



ACS Midwest Regional Meeting – Final Program

Blake R. Peterson, *Program Chair*

WEDNESDAY EVENING

KS Union
Ballroom

Sci-Mix

R. A. Altman, *Organizer*

6:00 pm - 8:00 pm

Poster Numbers: 66, 103, 200- 202, 206, 215, 226, 228, 231, 238, 240, 246, 248, 253, 256, 263, 270, 280- 283, 286, 289, 369, 377, 387, 395, 396, 454, 457, 466, 469, 473, 474, 501- 503, 505- 507, 510, 519, 522, 525.
See subsequent listings.

THURSDAY MORNING

KS Union
Alderson

Analytical Applications of Microfluidics

Cosponsored by ANYL

Financially supported by Center for Molecular Analysis of Disease Pathways, Adams Institute for Bioanalytical Chemistry

S. M. Lunte, *Organizer, Presiding*
M. A. Witek, *Presiding*

8:00 Introductory Remarks.

8:05 1. 3D nanostructuring of microfluidic devices by engineered colloidal self-assembly affords sensitive immunosensing of exosomal biomarkers. **P. Zhang**, Y. Shang, M. He, Y. Zeng

8:20 2. Chiral separation of Pacific Blue-labeled amino acids for the detection of biosignatures in extraterrestrial samples. **K.M. Schilly**, J. Creamer, M.F. Mora, P.A. Willis

8:35 3. Microfluidic devices for extracting cell-free DNA. **C.D. Campos**, M.A. Witek, S.A. Soper

8:50 4. Modular approach to microchip-based electrochemical detection using 3-D printing technology. **A.S. Munshi**, R.S. Martin

9:05 5. Integrated microfluidics system for the analysis of Circulating Multiple Myeloma Cells (CMMCs) using Fluorescent *in-situ* Hybridization (FISH) analysis. **K. Weerakoon-Ratnayake**, M.L. Hupert, M.A. Witek, S.A. Soper

9:20 6. Direct integration of microdialysis sampling with microchip electrophoresis separation for electrochemical detection of small molecule biomarkers in biological samples. **S. Gunawarhana** **UngawelDurayalage**

9:35 Intermission.

9:45 7. Microchip-based approaches for studying nitric oxide release from endothelial cells. **A. Townsend**, R.S. Martin

10:00 8. Microfluidic magnetic bead ELISA streamlined with pneumatic valves. **Y. Yang**, Y. Zeng

10:15 9. A novel detection method for microchip electrophoresis based on bipolar electrochemically generated fluorescence. **M.B. Wijesinghe**, D. Gunasekara, S.M. Lunte

10:30 10. Measuring the time-of-flight (ToF) of single molecules using dual beam laser-induced fluorescence. **B. Young**

10:45 11. High-efficiency and rapid separations of biological samples using flow-gated capillary electrophoresis. **M. Gong**

11:00 12. Optimization of hylene MP synthesis for production via microfluidics. **Z. Peacock**, S.M. Torres, T. Robison

KS Union
Kansas

Analytical Chemistry

Y. Zeng, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 13. Barriers in analytical chemistry: Broken instrumentation, and the modern instrumentation paradigm. **S.D. Abbott**

8:20 14. Fabrication of a mixed-scale fluidic device for comprehensive molecular profiling from circulating markers. **B. Gross**, V. Singh, J.M. Jackson, S.A. Soper

8:35 15. Electrochemical quantification of length mismatched DNA duplexes: Solution versus surface hybridization effect. **M. Shamsi**, M. Taki, H. Palmer

8:50 16. Untargeted identification of polyphenol secondary metabolites in *Sambucus nigra* (subsp. *canadensis*) flower extracts. **P.H. Bruner**, A.L. Thomas, C.M. Greenlief

9:05 17. Nanoscale electrophoresis separation of deoxynucleotide monophosphates. **C. Amarasekara**, C.E. O'Neil, K. Weerakoon-Ratnayake, B. Gross, S.A. Soper

9:20 18. Targeted analysis approach for efficient mapping of full *N*-glycosylation site profile of highly glycosylated proteins. **M.R. Wijeweera Patabandige**, E.P. Go, H.R. Desaire

9:35 19. Block copolymer-derived nanoporous films as platforms for electrochemical DNA sensors based on a steam-loop probe. **Z. Harandizadeh**, T. Ito

9:50 Intermission.

10:00 20. Cyanogenic glycosides analysis in American elderberry: picrate paper and LC MS/MS method development and validation. **M.K. Appenteng**, R. Krueger, H. Ingold, A.L. Thomas, C.M. Greenlief

10:15 21. A microfluidic IEF chip with scanning fluorescence detection. **K. Sellens**, A. Anye, C.T. Culbertson

10:30 22. Single-molecule studies of Nile red incorporated in block copolymer thin films. **H. Coceancigh**, T. Ito, D.A. Higgins

10:45 23. Expediting duplex specific nuclease (DSN) mediated microRNA detection using a microfluidic circulating device. **X. Zhou**, Y. Zeng

11:00 24. Diffusional studies of differently-charged molecules in self-assembled organic nanotubes using imaging fluorescence correlation spectroscopy. **G. Ghimire**, R. Espinoza, H. Xu, S. Nagasaka, N. Kameta, M. Masuda, D.A. Higgins, T. Ito

11:15 25. Improving brain delivery of a peptide via BBB (blood brain barrier) modulation and detection using LC-MS-MS. **K.R. Ulapane**, T.J. Siahaan, P. Kiptoo, T. Williams

KS Union
Pine

Biochemistry

H. R. Desaire, *Organizer*
J. Slusky, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 26. Role of fast protein dynamics in thymidylate synthase catalyzed hydride transfer. **A.K. Ghosh**, A. Kohen

8:30 27. Improved methods to accurately quantify methionine oxidation in glycoproteins. **J.T. Shipman**, E.P. Go, H.R. Desaire

8:50 28. Unraveling ionic liquid-iron porphyrin interactions to understand ionic liquid biodegradation. **A. Banerjee**, J. Shah

9:10 Intermission.

9:30 29. Effect of small organic molecules on the assembly of the 20S proteasome core particle. **A. Kante**, E.J. Deeds, D. Johnson, J. Karanicolas

9:50 30. Characterizing competitive binding of structurally diverse ligands with OSBP/ORP subfamily-1. **J.I. Nunez**, A.T. Le, N.R. Kothapalli, A.W. Burgett

10:10 31. Mechanism study of a peptide diastereomer with anti-cancer activity. **J. Yu**, A.I. Herrera, T.B. Shrestha, O. Prakash, D.L. Troyer, S.H. Bossmann

10:30 32. Electrostatic binding of wall teichoic acid re-sensitizes MRSA to oxacillin. **M. Foxley**, C.V. Rice

10:50 33. Interaction of 2-color multidrug resistance protein-1 biosensor with potential substrates in ensemble FRET-based assay. **B. Osa-Andrews**, K.W. Tan, S.H. Iram

Catalysts and Catalytic Technologies for Fuels, Chemicals, & the Environment

Cosponsored by ENFL

J. J. Bravo-Suarez, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 34. Hydrophobization of catalyst surfaces for biomass upgrading reactions in aqueous and biphasic systems. **D. Resasco**

8:35 35. Controlling product selectivity in the conversion of 2,3-butanediol to valuable products. **K.L. Hohn**, Z. Alauda, Q. Zheng

8:50 36. Water's unique influence on acid site distribution in low Si/Al zeolites. **J.L. White**, K. Chen, M. Abdolrahmani, S. Crossley, D. Resasco

9:05 37. Solid acid catalyzed depolymerization of various lignins into value added phenolic monomers. **K.Y. Nandiwale**, A.M. Danby, A. Ramanathan, R.V. Chaudhari, B. Subramaniam

9:20 38. Liquid phase propylene epoxidation with Nb based mesoporous silicates. **S.K. Maiti**, A. Ramanathan, B. Subramaniam

9:35 Intermission.

