin
233. Inhibitory activity of novel inverse agonists on the transcriptional function of human nuclear receptor RORgamma. **S. Bolin**, **H. Miller**, M. Huang, A. Dykeman, H. Ng
234. Investigating the inhibition of APEH in disease. **S. Geilmann**, T.M. Covey, D. Belnap
235. Investigating the modulation of SIAE and CASD1 gene expression and their influence on inhibitory receptor binding in cancer cells. **S. Grabenstein**, R. Willand-Charnley
236. Quantitative alcohol determination using infrared spectroscopy. **S. Johnson**, S. Burchett
237. Fibratol: Reduced fenofibrate. **T. Kuraan**, **A. Callow**, N. Piccirillo, A. Ferrucci, A. El-Khoury, A. Kotheimer, W. Haq, G. Balendiran
238. Developing a method to quantify glyphosate in soil samples. **T. Buettner**, **K. Ernest**, A.C. Moser
239. Red edge spectroscopic study of changes to BSA before and after UV photolysis with two fluorescence probes. **T. Mabile**, M. Marlow

240. Facile route to fabricate binder free Ni(OH)₂/RGO core-shell nanosphere for supercapacitor electrode. **Y. Khan**, P. Chandra Maity, A. Urade, S. Choudhary, I. Lahiri

Wichita Marriott
Salon F

Undergraduate Poster Session

M. Ahsan, *Organizer*

7:00 - 9:00

241. ANS photophysics in viscous solution: Concentration dependant lifetimes and fluorescence quenching. **A.M. Grabert**, M. Marlow

242. Electronic interaction in copolymers of vinylferrocene and vinylimidazole. **T. Flaske**, **B. Tayo**, C.J. Neef

243. Curcumin's derivative's anti-microbial effect. **A. Wu**, M. Seleem, M. Conda-Sheridan

244. Anion recognition properties of sulfonamide capped porphyrins. **A. Bass**, L. Latta, H. Story, H. Jemal, C. Cardenas, S.D. Starnes

245. Cofactor binding to aldose reductase. **A. Ferrucci**, **N. Piccirillo**, F.P. Schwarz, M.R. Sawaya, M. Verma, D. Cascio, G. Balendiran

246. UV/visible absorption studies of zinc selenide nanoparticles obtained using a controlled-growth, one-pot synthesis. **A.J. Cruz**, W.J. Engel, **D. Kee**, F.M. Schertz, D.P. Rillema

247. Porphyrin flanked phenyl-indole derivatives: Atropisomers for chiral recognition applications and the development of chiral switches. **A. Salazar**, L. Latta, W. Morrison, J. Ahumada Gonzalez, A. Bass, J. Lemieux, S.D. Starnes

248. Analysis of iridium in soil for identifying the K-Pg boundary. **B. Corbett**, Q. Zhang

249. Electrochemical reduction of nitro groups: From bioanalysis to lightweight high-energy density cathodic materials for lithium batteries. **B. Samuelson**, **M. Venzke**, P. Keller, B. Goeden, M. Balasingham, M.D. Koppang, H. Sun

250. Antioxidant activity of baicalein derivatives. **C. Holaway**, H. Butt, A. Vummenthala

251. Metal-assisted etching for nanoscale lithography. **C.D. Hunt**, S.B. Ulapane, C.L. Berrie

252. Molecular geometries of Fe(II) spin-crossover complexes. **C. Kirkvold**, B. Vlasisavljevich, B.A. Finney

253. Toward high-throughput single-cell organelle isolation using microfluidic electrokinetic lysis. **C. Johnson**, J.R. Sibbitts, C.T. Culbertson

254. SPME fiber derivatization of bisphenol A for gas chromatographic analysis. **D.W. Harak**, M. Vandenhul, C. List

255. Quantum chemistry simulations of rhodium(III) catalysts for hydrogen production. **D. Lynam**, M. Caricato
256. Proximate analysis of crude fiber content in wild and domestic elephant manure. **E. Griggs**, A. Arora, L. Jayawickrama
257. Synthesis of backbones for SIAE sugar-based inhibitors via carbanion and peroxide chemistry. **E. Sundall**, R. Willand-Charnley
258. Synthesis and study of the recognition properties of non-chiral and chiral porphyrin-calixarene hybrid hosts. **H. Story**, N. Feliciano, A. Kasetti, L. Mwangi, S.D. Starnes
259. Development of an anti-microbial surfactant-based nanovesicle coating for the prevention of biofilm formation on *in vivo* surgical implants. **H. Thurman**, L. Yahya, K. Roberts, D.S. English
260. Design, construction, and characterization of a low cost spectrometer with interchangeable parts. **J. Godek**, A.D. Gift
261. Catalytic and non-catalytic synthesis of *Chlorella vulgaris* into bio-oil via hydrothermal liquefaction. **J. Flores**
262. Determination of heavy metal levels in cosmetic foundations using ICP-AES analysis. **J. Johnson**, Q. Zhang
263. Isotope effect in optical rotation: Computational study. **K. Vander Laan**, T. Balduf, T. Aharon, M. Caricato
264. Development of a low cost, “stick anywhere” integrated heating device for on-chip temperature regulation during microfluidic cellular analysis. **K. Zuercher**, J.R. Sibbitts, C.T. Culbertson
265. Investigation of lanthanides as catalysts in oxygen reduction reaction and in CO₂ reduction using cyclic voltammetry. **K. Idarraga**, J. Draghicchio, K.L. Knoche
266. Caging ion-pairs. **K. Joseph**, S. Kaur, V. Day, K. Bowman-James
267. Thermal changes in ionic liquid solutions probed by differential scanning calorimetry. **K. Gudenkauf**
268. Investigating the thermostability of a heat shock protein DegQ protease, a bacteria analog to pregnancy related serine protease (HtrA3). **K. Constable**, N. Mikita
269. Effect of carbonization and chemical activation on the electrochemical properties of polyaniline. **L. Williston**, W. Lin, T. Ingsel, S.D. Bhoyate, G.S. Fernando, K.S. Siam, P.K. Kahol, R. Gupta
270. Synthesis of phenanthroline-based long-chain bridging ligands and their metal complexes. **L.D. Lewandowski**, A. Hussain, K. Mariappan, A.G. Sykes
271. Study of the composition changes of wood extracts from various extraction techniques. **M. Brockhaus**, J. Childears, B. Daro, C. Kamler, D. Ross, A. Snyder, K. Voichahoske, D.J. Peitz
272. Synthesis of phosphatidylglycerol receptor: Precursor preparation. **M. Ahsan**, K. Donavalli, D. Burns
273. Computational study of anthraquinone fluorescent chemosensors. **M. Koble**, A. Reuter, B. Vlaisavljevich