9:50 39. Microkinetic detail of ammonia decomposition through Y-procedure analysis of transient experiments. S. Lwin, L. Wang, R. Kunz, W. Diao, D. Constales, G. Yablonsky, **R. Fushimi**

10:20 40. Carbon nanotube-supported catalysts prepared by a modified photo-Fenton process for Fischer-Tropsch synthesis. H. Almkhelfe, X. Li, K.L. Hohn, **P.B. Amama**

10:35 41. Higher dispersion with increased activity of tungsten in bimetallic mesoporous silicates. **A. Ramanathan**, R. Maheswari, H. Zhu, B. Subramaniam

10:50 42. Withdrawn

11:05 43. Synthesis and characterization of biochar-based carbon supported metal nanoparticles. **S. Neeli**, H. Ramsurn

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Chemical Biology of Infectious Disease

Cosponsored by MEDI

T. E. Prisinzano, *Organizer, Presiding*

8:00 44. Chemical and macromolecular insights into ClpP modulation as an antibacterial strategy. **A.S. Duerfeldt**

8:25 Discussion.

8:30 45. From betulinic acid to BMS-955176, a second generation HIV-1 maturation inhibitor. **A. Regueiro-Ren**

8:55 Discussion.

9:00 46. Discovery of host-directed therapeutics for the treatment of Gram negative bacterial infections. **A.J. Duplantier, R.G. Panchal**

9:25 Discussion.

9:30 47. Antibody recruiting molecules: vetting a new modality. **M. Sender, B. Turunen, Y. Chen, C. Wells, D. Smith, C. Leach**

9:55 Discussion.

10:00 48. Development of first-in-class encephalitic alphavirus inhibitors with in vivo efficacy. **J.E. Golden**

Organic & Medicinal Chemistry

R. A. Altman, *Organizer*

H. Malinakova, *Organizer, Presiding*

8:00 49. Ni-catalyzed alkene carboacylation of *ortho*-allylbenzamides. **K.L. Vickerman**, J.A. Walker, J.N. Humke, L.M. Stanley

8:20 50. Directed stereoselective transition metal-catalyzed hydroboration and carbocupration of cyclopropenes. **A. Edwards**, M.A. Rubin

8:40 51. Formal α -C–H allylation of amines by quinone mediated oxidation / Pd catalyzed allylation. **L.M. Mori Quiroz**, M.D. Clift

9:00 52. Photo-induced oxidative decarboxylation-elimination for the synthesis of E/Z-enamides and enecarbamates. **K. Cartwright**, S.B. Lang, J.A. Tunge

9:20 53. Anodic cyclization: Pathway control and the construction of a 5,7,5-tricyclic ring system. **R. Feng**, R. Perkins, K.D. Moeller

9:40 Intermission.

9:50 54. Base catalysis enables access to α,α -difluoroalkyl(thio)ethers. **D. Orsi**, B.J. Easley, A.M. Lick, J.P. Sorrentino, R.A. Altman

10:10 55. Oxidative functionalization of amine-containing molecules through quinone catalysis. **X. Liu**, B. Haugeberg, J. Phan, T. O'Connor, S. Londhe, M.D. Clift, M. Leon

10:30 56. Applications of pyridine-oxazoline functionalized metal-organic frameworks for asymmetric transition-metal catalysis. **B.P. Schumacher**, T. Goh, W. Huang, L.M. Stanley

10:50 57. Computational study of Lawesson's reagent mediated fluorenone dimerization forming 9,9'-bifluorenylidene. **A.J. Eckelmann**, M.R. Siebert

11:10 58. Toward the development of a "universal" indole aryne generating platform: Synthetic and computational studies of trifluoroindoles, a new and versatile class of indole aryne precursor. **M. Rayhart**, Z. Albader, R. Glaser, C.J. Cramer, M. Wulser, M. Santos, C. Clements, K.R. Buszek

KS Union
Jayhawk

Starting Companies in the Biotech Industry

C. Berkland, *Organizer, Presiding*

8:00 Introductory Remarks by J. Sabol.

8:05 Session Overview by C. Berkland.

8:15 Introduction of Panelists: S.A. Soper, C. Marich, M. Flynn, L. Stehno-Bittel, C. Berkland.

9:05 Intermission.

9:20 Whiteboarding a company, group excercise.

9:50 Panel Discussion.

KS Union
Woodruff

Theory, Spectroscopy, & Materials

Cosponsored by COLL, INOR and PHYS

C. L. Berrie, J. D. Blakemore, C. G. Elles, C. K. Johnson, B. B. Laird, W. H. Thompson, *Organizers, Presiding*

8:00 59. Computer-aided nanomaterial and nanostructure research and design. **X.C. Zeng**

8:30 60. Single particle tracking: Recent advances in methods and applications. **C.F. Landes**

9:00 Intermission.

9:15 61. Interfaces large and small: Connecting molecular response to macrscopic phenomena. **C.J. Mundy**

9:45 62. Harnessing the optical properties of metal nanoparticles for targeted action. **A.J. Haes**

10:15 Intermission.

10:30 63. Ultrafast electronic and nuclear structural dynamics of excited state transition metal centers for solar energy conversion. **L.X. Chen**

11:00 64. Watching proteins dance. **C.M. Cheatum**

Undergraduate Symposium

Financially supported by Deciphera Pharmaceuticals, LLC
D. A. Vartia, *Organizer*

8:00 - 10:00

- 65.** ChemisTea: A quantitative chemical analysis of tea. **L. Nabulsi**, P. Morehouse
- 66.** Synthesis and structure-activity relationship (SAR) of carboxyl-substituted phenylalanine derivatives as LAT1 substrates. **L. Stoner**, **C. Hernandez**, S. Springer, H. Chien, K. Giacomini, C. Colas, A. Schlessinger, A.A. Thomas
- 67.** Characterization of cinnamic acid derivatives as novel pain medications: Role of adenosine pathway. C. Capellen, A. Priebe, M. Hunke, **M. Pattabiraman**, S. Chandra
- 68.** Heart phenotype of an aged mouse model with a targeted deletion causing reduced bone trabecular volume. **D. Warton**, J. Vallejo, N. Lara-Castillo, L.A. Wetmore, M. Johnson, M. Wacker
- 69.** Developing new derivatives of 1,8-naphthalimide dyes via Suzuki coupling reaction. M. Xie, T. Ding, **H. Cao**
- 70.** Co-crystallization of coumarin derivatives. **M. Reinmuth**, A. Sinha, C.B. Aakeroy
- 71.** Concentrate electrophoretically eluted DNA molecules in 3D printed devices. **A. Mashmann**, J. Dolphin, K. Kounovsky-Shafer
- 72.** Synthesis of a novel flavonoid dimer as a potential antibiotic. **A. Millhuff**, J.A. Morrill
- 73.** Quantitative analysis of CdSe/ZnS quantum dots by x-ray fluorescence. H.E. Maunders, A.J. Runia, A.L. Tietz, **D.E. Weisshaar**
- 74.** Role of $\alpha 5\beta 1$ integrin and Met in triple negative breast cancer metastasis. **J. Soukup**, S. Van slambrouck
- 75.** Optimizing the hydrogenolysis of 4-L-phenylspinacine. D.D. Smith, **A. Ghajarieh**, M.R. Hulce
- 76.** Synthesis of α -quaternary amino acids as potential LAT1 substrates. **B. Venteicher**, **C. Hall**, J. Campbell, C. Hernandez, K. Giacomini, H. Chien, C. Colas, A. Schlessinger, A.A. Thomas
- 77.** Biophysical characterization of *Burkholderia* type III secretion system minor translocon protein BipC. **M. Wilkinson**, S. Dey, S. Yadava, R. De Guzman
- 78.** Synthesis and evaluation of substituted-biaryl isothiocyanates. **C.C. Fanta**, **K.J. Tlusty**, A.L. Johnson, J.R. Mays
- 79.** Studying the binding interactions of alachlor and alachlor ESA using high performance affinity chromatography. **S. Trenhaile**, **A. Moser**

- 80.** Nanomaterial-based supports for ultra-thin layer chromatography and ellipsometry. **E. Johnson**, S. Beeram, E.L. Rodriguez, D. Peev, A. Nguyen, D.S. Hage, M. Schubert
- 81.** Role of nonpolar interactions in the recognition of highly polar histone peptides. **F. Poppinga**, D. Boamah, T. Lin, S. Basu, S. Chakravarty
- 82.** SBAP-linked bioconjugation of oligonucleotides to quantum dots. B. Eichler, **T. Hollinsworth**, **A. Kroeger**
- 83.** How halogens on azo-dyes effect solvatochromism. **P. Riegsecker**, D.J. Peitz, P.A. Karr
- 84.** Virtual screening of potential inhibitors of APOBEC3B: A promising cancer drug target. **Z.D. Smith**, E.M. Leddin, B. Miller
- 85.** Delivery of a peptide with anti-cancer activity using mesoporous silica nanoparticles. **D. Hassen**, J. Yu, T.B. Shrestha, H. Wang, D.L. Troyer, S.H. Bossmann
- 86.** Determination of electroendosmosis and electrophoresis in gel matrices for 3D printed devices. J. Lallman, R. Flaugh, **M. Kohlbek**, **K. Kounovsky-Shafer**
- 87.** Synthesis of analogues of Calcofluor White as antifungal agents. **N. Love**, D. Rane, B.R. Peterson
- 88.** Preparation of Boc-His(Bn)(Boc)-OH as its *tert*-butylamine salt. D.D. Smith, **J. Nguyen**, M.R. Hulce
- 89.** Identifying the binding location of atrazine and two of its metabolites on HSA using high performance affinity chromatography. **K. Frankenberg**, **A. Moser**
- 90.** Optimization of disulfide bond reduction for use in point-of-care microfluidic based devices with applications in early cancer diagnosis. **S. Cook**, J. Sibbitts, C.T. Culbertson
- 91.** Generation of benzyl isothiocyanate via photolysis of an *ortho*-nitrobenzyl-protected analogue. **C.W. Lang**, E. Voigt, E.H. Pauley, J.R. Mays
- 92.** Computational investigation of tryptophan dimer biosynthesis. **J. Lundervold**, J.A. Morrill
- 93.** Phenylalanine derivatives containing polar substituents as LAT1 substrates for use in drug delivery. **L. Stoner**, K. Finke, A. Anthony, J. Bauer, A. Flint, H. Chien, K. Giacomini, C. Colas, A. Schlessinger, A.A. Thomas
- 94.** Investigation of cybrid SH-SY5Y neuroblastoma cells as a model for mitochondrial contribution to cell death in Alzheimer's disease. **A. Brake**, L.A. Wetmore
- 95.** Development of microchip electrophoresis based separation sensor for analysis of catecholamine neurotransmitters in zebrafish brains. **S. Schoneich**, S. Gunawarhana UngawelDurayalage, S.M. Lunte
- 96.** Direct amide coupling to carboxylic acids using microwave techniques. **M. Brewer**, G.P. Nora
- 97.** Stability of BODIPYs towards trifluoroacetic acid: An experimental and computational study into the role of the substituents at boron. **D. Mason**, M. Wang, M.H. Vicente, P.N. Bobadova-Parvanova

- 98.** Construction of a genetic device to investigate bacterial DNA replication. **S. Anderson**, L. Rahn-Lee, L.A. Wetmore
- 99.** Computational study of (2 + 4) retro-cycloadditions of conjugated planar disilenes. P.P. Gaspar, **A. Seim**
- 100.** In silico drug design of heterocyclic cucurbitacin- inspired estrone analogs targeting EGFR in lung cancer. **T. Ostlund**, F.T. Halaweish, K. Alseud
- 101.** Synthesis and characterization of a DFDPP-CPDT polymer with ethynyl spacers by means of Sonogashira coupling. **H.P. Masching**, C. Benson, J.L. Duffy-Matzner
- 102.** Computational investigation of biflavonoid inhibitors of amyloid beta aggregation in Alzheimer's Disease. **S. Plassmeyer**, P. Windsor, D. Mattock, B. Miller, B.H. Han
- 103.** Using azide appended 2,3-naphthalimde as an approach for detection of H₂S. A. Ahmad, **H. Cao**
- 104.** Novel ethynyl-halo-hydroxyisoxazolines synthesis and investigation as potential antimicrobial agents. **K.G. Stevens**, C. Jensen, J.L. Duffy-Matzner
- 105.** Synthesis of water soluble rylene derivatives for sensor applications. **E.C. Olson**, C.H. Battle
- 106.** Detection and quantification of *N*-acyl-L-homoserine lactones from *Vibrio Harveyi* culture. **M.R. Wood**, T. Vasicek, K. Alkhatib, A. Diaz-Perez, P. Pysz, J.A. Stenken
- 107.** In silico drug design of Curcurbitacins Inspired Estrone Analogs (CIEA) targeting Small Cell Lung Carcinoma (SCLC). **Z. Khan**, F.T. Halaweish
- 108.** Determination of lambda DNA concentration in 3D printed devices. **C. Masters**, J. Dolphin, A. Maschmann, K. Kounovsky-Shafer
- 109.** Thiol modulation: Activity profiling of sulfur containing covalent modifiers and known drugs. **C. Clay**, J. Jun, S. Iqbal, P.R. Hanson

KS Union
Ballroom

Undergraduate Symposium

Financially supported by Deciphera Pharmaceuticals, LLC
D. A. Vartia, *Organizer*

10:10 - 12:10

- 110.** Catalytic activity of *bis*(2-pyridylmethyl)amine complexes containing coupled pendant arms in ATRA reactions. **J.M. Peterson**, K.D. Oshin
- 111.** Computational studies on the electrochemical reduction of CO₂ on Cu_xNi_y (x = 0-4; y = 4-x) clusters. **T. Creason**, A.Z. Clayborne