274. Cyclooxygenase-2 inhibitory activity of metal-curcumin complexes. **M. Vazquez**, J. Harder, A. Vummenthala
275. Cloning of a heat shock protein DegQ protease, a bacterial analog to pregnancy related serine protease (HtrA3). **M. Phillips**, N. Mikita
276. Activated carbon as an inexpensive alternative for counter electrode in dye-sensitized solar cells. **N. Ghee**, W. Wei
277. Interaction between type VI collagen and capillary morphogenesis protein 2 using fluorescence anisotropy. **P. Halimeh**, J. Bann
278. Taming two (photocatalytic) transformations: Reductive alkenylation and isomerization of heterocycles. **R.K. El Mokadem**, R. Overfield, J.D. Weaver
279. Chiral recognition properties of chiral piperidine capped porphyrins. **R. Gainzar**, S.E. Gonzalez Higgins, K. Mejia, A. Shammaa, S.D. Starnes
280. Identifying the prevalence of primary cilia on lymphatic endothelial cells in homeostasis. **R. Krump**, M. Latterell, D. Fink
281. Fourier transform spectroscopy of $\text{MgCCH} (\text{X}^2\Sigma^+)$ and an attempt to confirm its detection in IRC+10216. **S. Safarimaryaki**, L.N. Zack, J. Bernal, J. Min, L.M. Ziurys, M. Sun
282. Effect of changes in non-conserved regions of barracuda & tardigrade LDH on enzyme activity and thermal stability. **S. Khan**, C. Palmer, M.R. Beck
283. Determination of atrazine in Glacier Creek using gas chromatography-mass spectrometry. **S. Witte**, A.D. Gift, A. Miller
284. Co-crystallization: Can we make agrochemicals safer? **M. Vittengl**, N. Sarkar, A. Sinha, C.B. Aakeroy
285. Characterization of the dimerization domains of the mannose 6-phosphate/insulin-like growth factor II receptor. **T. Degener**, S. Dorn, J. Kreiling
286. Greener approach for the kinetic controlled-growth synthesis of quantum dot nanocrystals. **W.J. Engle**, D. Kee, A.J. Cruz, J. Bond, D.P. Rillema

FRIDAY MORNING

Wichita Marriott
Salon D

Analytical Chemistry

L. Shultz-Lockyear, *Organizer, Presiding*

8:00 287. Development of matrix metalloproteinase activity assay with fluorescently tagged magnetic nanoparticles and microchip isoelectric focusing. **S. Jia**, C.T. Culbertson, S.H. Bossmann

8:25 288. Continued development of a high-throughput single-cell analysis device for the measurement of nitric oxide levels in microglia. **J.R. Sibbitts**, C.T. Culbertson

8:50 289. Kinetics of mediated microfluidic electrochemistry on complexes in the intact mitochondrial electron transport chain. **N.L. Frantz**, G. Brakoniecki, K. Voorhis, Y. Levitsky, D. Proshlyakov

9:15 290. Electrochemical activity assay for protease analysis using carbon nanofiber nanoelectrode arrays with optimized peptide substrate length and temperature. **Y. Song**, H. Fan, M. Anderson, J. Wright, D.H. Hua, J. Koehne, M. Meyyappan, J. Li

9:40 291. Monitoring MVOCs over time from *Rhizopus stolonifer* using SPME GC/MS. **C. Gamlath Mohottige**, T. Mlsna, R. Baird

10:05 Intermission.

10:15 292. Proteomics analysis reveals docosahexaenoic acid-mediated protective effects in lipopolysaccharide-stimulated microglial cells. **C.M. Greenlief**, B. Yang, R. Li, X. Geng, J. Lee, B. Mooney, K. Fritsche, D. Beversdorf, G. Sun

10:40 293. Identification of two novel trace impurities in mobile phase prepared with commercial formic acid. **E. Bakota**, R.A. Levine

11:05 294. Investigation of polycyclic aromatic hydrocarbon (PAH) and chiral-PAH analogues-methyl- β -cyclodextrin guest-host inclusion complexes by fluorescence spectrophotometry and partial least square regression analysis. **S. Fakayode**, L. Greene, B. Elzey, M. Franklin

11:30 295. Chromium removal from aqueous systems by polyaniline treated biochar. **A. Herath**, C. Reid, T. Mlsna

Wichita Marriott
Salon E

Biochemistry

J. Balthazor, *Organizer, Presiding*

8:00 296. Structural characterization of glycomembrane proteins involved in human disease. **G.A. Cook**

8:25 297. Withdrawn

8:50 298. Structural and functional characterization of pheromone binding protein from *Ostrinia furnacalis*. **S.R. Dahal**

9:15 Intermission.