- 112.** Development of a microbial transformations research project for the organic chemistry laboratory curriculum. **A. Cribb**, C. Hillebrand, J.L. Torres Y Torres
- 113.** Structural and functional characterization of a *Yersinia pestis* opine dehydrogenase involved in metallophore biosynthesis. **C.L. Davis**, A.L. Lamb, J.S. McFarlane
- 114.** Computational investigation of the aggregation of asphaltenes with various solvents and aggregation inhibitors. **B. Lawson**, K.L. Humphries, J.D. Bickel, B. Miller
- 115.** Utilizing *tris*(2-pyridylmethyl)proazaphosphatrane complexes as catalysts in ATRA reactions. **K.L. Sandquist**, K.D. Oshin
- 116.** Probing electron delocalization in low-valent organometallic platforms featuring the isocyanide junction unit via a new ^{13}C NMR approach. **Z.A. Wood**, M.D. Hart, M.V. Barybin
- 117.** Synthesis, characterization, and catalytic activity of hollow Mn_3O_4 nanoparticles for cyclohexene oxidation. **C.M. Karki**, J.D. Hoefelmeyer
- 118.** Isolation of trace impurities in Antarctic ice for the purpose of analyzing "Old Faithful". **L. Dirks**, J. Cole-Dai, K.M. Peterson
- 119.** Selenium sorption to hematite at elevated temperature. **J. Dunn-Wall**, C. Freemyer, A. Miller
- 120.** Fluorescent detection of the post-translational modification of PvdJ module 2 in *Pseudomonas aeruginosa*. **K. Brewer**, T.A. Ronnebaum, A. Chilton, A.L. Lamb
- 121.** Photon detection for precision laser spectroscopy. **C. Kujawa**, S. Pineda, A. Klose
- 122.** Non-resonant two-photon excitation of phototriggers. **E. Lorenzo**, S. Senadheera, A.L. Houk, R.S. Givens, C.G. Elles
- 123.** Manipulation of femtosecond laser processed aluminum-1100 surface wetting behavior *via* coating by silanes with long-chain alkyl or fluoroalkyl substituents. **A. Tanbouza-Husseini**, K.R. Everitt, S.A. Darveau, C.L. Exstrom
- 124.** Calculating activation rate constant values (k_{act}) in ATRA reactions utilizing modified *tris*(2-pyridylmethyl)amine (TPMA) based complexes. **I.J. Bazley**, K.D. Oshin
- 125.** Chemobrain in zebrafish: Neurochemical assessments and evaluation of potential therapeutic treatments. **J. Loomis**, T. Field, C. Stucky, M. Shin, M.A. Johnson
- 126.** Investigating peptide selectivity and affinity to metal ions: Developing qualitative assays of peptide-metal ion interactions using metal ion dependent dyes and cellulose membranes. **M. Guile**, C. Obinwa, K. Yoshimatsu
- 127.** Computational analysis of the anti-cancer drug cisplatin with the *Thermus thermophilus* ribosome. **J.D. Bickel**, B. Miller
- 128.** Mechanism elucidation of gold-catalyzed three-component reactions forming furans. **M.J. Bakker**, M.R. Siebert

- 129.** Isolation and characterization of a manganese(III) intermediate. **E.G. Stewart-Jones**
- 130.** Enhancement of the hydrogen atom abstraction ability of $[\text{Mn}^{\text{III}}(\text{OH})(\text{dpaq})]^+$ by the addition of a redox inactive Lewis acid. **A.M. Donovan**, D. Rice, T.A. Jackson
- 131.** Detection of anti-staphylococcal activity by utilizing copper-dependent inhibitors with an extended thiourea group. **F. Rahman**, A.P. Malalasekera, A. Delpe Acharige, M. Kalubowilage, A.G. Dalecki, K.R. Schaaf, O. Kutsch, F. Wolschendorf, S.H. Bossmann
- 132.** Cobalt(II) metal ion complexes of tapa with exogenous anionic ligands bound in the H-Bonding pocket. N. Stumme, N. Sedore, K. Chabal, C. Milius, A. Ellern, D. Swenson, **M. Zart**
- 133.** Effects of acid catalysts on the preparation of ambient-dried titania aerogels. **L.M. Hansen**, S.A. Darveau, **C.L. Exstrom**
- 134.** Syntheses and crystal structures of lanthanide dithiooxamide complexes. **A. Bohanon**, E.M. Villa
- 135.** Removal of alkaline earth metals from produced brine using poly-acrylic acid. **E. Albertson**, K. Shafer-Peltier, S. Randtke, E.F. Peltier
- 136.** Photochromic switching in the plasmonic field of gold nanoparticles. **W. Harmon**, C.J. Otolski, C.G. Elles
- 137.** Investigating the use of CYCLAM derivatives as catalysts for ATRA reactions. **C.J. LeWarne**, K.D. Oshin
- 138.** Exploring actinide chemistry in environmentally relevant systems: Th(IV), U(VI), & Np(IV,V,VI) bound by macrocyclic ligands. **A. Blanes**, E. Cole, M.C. Basile, T. Forbes
- 139.** Tuning the reactivity of Mn(III)-hydroxo model complexes via ligand substitution. **A.D. Burr**, G.B. Wijeratne, T.A. Jackson
- 140.** Reaction dynamics of the $\text{TeMo}_6\text{O}_{24}^{6-}$ ion in water. **G. Kuhl**, E.M. Villa
- 141.** Supercell crystal structure of $\text{Na}_2\text{Ga}_2(\text{BO}_3)_2\text{O}$. **G. Brown**, R. Smith
- 142.** Facile one-pot synthesis of WSe_2 nanoparticles from the reaction between diphenyl diselenide and tungsten hexacarbonyl. **J.R. Blum**, W.M. Colling, S.A. Darveau, C.L. Exstrom
- 143.** An investigation of biaxial and uniaxial strain-induced effects in smectic and nematic liquid crystals. **K. Kurtenbach**, M. Sadati
- 144.** Effects of surface capping and pH on seeded growth. **M.M. Scanlan**, A.N. Chen, S.E. Skrabalak
- 145.** Role of transition metal linkers in germanium cluster assemblies. **D.D. Nguyen**, A. Schnepf, A.Z. Clayborne
- 146.** Fabrication of WSe_2 thin films *via* a mild-temperature selenization of chemical bath-deposited tungsten oxide. **M.E. Falconer**, S.A. Darveau, C.L. Exstrom

147. Rotational analysis of the $\beta\ ^2\Delta_i - X\ ^2\Pi_i$ transition of CuO using Intracavity Laser Spectroscopy (ILS). J. Harms, **T. Nair, R. Russell**, L.C. O'Brien, J.J. O'Brien

148. Syntheses and crystal structures of lanthanide periodate compounds. **R. Colin**, E.M. Villa

149. Calibration of dye laser using laser absorption spectroscopy of iodine. **S. Pineda**, C. Kujawa

150. Effects of silica aerogel embedment on the wetting properties of femtosecond laser processed aluminum 1100 surfaces. **K.R. Everitt**, A. Tanbouza-Husseini, S.A. Darveau, C.L. Exstrom, E. Peng, J.E. Shield, G. Gogos, R. Bell, C.A. Zuhlke, D.R. Alexander

151. Characterization of dentin slices and monitoring their remineralization by AFM-IR and nano-indentation. **A. VanLaecken**, G. Sereda, J. Turner

152. Uniquely engineered doxorubicin-based pH responsive polymeric drug delivery device against breast cancer. **C. Crane**, T. Nguyen, C. Ferrel, S. Aryal

153. Chemistry of tungsten-selenium nanocrystalline product formation from a mild-temperature reaction between tungsten hexacarbonyl and selenium. **W.M. Colling**, J.R. Blum, S.A. Darveau, C.L. Exstrom

154. Characterization of metal-doped amorphous silica clusters via DFT simulations of py-FTIR. **H. Leblanc**, A. Jystad, M. Caricato

155. Examination of the effect of different mole ratios of internally mixed sodium chloride-alanine aerosols on their hygroscopic properties. **M. Alfarra**, D. Woods, S. Gottuso, J.P. Darr

THURSDAY AFTERNOON

KS Union
Malott

Catalysts and Catalytic Technologies for Fuels, Chemicals, & the Environment

Cosponsored by ENFL

J. J. Bravo-Suarez, *Organizer, Presiding*

12:30 Introductory Remarks.

12:35 156. Molecular and microkinetic modeling in catalysis. **L. Arnadottir**

1:05 157. Density functional theory and kinetic modeling for rational catalyst design. **B. Liu, M. Zhou**

1:20 158. Theoretical characterization of metal-doped amorphous silicates. A. Jystad, H. Leblanc, A. Biancardi, **M. Caricato**

1:35 159. Using density functional theory calculations to determine Brønsted site acidity in zeolite. **M. Zeets, B. Wang**

1:50 160. Investigation acidity inside pores of SBA 15 via single molecule spectroscopy. J. Xie, **J. Xu, H. Wang, K.L. Hohn**

2:05 Intermission.

2:20 161. Catalysis for sustainable chemistry: Process development and catalyst characterization. **A. Allgeier**

2:50 162. Vapor phase ring rearrangement of furanic species over TiO₂ supported catalysts. **L.V. Herrera, S. Crossley**

3:05 163. Facet effect of ceria nanostructures on catalytic generation of hydroxyl radicals. **T.J. Fisher, C.L. Cheung, N. Shao, W. Mei, R. Sabirianov, N. Al-Aqtash, K. Tarawneh**

3:20 164. Nanostructured electrocatalysts for hydrogen and oxygen evolution reactions. **R. Gupta**

3:35 165. New process to synthesize Rh₂S₃ precursor for Rh_xS_y catalyst by Na₂S and pretreated carbon for HER/HOR in HBr solution. **Y. Li, T.V. Nguyen**

KS Union
Alderson

From Molecules to Nanomaterials: Applications in Energy & Catalysis

Cosponsored by COLL and INOR

C. L. Berrie, J. D. Blakemore, *Organizers, Presiding*

12:30 166. Artificial photosynthesis: Light capture, charge separation, and fuel production. G. Mohandass, Y. Jang, M. Kincaid, C. Obondi, S. Yellappa, **F. D'Souza**

1:00 167. Effects of an unconjugated bipyridine ligand on H₂ evolution with organometallic rhodium complexes. **D. Lionetti**, V.W. Day, J.D. Blakemore

1:20 168. Vertically aligned carbon nanofibers with ultra-low platinum loading for oxygen reduction reaction. **A. Elangovan**, J. Li

1:40 Intermission.

1:50 169. Bubble residence during water splitting reactions at structured semiconductor-electrocatalyst interfaces. **R. Coridan**

2:20 170. Multifunctional metal-organic framework materials for applications in asymmetric catalysis. **T. Gadzikwa**, K.P. Samarakoon, C.S. Satterfield

2:40 171. Supramolecular chemistry of phytate, *myo*-inositol hexakisphosphate. **E. Haque**, V.W. Day, K. Bowman-James

3:00 172. Local hybrid perovskite photophysics. **M.K. Kuno**

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KS Union
Big 12

Midwest ACS Graduate Awards Symposium

Financially supported by Wakarusa Valley ACS Local Section
M. A. Witek, *Organizer, Presiding*

12:30 Introductory Remarks & the Award Ceremony.

12:40 173. Beyond the diffraction limit: Super high resolution using microlens based nanoscopy. **R. Balaraman**, J. Sharma, A. Pond, C. Zhou, P. Kohli

1:00 174. Shape memory superelastic poly(isocyanurate-urethane) aerogels (PIR-PUR) for deployable panels and biomimetic applications. **S. Donthula**, C. Mandal, T. Leventis, J. Schisler, M. Adnan Saeed, C. Sotiriou-Leventis, N. Leventis

1:20 175. First symmetric π -conjugated molecular linker asymmetrically anchored with isocyanide and thiolate junctions. **J. Applegate**, N.R. Erickson, N. Gerasimchuk, M.V. Barybin

1:40 176. Design and synthesis of a series of bidentate ligands for coordinating with Re (I) and Ru (II) metal centers as dyes for harvesting sunlight. **V. KomReddy**, D.P. Rillema

2:00 Intermission.

2:10 177. Mechanistic study of dye-decolorizing peroxidase from *Enterobacter lignolyticus* using kinetic isotope and viscosity effects. **R. Shrestha**, G. Huang, D.A. Meekins, B.V. Geisbrecht, P. Li

2:30 178. Characterization of LiZnP nanoparticles by advanced solid-state NMR spectroscopy. **A. Venkatesh**, M.A. White, J. Vela , A.J. Rossini

2:50 179. Synthesis and biological activity of siderophores from human pathogenic *A. baumannii*. **T. Bohac**, J.A. Shapiro, T.A. Wencewicz

3:10 180. Withdrawn

KS Union
Centennial

Organic & Medicinal Chemistry

R. A. Altman, H. Malinakova, *Organizers*
J. D. Weaver, *Presiding*

12:30 181. Stereoselective syntheses of allenols and alkenols by 1,2-, 1,4- double hydride reductions of 3-alkynyl- and 3-alkenyl-2-cycloalkenones. **M.R. Hulce**, B.L. Callahan

12:50 182. Synthesis and evaluation of oxygen analogues of a promising anticancer drug. **R.A. Bunce**

1:10 183. Iterative photocatalytic C—H functionalization: Rapid and programmable access to oligoarenes. A. Arora, **J.D. Weaver**

1:30 184. Extension of the cavitand-mediation photocycloaddition approach: Interplay of weak interactions on the 2+2 photocycloaddition of substituted cinnamic acids. **M. Pattabiraman**, T. Bokoskie, N. Vuong, A. Kashyap

1:50 Intermission.

2:05 185. Ring-degenerate rearrangements of 1-substituted-4-imino-1,2,3-triazoles. J. Christensen, M.D. Hanson, R.K. Zawistowski, **J.T. Fletcher**

2:25 186. Fluorescent logic gates as multi-input chemical sensors for neuronal imaging. L. Zhang, K.S. Hettie, J.L. Klockow, C. Yin, **T.E. Glass**

2:45 187. Withdrawn

KS Union
Kansas

Spectroscopy Applied to Structure, Dynamics, & Imaging

Cosponsored by PHYS

C. G. Elles, C. K. Johnson, *Organizers, Presiding*

12:30 188. Surface plasmon coupled emission Raman spectroscopy measurements of the chemical composition and thickness of thin films. **E.A. Smith**, C. Nyamekye, S. Weibel, J.M. Bobbitt

1:00 189. Extended photoluminescence lifetimes in optically enhanced CdTe/CdS QWs. **W.M. Sanderson**, F. Wang, W.E. Buhro, R.A. Loomis

1:20 190. Charge transfer exciton and spin flipping at organic-TMD interfaces. **T.R. Kafle**, B. Kattel, T. Wang, W. Chan

1:40 191. Temperature effect on bulk and thin film ionic liquids examined using vibrational spectroscopy and calorimetry. **J. Wrona**, S.K. Shaw

2:00 Intermission.