9:25 299. Potentiating Antibiotics using a β -stranded ligand. **P. Sukthankar**, C.B. Cook, J. Slusky

9:50 300. Role of myopalladin in cardiac muscle function and disease. **V. Kadarla**, M.R. Beck

10:15 301. Computer-aided discovery of novel inverse agonists to inhibit the transcriptional function of human nuclear receptor RORgamma. **M. Huang**, S. Bolin, H. Miller, A. Dykeman, H. Ng

10:40 Intermission.

10:50 302. QM level investigation into the catalytic cycle of cytochrome P-450 involving imidazolium-based ionic liquid cations as substrate. **A. Banerjee**, J. Shah

11:15 303. Development of a novel gene delivery nanocarrier. **O. Covarrubias-Zambrano**, T.B. Shrestha, M. Montes-Gonzalez, S.H. Bossmann

11:40 304. Microstructured hydrogel surfaces for stem cell differentiation. **Y. Vasquez**, H.G. Jayasinghe, S. Madihally

Wichita Marriott
Salon 1

Chemical Education with a Focus on Online Chemical Education

Cosponsored by CHED
J. L. Torres Y Torres, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 305. Taking the classroom out of chemistry: Journey in the world of online chemical education. **S. Burchett, J.L. Hayes**

8:35 306. Status on chemistry online courses at Missouri Western State University. **S. Svojanovsky**

9:00 307. Using technology to our advantage: Tales from a partially flipped organic chemistry classroom. **J.S. Rhoad**

9:25 308. Effect of argumentative writing to promote nonscience major students' learning in an introductory chemistry course. **C.P. Aguirre-Mendez**, Y. Chen, T. Terada

9:50 Intermission.

10:10 309. Development and first year of WGU's online competency-based general chemistry course series. **D. Branan**

10:40 310. Learner-centered strategies for teaching biochemistry online. **M.K. Zimmerli, J.L. Torres Y Torres**, C.D. Rogers, A.L. Reno, M.L. Brulotte

11:05 311. Assessment of student reasoning and interactions during online synchronous chats. **R.S. Cole**, E. Kartsonaki, G. Lawrie

11:30 312. Creating custom Foldit puzzles for teaching biochemistry. **S. Horowitz**

11:55 Concluding Remarks.

Wichita Marriott
Salon 2

Drug Discovery & Development

Cosponsored by MEDI
W. Groutas, *Organizer, Presiding*

8:00 Introduction.

8:05 313. Repurposing clinically-used drugs for the treatment of neurological problems associated with inactivating mutations in the enzyme ALDH7A1. **K.S. Gates**, J. Wyatt, C. Nel, D. Ahire, J. Jha, D. Greenan, J. Tanner, F. Gallazi

8:40 314. Methylenecyclopropane nucleoside analogs as broad-spectrum anti-herpes agents. **T.L. Bowlin**

9:15 315. Glycomimetics and peptidomimetics for drug-resistant bacterial infections and cancer. V. Damalanka, A. Maddirala, L. McGrane, J. Voss, J. Pinkner, L. Klampfer, T. Hannan, S. Hultgren, **J.W. Janetka**

9:50 Intermission.

10:00 316. Structural biology in drug discovery: Development of viral protease and protein–protein interaction inhibitors. **S. Lovell**

10:35 317. Dimensionally enhanced antibacterial library screening. **W.G. Gutheil**, N.J. Ayon

Wichita Marriott
Salon C

Energy Conversion with Molecules & Interfaces

Cosponsored by INOR
Financially supported by Shimadzu Instrument Co. and MDPI Molecules
C. L. Berrie, J. D. Blakemore, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 318. Redox-active block copolymer thin films for electrochemically-controlled catalysis. **T. Ito**, G. Ghimire, H. Coceancigh, Y. Yi

8:45 319. Asymmetric functionalization of azulene and 6,6'-biazulene π -linkers with isocyanide and mercapto junction groups along their molecular axes. **J. Applegate**, M.K. Okeowo, N. Gerasimchuk, M.V. Barybin

9:05 320. Nanoscale imaging of photocatalytic activity in semiconductor nanostructures using super-resolution fluorescence microscopy. **B. Sadtler**

9:45 Intermission.

10:00 321. Biomolecular electrocatalysts for energy applications. **S.D. Minteer**

10:40 322. Electrochemical kinetic studies of [Cp*Rh] complexes featuring substituted dipyritylmethane ligands. **J.A. Hopkins**, D. Lionetti, J.D. Blakemore

11:00 323. C–H activation and hydrogen/deuterium (H/D) exchange: Mechanistic insight into heterogeneous catalysts. **A. Sadtler**

11:40 Concluding Remarks.

Wichita Marriott
Arkansas

Inorganic Chemistry

D. A. Hanna, *Organizer*
J. Townsend, *Presiding*

8:00 324. Assembly and characterization of heterobimetallic complexes of palladium with redox-inactive metals. **R.R. Golwankar**, A. Kumar, V. Day, J.D. Blakemore

8:25 325. Use of Ce(IV) ammonium nitrate for Mn(IV)-oxo formation and oxidation reactivity. **Y. Lee**, S. Jones, T.A. Jackson

8:50 326. Synthesis, structure, and properties of the branched oligogermane (Ph₃Ge)₃GeF. **C.S. Weinert**, A. Hayatifar

9:15 327. Synthesis and characterization of aryl and alkyl substituted oligogermanes. **M. Leal**

9:40 Intermission.

10:05 328. Synthesis, structure, reactivity and properties of fluorinated pyridyl and bipyridyl ligands and their metal complexes (Pt, Pd, Ir, etc.). **N. Lu**, C. Chang

10:30 329. Boron-based molecular bis-tweezers: Crystal engineering of a host for separation of thiophene from benzene. **G. Campillo-Alvarado**, H. Morales-Rojas, H. Hopfl, L. Macgillivray

10:55 330. Pincer-type N-heterocyclic carbene copper (I) complexes and their utilization in transfer hydrogenation reaction. **J. Minnick**, L. Tahsini

Wichita Marriott
Salon B

Organic Chemistry in the 21st Century

B. A. Atwater, *Organizer, Presiding*

8:00 331. Chemical and physical tuning of polyphosphazene membranes for gas separation processes. **J. McNally**, C. Orme, J. Klaehn, F.F. Stewart

8:25 332. Benzophenone glycosides and a microwave: Beginning of a career at a PUI. **A.L. Pirinelli**

8:50 333. Strategies for targeted therapies of cancer: Development of small molecule drug conjugates with folate targeting ligands. **A.E. Felten**, I.R. Vlahov, C.P. Leamon

9:15 334. Selective functionalization of pyridines, diazines and pharmaceuticals via heterocyclic phosphonium salts. **A. McNally**

9:40 Intermission.

9:50 335. Carbohydrate-protein interactions that promote natural killer cell activation and degranulation. **M.P. Farrell**

10:15 336. Beyond total synthesis: Synthetic adventures in chemical screening library construction, therapeutic agent potentiation, and facilitated transport. **R. Rafferty**

10:40 337. Towards the development of a green double allylation methodology. **B.A. Atwater**, L. Boese, S. Champagne, J. Placzek

11:05 480. Solution to “Anomalous” Asymmetric Halocamphor Dissociation Reactions.. **J.D. Van Horn**

Wichita Marriott
Sedgwick

Solvent & Solute Interactions with Macromolecules

K. R. Mitchell-Koch, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 453. Advanced studies of Kevlar[®] pulp characterization using low-field nuclear magnetic resonance (NMR) relaxometry. A.M. Allgeier, **M. Toledo Suekuni**, T. Myers, S. Shelburne, M. McNeil, W. Shepperson, A. Prisco

8:30 454. Predicting the solvent structure around macromolecules in solutions with the integral equation theory of molecular liquids. **A. Kobryn**

9:10 455. Olfaction in moths: Structural and functional studies of pheromone-binding proteins. **S. Mohanty**

9:50 Intermission.

10:00 456. Removing the barrier to the calculation of activation energies: Aqueous hydration dynamics. A.K. Borkowski, E.A. Piskulich, **W.H. Thompson**

10:40 457. Extraordinary solvation of a substrate analog within an enzyme active site observed with 2D IR spectroscopy. **S.D. Moran**

11:20 Concluding Remarks.

Wichita Marriott
Salon A

Ultra-sensitive, High Resolution Fluorescence Spectroscopy

D. S. English, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 338. Conformations and dynamics in nitric oxide synthases: Insights from time-resolved and single-molecule fluorescence. **D.C. Arnett**, B.C. Smith, C.K. Johnson

8:35 339. Studying highly-dynamic proteins involved in protein targeting to the thylakoid membrane using single molecule fluorescence. **C.D. Heyes**

9:05 340. Single-molecule conformational analysis of apolipoprotein E. M. Stuchell-Brereton, M. Zimmerman, B. Baban, G. DeKoster, G.R. Bowman, C. Frieden, **A. Soranno**

9:35 341. Disordered RNA-folding chaperones enhance nucleic acid folding via local charge screening. **E.D. Holmstrom**

10:05 Intermission.

10:15 342. Unique solvent-swelling behavior of PEO microdomains revealed using fluorescence methods. **H. Coceancigh**, D.A. Higgins, T. Ito

10:40 343. Fluorescence imaging of whispering gallery mode resonances. **R. Dunn**, T. Pak

11:05 344. Fluorescence-based studies to evaluate binding and release of a new class of antimicrobials. **D.S. English**, T. Dinh, D. Burns, M. Alsuri, B. Seelam

Wichita Marriott
Salon F

Inorganic Chemistry

A. Oberley, *Organizer, Presiding*

8:30 - 10:30

345. Cyanoxime derivatives of main group V elements. **K.A. Pinks**

346. Variable temperature studies of new NIR fluorescent 1D platinum wires. **B. Lottes**, N. Gerasimchuk, M.Y. Berezin

347. Photo-catalyzed click chemistry with strain loadable alkene on gold nanoparticles. **S. Sulthana**, K. Singh, J.D. Weaver, Y. Vasquez

348. Determining inorganic selenium speciation in water samples by graphite furnace atomic absorption spectroscopy. **S. Ehsani**, D. James, V. Hodge

349. Synthesis of phase pure gold phosphide nanoparticles. **D.G. Fernando**, T. Nigro, S.M. Alia, B.S. Pivovar, Y. Vasquez

350. Pyruvic acid oxime and oxalate precursors for production of nanocrystalline metal oxide catalysts. **A. Alayyaf**, A.W. Apblett