2:20 192. Towards super-resolution ultrafast Raman imaging. **R.R. Frontiera**

2:50 193. Assignment of excited-state vibrational spectra from resonance-enhanced femtosecond stimulated Raman scattering: Combining experiment and theory. **M.S. Barclay**, T.J. Quincy, C.G. Elles, M. Caricato

3:10 194. Probing higher-lying electronic states via mode-specific enhancement of excited-state resonance Raman spectra. **T. Quincy**, M. Barclay, M. Caricato, C.G. Elles

KS Union
Jayhawk

Theory of Interfaces

B. B. Laird, W. H. Thompson, *Organizers*
K. R. Mitchell-Koch, *Presiding*

12:30 195. Rich phase behavior of confined water: Nano ice, nano bubble, low-density and high-density liquid water. **X.C. Zeng**

1:10 196. Morphometric thermodynamics in 2D: Comparing theory to simulation. **S. Martin**, B.B. Laird

1:30 Intermission.

1:50 197. The role of substrate structure on heterogeneous nucleation. **J.P. Palafox - Hernandez**, B.B. Laird

2:30 198. Structure of the Al-Ga solid-liquid interface. **P.R. Barry**, J. Kern, B.B. Laird

2:50 199. Understanding the wetting behavior of octane-water-silica systems using Monte Carlo simulation. W. Guo, **J. Errington**

KS Union
Ballroom

Organic & Medicinal Chemistry

R. A. Altman, H. Malinakova, *Organizers*

1:00 - 3:00

200. Synthetic lethal targeting of growth factor receptors. **K. Knewtson**, C. Perera, M.M. Lee, D. Hymel, B.R. Peterson

201. New approach to disable resistance in MRSA. **C.V. Rice**, M. Foxley, S.N. Wright, A.K. Lam

202. Magnetic resonance characterization of peritoneal mesothelioma, psuedomyxoma peritonei and cirrhosis ascites. **M.R. Hulce**, B.W. Loggie, G.K. Sirineni, P. Thomas

203. Synthesis and characterization of Chitosan derivatives for high performance gene delivery. **Q. Wyatt**, A.M. McMullen, L. Kwok, R.S. Herati

204. Synthesis of functionalized bile acid macrocycles towards the construction of steroid-based molecular cages. **C.A. Knudtson**, J.R. Dias

205. Cell permeable dibenzothiophene based fluorescent dye and O^{3P}) generators. **J.T. Petroff**, R.D. McCulla

206. Multi-antigen I-domain conjugates against antigenic spreading in animal models for multiple sclerosis. **M.G. Moral**, P. Kiptoo, T.J. Siahaan

207. Synthesis of small molecules to understand the mechanism of methylation of 2'-deoxyuridine-5'-monophosphate byin flavin-dependent thymidylate synthase. **D. Mondal**, J. Yao, A. Kohen

208. Restoring susceptibility to methicillin-resistant *Staphylococcus epidermidis*. **A.K. Lam**, M. Foxley, C.V. Rice

209. Conjugate addition of N-acetylcysteine to bisphenol A-3,4-quinone. D.E. Stack, **B. Mahmud**

210. Concept of copper-activatable drugs. **T. Shrestha**, A. Delpe Acharige, M. Kalubowilage, F. Wolschendorf, S.H. Bossmann

- 211.** Diastereoselective 7-*exo-trig* nucleophilic cycloaddition of tethered alkoxides to cyclopropenes *en route* to homochiral medium ring scaffold with anti-mycobacterial activity. **V. Maslivetc**, A. Philippova, M. Rubina, M.A. Rubin
- 212.** Synthesis and efficacy evaluation of naphthalimide intercalating agents. **R. Oelrich, M. Schneider, Y. Salha**, M.A. Lewis
- 213.** Design and synthesis of novel OSW-1 scaffolds as precision cancer therapeutic agents. **C.A. Malinky, A.T. Le, S. Sakers, G. Nguyen, G. Manginelli, A.W. Burgett**
- 214.** Synthesis of five-membered SHetA2 Flex-Het analogues for preventing human ovarian cancer. **D. Bryant, D. Berlin, R.A. Bunce**
- 215.** Applications of the radical-polar crossover reaction to medicinal chemistry. **S. Cullen, G.K. Friestad**
- 216.** Modular total synthesis of salvinorin A inspired designer opioids. A. Sherwood, **S. Williamson, R. Crowley, T.E. Prisinzano**
- 217.** Design, synthesis and biological study of hybrid drug candidates of nitric oxide releasing cucurbitacin-inspired estrone analogs for treatment of hepatocellular carcinoma. **M.A. Abousalim, M.A. Shaaban, M.K. Abd El Hamid, Y.A. Elshaier, M.H. Abdelrahman, F.T. Halawehish**
- 218.** Design, synthesis and characterization of 1-(2-((4-(4-methoxyphenyl)-2,2-dimethyl-3-phenylchroman-7-yl)oxy)ethyl)pyrrolidine (JAK15) analogs for treatment of ovarian cancer. **J. Apraku, C.C. Subhash, F.T. Halawehish**
- 219.** Development of novel electrophilic probes for chemical biology: Synthesis and reactivity profiling studies using ¹⁹F NMR. **J. Jun, A. Cassity, J.S. Jha, C. Clay, P.R. Hanson**
- 220.** Modular synthesis and reactivity profiling studies of diverse and stereochemically enriched *C*-, *S*-, and *P*-based electrophilic macrocycles. **G.C. Dissanayake, S. Javed, D. Vithanage, A. Ganguly, P.R. Hanson**
- 221.** Novel tetramic acid analogs: Synthesis and reactivity profiling of cysteine-reactive β -keto-vinyl sultams. **J.S. Jha, J. Jun, P.R. Hanson**
- 222.** Design, synthesis and reactivity profiling of cysteine-reactive electrophilic acyl sultams. **S. Iqbal, M.A. Khan, Q. Zang, C. Clay, E. Gao, J. Loh, N. Asad, P.R. Hanson**
- 223.** Study of epimetalated intermediates towards functional group transformations of *pi*-bonded organic compounds. **J. Gitua**
- 224.** Synthesis of vinyl cyclopropanes via anion relay cyclization. **K.M. Allegre, N. Brennan, J.A. Tunge**
- 225.** Radical [1,3] rearrangements of Breslow intermediates. **H. Wallace**
- 226.** Stereospecific decarboxylative benzylation of enolates: Scope, application, and mechanistic insights. T. Li, **M.L. Maliszewski, J.A. Tunge**
- 227.** Mechanism for the formation of benzo[e]-1,3-oxazin-4-ones from reactions of salicylic acids and anilines with HATU. **D. Leas, J. Wu, Y. Dong, J.L. Vennerstrom**