351. Selective fluorescence sensing of metal cations with imine based macrocycles. **D. Cork**

352. Novel cyanopyrazole scorpionate complexes. **J. Kromer**, D.M. Eichhorn

353. Scorpionate, pyrazolate, and pyrazole complexes of palladium, platinum, and iron. **A. Oberley**, D.M. Eichhorn

- 354.** Utilizing scorpionate ligands to generate thermally stable Schrock-type molybdenum catalysts for alkane metathesis applications. **E. Goentzel**, P.E. Sues
- 355.** Influence of Lewis acids on a $\text{Mn}^{\text{III}}\text{OH}$ system. **E. Grotemeyer**, D. Rice, A. Donovan, T.A. Jackson
- 356.** Exploiting aurophilic interactions in a [2+2] photocycloaddition: Single-crystal reactivity with changes to surface morphology. **C. Li**
- 357.** Substituent effects on the HOMO-LUMO absorption and emission of Pt(II)-biphenyl complexes containing 1,10-phenanthroline derivatives. **A.J. Cruz**, D.P. Rillema, S.R. Stoyanov, A. Jehan, K.S. Siam
- 358.** Reactivity and luminescent properties of heteroleptic Cu(I) complexes supported by chelating triaminoborane-bridged diphosphorus and nitrogen ligands. **J.C. Zgrabik**, K. Lee, C.M. Donahue, J.D. Culpepper, S.R. Daly
- 359.** Investigating the effect of hydrogen bonding on redox reactivity of Mn^{III} -hydroxo complexes. **A.A. Opalade**, T.A. Jackson
- 360.** Rhenium complexes containing carboxylate linkages attached to TiO_2 for dye-sensitized solar cells. K.M. Ensz, V. KomReddy, **D.P. Rillema**
- 361.** Syntheses and crystal structures of novel heterobimetallic $4d\text{-}4f$ sulfite structures. **K.S. Ogura**, E.M. Villa
- 362.** Advances in new hybrid lanthanide sulfite structures. **A.D. Tran**, E.M. Villa
- 363.** Synthesis and characterization of transition metal complexes as catalysts for proton-coupled electron transfer. D.P. Rillema, **H. Nguyen**
- 364.** Influence of the equatorial ligand field in tuning the reactivity of the manganese(IV)-oxo complexes in oxygen atom transfer reactions. **P. Singh**, M. Denler, E.G. Stewart-Jones, T.A. Jackson
- 365.** Preparation and characterization of a series of platinum(II) biphenyl complexes containing bipyridine ligands with substituents in the 4,4'-position. **D.P. Rillema**, **A. Jehan**, H. Nguyen, A.J. Cruz, C. Moore
- 366.** Synthetic and crystallographic investigations into rhenium–manganese silicides and rhenium–ruthenium silicides. **D. Meyer**, F. Wang
- 367.** New analogue of $[\text{Ru}(\text{bpy})_3]^{2+}$ bearing 9,9'-dimethyldiazafluorene ligands. **M.L. Anderson**, W. Henke, J. Hopkins, V. Day, J.D. Blakemore
- 368.** Second-shell hydrogen bonding's impact on HAT reactions of Mn(III)-hydroxo complexes. **L. Hessefort**, A. Opalade
- 369.** Heptanuclear organometallic Cr(0) complex featuring 12 azulene units. **D. Maldonado**, J. Applegate, M.V. Barybin
- 370.** Self-assembled monolayer films of cyano- and isocyano-functionalized mercaptoazulenes. **X. Ortiz-Medina**, C.L. Berrie, M.V. Barybin
- 371.** Toward terazulenenic π -linkers with complementary orbital density distributions within their frontier molecular orbitals. **T. Vo**, N.R. Erickson, M.V. Barybin

372. Design and performance of dioxomolybdenum(VI) complexes of chiral modular ligands for enantioselective oxygen atom transfer reactions. **T.A. Rusmore**, K.M. Nicholas, D.T. Glatzhofer

373. Influence of ligand field on hydrogen atom transfer reactions by oxomanganese(IV) species. **J.R. Mayfield**, A. Massie, M. Denler, D. Leto, T.A. Jackson

Wichita Marriott
Salon F

Organic Chemistry

E. L. Trump, *Organizer, Presiding*

10:30 - 12:30

374. Synthesis and characterization of chitosan derivatives for high performance gene delivery. **A.M. McMullen**, R.S. Herati

375. Battle for dominance: Hydrogen, halogen and chalcogen bonding. **V. De Silva**, V. Day, A. Sinha, C.B. Aakeroy

376. Electronic interaction in copolymers of vinylferrocene and vinylimidazole. **S. Mahbub**, C.J. Neef

377. Investigation of palladium-mediated cyclizations of α,β -unsaturated oximes. **S. Weber**, M.D. Mosher

378. Design of a flow-based ATR-FTIR spectrometer for detection of diacetyl in beer. **A. Campanella**, C. Toe, M.D. Mosher

379. Progress report on the synthesis and biological evaluation of hydroxylaminoacridines. **J. Forster**, C. Taylor, M.D. Mosher

380. Understanding intermolecular competitions between chalcogen and halogen bonds. **V. Panikkattu**, C.B. Aakeroy, V. Day, A. Sinha

381. *In silico* investigation of conversion of biodiesel to gasoline. **A. Roy**, M.R. Siebert

382. Synthesis of complexes of N-heterocyclic carbenes (NHCs) of silver(I) and copper(I) with potential antibiotic properties. **H. Palencia**, I. Monreal-Leyva, O.A. Lozano-Ramos, E.F. Arias-Rodriguez, A. Nuxoll

383. Synthetic approaches to 4*H*-benzo[*d*][1,3]oxazin-4-ones. **J.K. Annor-Gyamfi**, R.A. Bunce

384. Effects of porphyrin molecules that bind to the phosphatidylglycerol (PG) head group, a lipid found in the bacterial plasma membrane. **B. Seelam**

385. Biodiesel conversion through pyrolysis: Density functional theory analysis of methyl linoleate. **M. Bakker**

386. Withdrawn

387. Oxidatively and reductively-cleavable protecting group strategies for array-based parallel synthesis. **N. Yeh**, **R.L. Krueger**, K.D. Moeller

- 388.** New approach to selectivity in a preparative electrochemical reaction. **Q. Jing**, K.D. Moeller
- 389.** Chirality-directed self-assembly of novel dual catalytic dendrimers: Applications toward tandem two step catalysis. **J. Zhou**, G.R. Still, S.A. Moteki
- 390.** Devising a scalable solution phase synthesis of peptidomimetics to probe the G protein cell receptor signaling pathway. **Y. Zhu, Z.T. Medcalf, R.L. Krueger**, K.D. Moeller
- 391.** Synthesize a new multi-target AMPK activator based on natural activators and improve its physiochemical properties for treating cancer and Alzheimer's diseases. **B. Sharma**
- 392.** Paired electrochemistry: Powerful and general tool for on-site generation of chemical reagents. **T. Wu**, K.D. Moeller
- 393.** Stereoselective synthesis of homoallylic alcohols by double hydride reduction. **M.R. Hulce**, B.L. Callahan
- 394.** Synthesis of concentrative nucleoside transporter 2 ligands. **H. Way, B. Venteicher**, H. Ngo, H. Chien, A. Schlessinger, K. Giacomini, A.A. Thomas
- 395.** Synthesis optimization toward 1,2,3-triazolyl β -amino acid prodrugs for LAT1 targeted drug delivery. **J. Griffith, J. Engberg**, C. Hall, H. Wolfe, A. Wells, A. Duncan, H. Ngo, H. Chien, C. Colas, A. Schlessinger, K. Giacomini, A.A. Thomas
- 396.** Synthesis and properties of super stable DOTA cations. **E.L. Trump**, D. Reese
- 397.** Investigating the effect of the ester linkage between phenylalanine and ketoprofen in a LAT1 targeted prodrug. **K. Merklin**, B. Venteicher, H. Way, J. Griffith, C. Alvarado, S. Springer, K. Finke, L. Stoner, E. Augustyn, H. Ngo, H. Chien, C. Colas, A. Schlessinger, K. Giacomini, S. Chandra, E. Hill, A.A. Thomas
- 398.** Platinum bis(fluoro-ponytailed) bipyridine complex catalyzed hydroxylation of alkynes under thermodynamic condition. **N. Lu**, T. Tsai
- 399.** Investigating the effect of electron withdrawing group to an nucleophilic addition reaction for the detection of thiol-containing species. **K. Everitt**, H. Schmitz, H. Cao
- 400.** Chemical investigation of curcumin derivatives for cyclooxygenase-2 inhibition. **J. Harder, M. Vazquez**, A. Vummenthala
- 401.** Curcumin-metal complexes as inhibitors of beta-amyloid aggregation. **M. Dervisevic**, J. Brabant, A. Vummenthala
- 402.** Sulfonyl linchpins: Building block for electrophilic probes. **E. Plouch**, V. Thomas, P.R. Hanson
- 403.** Synthesis of ω -amino isoprenoid bisphosphonates as potential GGDPS inhibitors. **A. Fairweather**, M.L. Varney, S.A. Holstein, D.F. Wiemer
- 404.** Synthesis of small bis phenolic ether scaffold cationic molecules. **K. Donavalli**, D. Burns
- 405.** Synthesis of chiral selectors with proline amino acid ionic liquids for enantioseparation. **P.P. Pham**
- 406.** Enantioselective synthesis of proline derivatives for use in the synthesis of aclidinomycin A and B. **G.P. Nora**

- 407.** Asymmetric transfer hydrogenation of ketophosphonates catalyzed by imidazolium ion tethered TsDPEN ligands with iridium(III) in water. **P. Quan**, M. Sun, B. Ni
- 408.** 4-fluoroacetophenone-(4'-phenoxyphenylethylidene) hydrazone, an unsymmetrical acetophenone azine: Synthesis, structure and computational study. **H. Bhoday**, R. Glaser
- 409.** Toward peptide-polymer amphiphiles with different properties for studying biological interactions. A.J. Nasrazadani, S.A. Innes, E.L. Torrey, H.A. Hernandez, M.P. Thompson, N.C. Gianneschi, **A.J. Luthi**
- 410.** Anion recognition properties of chiral porphyrin atropisomers: Chiral switches? **L. Latta**, A. Salazar, J. Lemieux, J. Ahumada Gonzalez, W. Morrison, A. Bass, M. Waites, S.D. Starnes
- 411.** Applications of hydrogen- and halogen-bonding in the crystal engineering of photoreactive solids. **J.Q. Bell**, L. Macgillivray
- 412.** Non-linear optical properties of crystalline unsymmetrical 4-halo-4'-*n*-alkoxyacetophenone azines and of butadiene analogs: Structural and computational analysis of the crystal architectures. **K. Yang**, **S. Murphy**, N. Corretjer, S. Gadban, R. Glaser
- 413.** Dienylation of alpha-aryl malonates with Diels-Alder applications. **T. McQuillan**, M. Maliszewski, J.A. Tunge
- 414.** Competition studies to compare reactivity of different electrophiles in Tsuji-Trost reactions. **J.E. Super**, M. Duncan, J.A. Tunge
- 415.** Intramolecular cyclization of thiol-functionalized triazolyidenes salts through disulfide intermediate. **L. Ardon Munoz**
- 416.** Chemical defenses of pioneer plants. **E. Plouch**, E. Berens, N. Weigle, E. Sanford, K. Murray

FRIDAY AFTERNOON

Wichita Marriott
Salon D

Analytical Chemistry

L. Shultz-Lockyear, *Organizer, Presiding*

1:00 417. Optimization of extraction conditions for lignin from wheat biomass. **R. Roy**, **D.E. Raynie**

1:25 418. Spectroscopic characterization of interactions in aqueous solution between poly(methacryloxyethyltrimethylammonium) chloride and halogenated fluorescein dyes. E. Sowers, L. Duvall, C. Graham, J. Palakeel, M. Hammar, F.A. Jutton, **E.E. Remsen**

1:50 419. Red edge spectroscopic study of two fluorescence probes in several sugar glasses at ambient temperature. **M. Marlow**

2:15 Intermission.