- 228.** Benzo[*b*]naphtho[2,1-*d*]selenophene-*Se*-oxide, Benzo[*b*]naphtho[1,2-*d*]selenophene-*Se*-oxide as potential triplet atomic oxygen precursors. **S.M. Chintala**, R.D. McCulla
- 229.** Synthesis of 5-amino-2-sulfonamido-thiazole-4-carboxylic acids using microwave techniques. **G.P. Nora**
- 230.** Directed nucleophilic addition of phenoxides to cyclopropenes. **P. Yamanushkin**, M. Lu-Diaz, A. Edwards, M. Rubina, M.A. Rubin
- 231.** Developing methods for diversifying molecular scaffolds directly on a microelectrode array. K.D. Moeller, **N. Yeh**
- 232.** Study on the compatibility of manganese-mediated radical addition reaction with aromatic heterocycles. **M. Li**, L. Goff, G.K. Friestad
- 233.** Scope of the electrophilic groups for cyclization in the type-II Mn-mediated radical-polar crossover annulation. **R.L. Hein**, G.K. Friestad
- 234.** Novel triazole-containing tricyclic sultams: Intramolecular C–H functionalization of triazoles to generate a small molecule library. **V.U. Thomas**, M.A. Khan, Q. Zang, E. Gao, P.R. Hanson
- 235.** An efficient synthesis of *P*-sterogenic mono-, bi- and tricyclic *P*-heterocycles via one-pot sequential enyne ring-closing metathesis/Diels-Alder protocol. **D.A. Vithanage**, S. Javed, A. Ganguly, G.C. Dissanayake, P.R. Hanson
- 236.** Diastereoselective six- and seven-membered ring closure *via* intramolecular nucleophilic attack by nitrogen ylides on C=C bond of cyclopropenes. **V. Maslivetc**, A. Maslivetc, M. Rubina, M.A. Rubin
- 237.** Exploring reactivity of N-heterocyclic carbenes (NHCs). **H. Palencia**, I. Monreal-Leyva, L. Berdugo
- 238.** Synthesis of oxacycles via reaction of stabilized carbanions with peroxides. **A. Horn**, P.H. Dussault
- 239.** Efficient synthesis of substituted 1*H*-indazoles. **J. Annor-Gyamfi**, R.A. Bunce
- 240.** Practical and scalable total syntheses of complex benzannulated indole natural products via indole aryne cycloaddition methodologies. Total synthesis of the trikentrins and herbindoles. Z. Albader, M. Rayhart, O. Talavera, **K.R. Buszek**
- 241.** Synthesis, characterization, and catalytic activity of chiral covalent organic frameworks. **A. Volkov**, L.M. Stanley
- 242.** Synthesis and biological screening of cucurbitacin-inspired estrone analogues targeting JAK/STAT3 pathway in pancreatic cancer. **K. Alseud**, F.T. Halaweish
- 243.** Intramolecular C–H functionalization via *C*-vinylation: Synthesis of structurally unique triazole-fused vinyl sultams. **A. Cassity**, J. Jun, N.M. Windmon, N. Asad, A. Diepenbrock, P.R. Hanson, K. Jeon
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KS Union
Woodruff

Midwest Plenary Symposium

Financially supported by St. Louis Local Section

J. A. Heppert, *Organizer*

T. E. Prisinzano, *Presiding*

3:45 244. Can ionic liquids be disruptive enough to save the world? **R.D. Rogers**

4:35 Intermission.

4:40 245. From molecular dating to functional materials. **C.B. Aakeroy**

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FRIDAY MORNING

KS Union
Ballroom

Biochemistry

H. R. Desaire, J. Slusky, *Organizers*

8:00 - 10:00

- 246.** Perturbing the BfrB:Bfd interaction of *Pseudomonas aeruginosa* by chemical and genetic intervention causes irreversible accumulation of iron in BfrB. **A. Punchi Hewage**, H. Yao, B. Nammalwar, K.K. Gnanasekaran, S. Lovell, R.A. Bunce, J. Chandler, M.E. Rivera
- 247.** Determination of the interaction of the transmembrane helices of IpaB in micelles by EPR Spectroscopy. **A. Chakravarty**, R. N De Guzman
- 248.** Identification of novel inhibitors of multidrug resistance protein 1 (MRP1). **A. Sampson**, K.W. Tan, B.G. Peterson, S.H. Iram
- 249.** Dynamic ligand-dependent FRET changes of 2-color Multidrug resistance protein-1 biosensor. **B. Osa-Andrews**, K.W. Tan, S.H. Iram
- 250.** Cellular effects of ligand binding to the oxysterol-binding protein family (OSBP/ORP4). **B. Roberts**, Z.C. Severance, R. Bensen, N.R. Kothapalli, J.I. Nunez, M. Hongyan, S. Wu, A.W. Burgett
- 251.** Neuroprotective properties of Ascorbic Acid against N-substituted derivative of Parkinsonian toxin 1-methyl-4-phenylpyridinium (MPP+). **B. Lickteig**, D. Murphy
- 252.** Solving the MSTery: Determining the Chemical Mechanism of Lyase Activity. **C. Shelton**
- 253.** Interactions between the CS and cytochrome b5 reductase domains of human Ncb5or revealed by X-ray crystallography. **D.R. Benson**, S. Lovell, N. Mehzabeen, K.P. Battaile, H. Zhu
- 254.** Effects of macromolecular crowding and lipid composition on CYP2J2 stability and substrate metabolism. **H. Huff**, A. Das
- 255.** *Pa*-Bfd (*Pseudomonas aeruginosa*-bacterioferritin associated ferredoxin) fold is stabilized by a phosphate ion. **H.N. Wijerathne**, H. Yao, S. Lovell, M.E. Rivera
- 256.** Biosynthesis of opine metallophores by bacterial pathogens. **J.S. McFarlane**, C.L. Davis, A.L. Lamb
- 257.** Importance of the C-terminus of ALDH7A1 for catalytic activity and oligomerization. **J.W. Wyatt**, D.A. Korasick, A.R. Laciak, K.S. Gates, J. Tanner
- 258.** Cloning of a periplasmic serine endoprotease of *Escherichia coli*. **N. Mikita**

- 259.** PvdF as potential novel transformylase from *Pseudomonas aeruginosa*. **N. Kenjic**, A.L. Lamb
- 260.** EPR reveals different conformations of *Yersinia* LcrG and *Pseudomonas* PcrG proteins. **P. Guha Biswas**, P. Kaur, K. Kaur, A. McShan, S. Tachiyama, L. Song, R. De Guzman
- 261.** 3D reconstruction of tetanus neurotoxin using negative stain electron microscopy and electron tomography. **P. O'Neil**, A. Machen, M.T. Fisher
- 262.** Mutagenesis study on bio-orthogonal protein-peptide isopeptide bond forming systems. **S.P. Kasson**, K. Yoshimatsu
- 263.** Withdrawn
- 264.** Study of anti-proliferative activity of cucurbitacins inspired esterione analogs on hepatocellular carcinoma. **S. Elgazwi**, F.T. Halaweish, M. Mahnashi
- 265.** Investigation on innate and adaptive immune response of Macrophage. **S. Jo**
- 266.** G-quadruplex driven self-assembly of DNA origami dimer. **S. Yang**, W. Liu, R. Wang
- 267.** Small molecules binding to *Shigella* Type III Secretion System (T3SS) tip protein IpaD. **S. Dey**, A. Anbanandam, B. Mumford, R. De Guzman
- 268.** 2-alkyl-4-quinolones of *Pseudomonas aeruginosa* as iron chelators in bacterial iron homeostasis. **T. Pahattuge**, T. Williams, J. Chandler, M.E. Rivera
- 269.** Investigating “stuffed” domains of NRPS assembly lines: PchF and PchE of pyochelin biosynthesis. **T.A. Ronnebaum**, G.P. Horsman, S.J. Booker, T.E. Prisinzano, A.L. Lamb
- 270.** Myopalladin's role in cardiac muscle function and disease. **V.K. Kadarla**, M. Beck, M.L. Bang
- 271.** Synthesis of (5-oxo-2-dibenzothienylmethyl)triphenylphosphonium and its localization in mitochondria to study oxidative stress. **A. Isor**, R.D. McCulla
- 272.** Towards synthetic cell surface receptors that control signal transduction. **Y. Yin**, C. Perera, D. Hymel, B.R. Peterson
- 273.** Synthetic mimics of cytochrome b5 as cell surface receptors. **A. Andres**, B.R. Peterson
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Chemical Biology of Microbial Processes

M. E. Rivera, *Organizer*

A. L. Lamb, *Presiding*

8:00 274. Chemical biology of bacterial nanoinjectors. **R. De Guzman**

8:35 275. Functional models of chromosomal ParDE toxin-antitoxin systems. **C. Bourne**

9:10 276. Using biolayer interferometry to assess the kinetic stability of bacterial toxins for accelerated drug discovery. **M.T. Fisher**

9:45 Intermission.