2:25 420. Indirect determination of mica present in cosmetics via rubidium content. **S. Alsherari**, A.W. Apblett

2:50 421. Application of attenuated total reflection infrared microscopy to the forensic examination of automotive paint smears. **G.P. Affadu-Danful**, F. Kwofie, L. Zhang, K. Kalkan, K. Dahal, H. Zhong

3:15 422. Infrared imaging applied to problems in forensic automotive paint analysis. **K. Sharma Dahal**, F. Kwofie, H. Zhong, B.K. Lavine

Wichita Marriott
Salon E

Biochemistry

J. Balthazor, *Organizer, Presiding*

1:00 423. Development of new analytical peptides (WTAS-DAPK1 and WTAS-calpain-1) for improved targeted uptake and toxicity. **S. Ehsan**, O. Covarrubias-Zambrano, S. Jia, C.T. Culbertson, S.H. Bossmann

1:25 424. RNA interference of X-box binding protein 1 in *Acyrtosiphon pisum*. **J. Lutgen**, J. Ridder, J. Balthazor

1:50 425. NMR and molecular dynamics simulation reveal the impact of V23D mutation on the function of yeast oligosaccharyltransferase subunit Ost4p. **B.P. Chaudhary**

2:15 426. Characterization of γ -sarcoglycan by NMR. **M.S. Harris**, M. Jamaledine, G.A. Cook

2:40 Intermission.

2:50 427. Expression, purification, and characterization of the syndecan-1 ectodomain: Potential biomarker for cancer diagnosis and prognosis. **A.R. Anderson**, G.A. Cook

3:15 428. OSW-1 induced prophylactic antiviral response through long-term oxysterol-binding protein (OSBP) repression. **Z.C. Severance**, B.L. Roberts, R.C. Bensen, N. Kothapalli, C. Malinky, A.T. Le, H. Ma, W. Reddig, S. Wu, E. Blewett, A. Burgett

3:40 429. Aromatase inhibition by potent inhibitors AR11 and AR13. **S.A. Souza**

4:05 Concluding Remarks.

Wichita Marriott
Salon B

Environment & Human Health

K. Wimalasena, *Organizer, Presiding*

1:00 430. MPP⁺ scaffold containing lipophilic compounds are selective dopaminergic toxins *in vivo*. **K. Wimalasena**, D. Murphy, B. Lickteig

1:25 431. Identification and optimization of aspartic protease inhibitors as antimalarial agents. **M.J. Meyers**

1:50 432. Further developments of a novel class of inhibitors of *Aedes aegypti* Kir1 (AeKir1) channel. **C.D. Aretz**, C.R. Hopkins, J. Denton, J. McCarthey, M. Kramer, S. Kharade, P. Piermarini, R. Rusconi Trigueros

2:15 433. Drug targeting of oxysterol-binding proteins: Design and synthesis of natural product-derived anti-viral and anti-cancer lead compounds. **C. Malinky**, A.T. Le, R. Fogle, A. Burgett

2:40 434. Do effective antibiotics require stereocenters? They do not. **K. Eschliman**, T. Lewis, S. Leonard, F. Al Ibrahim, A. Tebeje, S.H. Bossmann

3:05 435. Development of ClpP2 cctivators to treat chlamydial infections. M. Seleem, N. Rodrigues de Almeida, S. Ouellette, **M. Conda-Sheridan**

Wichita Marriott
Salon A

Methods, Molecules & Materials

D. P. Rillema, *Organizer*
N. E. Schmidt, *Presiding*

1:00 436. Light-controlled dynamic self-assembly of a spiropyran-modified tetrapeptide. **C. Creemer**, J.R. Parquette, M. Liu, T. Reardon

1:25 437. Profiling the cancer secretome by exploiting metabolic bioorthogonal labeling and enrichment of tumor-associated glycans. **C. Agatemor**, V. Dharharma, A. Osman, L. Ha, K. Muthiah, M. Jukes, B. Robertson, H. Li, C. Saeui, J. Song, R. Ariss, M. Buettner, H.E. Katz, Q. Le Thi, K.J. Yarema

1:50 438. Understanding the chemistry of manganese nitrides for atmospheric ammonia production. **B. Liu**, N. Shan, C. Huang, R. Lee

2:15 439. Radio frequency-controlled delivery of therapeutic peptides to cancer sites. **J.L. Hammer**, L. Chlebanowski, J. Yu, P. Thapa, S.H. Bossmann

2:40 440. Fabrication and characterization of a protein composite conduit for nerve regeneration. **L. Yao**, A. DeBrot

3:05 441. Self-healable superomniphobic surfaces for corrosion protection. **M. Ezazi**, B. Shrestha, N. Klein, D. Lee, S. Seo, G. Kwon

Wichita Marriott
Salon 1

Midwest Regional Award Symposium

N. A. LaFranzo, *Organizer*
R. D. Little, *Presiding*

1:00 442. Organic electrochemistry: Potpourri of synthesis and mechanism. **R.D. Little**

1:30 443. Stereoselective electrocatalysis of radical reactions. **S. Lin**, N. Fu, L. Song, W. Lee

2:00 444. Urinary FSH glycoform evaluation by automated Western blotting. **S. Katta**, G.R. Bousfield

2:30 445. Application of visible-light photoredox catalysis in polymer networks to control large amplitude movement and mechanical properties of gels. **J.C. Barnes**

3:00 446. Development of tripodal ligand frameworks and first-row transition metal reagents for selective C–N bond construction methodologies. **A. Kalra**

Wichita Marriott
Salon C

Scorpionate Transition Metal Complexes

D. M. Eichhorn, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 447. Recent developments in cyanoscorpionate chemistry. **D.M. Eichhorn**, J. Kromer, A. Oberley, L. Kadel

1:35 448. Nitrene transfer catalysis using first-row transition metal scorpionate complexes. **M.P. Jensen**

2:00 449. Multiple bond metathesis of organometallic uranium complexes supported by scorpionate ligands. **C. Tatebe**, S.C. Bart

2:25 Intermission.

2:35 450. Tris(oxazolinyl)borate scorpionate compounds and catalytic chemistry. **A.D. Sadow**

3:00 451. Structure-property relationships in photoresponsive pyrazolylborates. **S.M. Holmes**, Y. Zhang, N.P. Rath, R. Clerac, C. Mathoniere

3:25 452. Scorpionates for stabilizing Mn(III)-peroxo adducts, low-spin Mn(III) species, and high-valent Mn(IV) compounds. **T.A. Jackson**, H. Colmer, A. Forshaw, J.M. Smith, J.A. Telser

Wichita Marriott
Salon F

Physical Chemistry

K. S. Siam, *Organizer, Presiding*

1:30 - 3:30

458. Effects of covalent and non-covalent interactions at a molecule–semiconductor interface. **B. Dhital**

459. Approaches towards time-effective MRI diffusion tensor imaging. **M. Payne**, T.B. Shrestha, I. Mali, S.H. Bossmann

460. Computational study of CO₂ capture by the Rubisco-inspired tetrapeptide KDDE: Sequence of carbamate formation and Mg²⁺ complexation. **K. Yang**, **R. Glaser**

- 461.** Using an energy cascade trilayer structure to dissociate photoexcited excitons at organic semiconductor interfaces. **S.S. Wanigasekara**, B. Kattel, T.R. Kafle, W. Chan
- 462.** Development of MRI imaging methods to quantify cerebellar regional gray matter in rats. **I. Mali**, T.B. Shrestha, M. Payne, B.P. Anderson, S.H. Bossmann
- 463.** Development of high-performance supercapacitors using waste coffee powder: Importance of nitrogen-doping on electrochemical properties. **J. Choi**, C. Zequine, S.D. Bhoyate, X. Li, P.K. Kahol, R. Gupta
- 464.** Comparison of stability of native to D-retro-inverso amylin and the effect of forcefield on conformational preferences. **N. Nguyen**, U. Hansmann, P. Pandey
- 465.** Theoretical study of the volatile aluminum hydroxides AlOH , $\text{Al(OH)}_2(\text{g})$ and $\text{Al(OH)}_3(\text{g})$. **D.L. Myers**, U. Pustina
- 466.** Simulations of solution-phase Raman spectra with the coupled cluster single and double-polarizable continuum model (CCSD-PCM) method. **R. Lampton**, M. Caricato, M. Barclay
- 467.** Use of a dithiocarbamate-modified redox polymer attached to gold for the layer-by-layer construction of enzymatic bioanodes. **S. Wilson**, D.T. Glatzhofer
- 468.** ONIOM computational study of the thermochemistry of activation and carbamylation reactions of Rubisco. **K. Knobbe**, **J. Schell**, R. Glaser
- 469.** ^1H and ^{31}P NMR analysis of a $1, \text{N}^6$ -ethenoadenine lesion incorporated in DNA. **K. Ljunggren**, G.A. Meints
- 470.** Plasmon-mediated photocatalysis using electron dynamics calculations. **P. Pandeya**, C.M. Aikens
- 471.** Effect of uracil in different sequence contexts on DNA properties by 2D ^1H and ^{31}P solution NMR. **J. Becker**, **A.C. Pilarski**, G.A. Meints
- 472.** Structure and dynamics of native and mutant serine/threonine kinase 11 (STK11) by molecular dynamics simulation. **M. Halim**, M. Islam, A. Khan, M. Parves, M. Hossain
- 473.** Solid state reactions of silicon dioxide, titanium dioxide, and yttrium(III) oxide. F. Salazar-Salas, L.Y. Robles-Fernandez, **D.L. Myers**
- 474.** ^1H and ^{31}P solution NMR investigation of G:T mismatches in DNA. **M. Westwood**, G.A. Meints
- 475.** Conversion of algae into bio-oil through hydrothermal liquefaction. **E. Cardenas**, K. Largent, B. Jang
- 476.** Using replica-exchange-with-tunneling to access the lymphotactin folding switch. **A. Ray**, P. Khatua, U. Hansmann
- 477.** Rapid analysis of regional protein hydration shell dynamics from dydration shell structural data. **E. Shahryari**, K.R. Mitchell-Koch, J.N. Dahanayake
- 478.** Mapping order in liquid and crystalline water. **R. Maharjan**

FRIDAY EVENING

Wichita Marriott
Salon D

Midwest Research Award Lecture

Financially supported by St. Louis Local Section

N. A. LaFranzo, *Organizer*

R. D. Little, *Presiding*

4:00 479. Exploring the synergistic relationship between organic synthesis and electrochemistry. **K.D. Moeller**