10:05 277. Iron-clad strategies of microbial growth: chemical biology of siderophores. **A. Butler**, Z. Reitz, G. Maier, K. Dulaney

10:40 278. Developing microdialysis sampling as an in situ analysis tool for quorum sensing from biofilms. **J.A. Stenken**

11:15 279. Copper-activated drugs to maximize the effects of nutritional immunity. **S.H. Bossmann**, F. Wolschendorf

KS Union
Ballroom

Chemical Education

J. E. Headrick, *Organizer*

8:00 - 10:00

280. Developing teaching modules that incorporate next generation science standards in the secondary science curriculum. **N. Jackson**, B.D. Hidaka, C.G. Elles

281. Addressing retention of general chemistry students via a new supplemental problem solving course: CHE 198 at Missouri Western State University. **S.L. Hiley**, M.W. Ducey, D. Stasko

282. Withdrawn

283. VIVED Chemistry, a new interactive, educational, 3D platform for educators and students to enhance learning chemistry. **A.M. Cannon**, J. Kersten, W. Baltz, Y.A. Letuchy, A. Patrick

284. Student produced videos for teaching. **J.C. Easdon**

- 285.** Instrumental analysis project that teaches aspects of liquid chromatography. **J. Hahn**, D.W. Harak
- 286.** Electrocatalysis projects for the undergraduate instrumental analysis laboratory. **T.P. Ratz**, D.W. Harak
- 287.** Drafting and using a novel standard exam to measure how students apply chemistry to biology. **D. Morrone**
- 288.** Safety considerations when designing a new chemical engineering research laboratory. **W.J. Gilbert**, M. Shiflett
- 289.** ACS Division of Small Chemical Businesses (SCHB): Opportunities and benefits. **J.E. Sabol**
- 290.** Calculation of wavefunctions made easy. **J.R. Dias**
-

KS Union
English

Chemical Education

J. E. Headrick, *Organizer*
A. A. Vartia, *Presiding*

8:00 291. Ad astra per exceLCA: Chemical accounting for the undergraduate researcher. **J.R. Silverman**, B. Subramaniam

8:20 292. Lab for the pack: Redesigning first semester general chemistry lab for the students we have. **B.M. Neal**, D.J. Styers-Barnett, A.R. Cutler, L.A. Bolyard

8:40 293. Revolutionizing undergraduate labs with benchtop NMR: An active learning approach. **M.T. Zamora**, J.F. Araneda, S.D. Riegel

9:00 294. Incorporating an interdisciplinary course-based undergraduate research experience into an introductory organic and biochemistry lab course. **M.J. Harvey**

9:20 Intermission.

9:35 295. Professionalism in chemistry II. **S. Gamagedara**

9:55 296. Flipping an organic chemistry class. **M.A. Lewis**

10:15 297. New organic chemistry reaction simulation that allows students to simultaneously view the 2D scheme and 3D animation of reactions. **A.M. Cannon**, J. Kersten, W. Baltz, Y.A. Letuchy, A. Patric

From Molecules to Nanomaterials: Applications in Energy & Catalysis

Cosponsored by COLL and INOR

C. L. Berrie, J. D. Blakemore, *Organizers, Presiding*

8:00 298. X-ray transient absorption spectroscopy. **L.X. Chen**

8:30 299. Fabrication of micro and nano sized metal structures on Si (111) and Mica substrates: An Atomic Force Microscope (AFM) and Particle Lithography (PL) approach. **S.B. Ulapane**, A.K. Borkowski, M.K. Okeowo, J. Tottleben Doolin, C.L. Berrie

8:50 300. Electrochromic diisocyanide-terminated bi- and terazulenic platforms chemically accessible with three different molecular charges. **N.R. Erickson**, A.D. Spaeth, D.M. McGinnis, M.V. Barybin

9:10 Intermission.

9:20 301. Promoting adsorption of non-thiolated molecules to gold nanostars. **A.J. Haes**, W. Xi, H.T. Phan, G. Lu

9:50 302. Design of ultrasmall intermetallic compound nanoparticles for electrocatalysis. **Z. Qi**, C. Xiao, T. Goh, Y. Pei, W. Huang

10:10 303. Synthesis of highly dispersed and highly stable supported Au-Pt bimetallic catalysts by a two-step method. **X. Wang**, X. Liang

10:30 Intermission.

10:40 304. Size-selective catalysts with an ultra-thin porous shell prepared by molecular layer deposition. **Z. Shang**, X. Liang

11:00 305. Breaking the intrinsic limits of electrode materials in electrical energy storage using a hierarchical core-shell structure. **J. Li**, J.E. Brown, G.P. Pandey, S. Klankowski, J. Acharya, J. Wu

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Inorganic Chemistry

J. D. Blakemore, *Organizer*
D. Lionetti, *Presiding*

8:00 Introductory Remarks.

8:15 306. Hydrogen atom transfer reactivity by a series of N5-ligated oxomanganese (IV) complexes. **A.A. Massie, D. Rice, T.A. Jackson**

8:30 307. Oxygen-exchange kinetics of the Anderson-type polyoxometalate ion $\text{IMo}_6\text{O}_{24}^{5-}$. **M. Spriet, E.M. Villa**

8:45 308. Theoretical investigation into the reaction landscape of hydrogen atom abstraction by a $\text{Mn}^{\text{IV}}(\text{O})$ complex. **D. Rice, A.A. Massie, T.A. Jackson**

9:00 309. Distinguishing between homogeneous and heterogeneous hydrogen-evolution electrocatalysis with a quartz crystal microbalance. **D.J. Sconyers, J.D. Blakemore**

9:15 Intermission.

9:30 310. Synthesis and characterization of $(\text{Cp}^*\text{H})\text{Rh}(\text{diimine})$ complexes. **Y. Peng, D. Lionetti, J.D. Blakemore**

9:45 311. Multielectron processes in a rhodium bipyridine complex relevant to hydrogen fuel production. **W. Moore, W. Henke, K. Prather, J.D. Blakemore**

10:00 312. d-Electron count, ion-pairing and diagonal twist angles in metallo-bis(dithiolene) complexes. **C.C. Kirkpatrick, J.N. Truong, B.A. Kowert**

10:15 Intermission.

10:30 313. Highly stable two and three lithium insertion in conformal amorphous V_2O_5 shells electrodeposited on electrospun carbon nanofiber network as a flexible lithium ion battery cathode. **J.E. Brown**

10:45 314. Varied extended singlet excited state lifetime via excimer formation as a MOF topology-dependent function. **J. Yu, P. Deria**

11:00 315. Quantitative control of metal doping in TiO_2 nanocrystals. **S. Mia, S. Varapragasam, C. Balasanthiran, J.D. Hoefelmeyer**

11:15 316. Ag-TiO₂ hybrid nanoparticles as active photocatalyst for hydrogen evolution. **S. Varapragasam, S. Mia, C. Balasanthiran, J.D. Hoefelmeyer**

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Materials Chemistry

F. Tao, *Organizer, Presiding*

8:00 317. Crystal engineering of energetic materials: Co-crystals of tetrazole based explosives with modified performance. **J.C. Gamekkanda**, C.B. Aakeroy, A. Sinha

8:20 318. Study of microwave effect on synthesis of hyperbranched CdS_{1-x}Se_x supra quantum dots. **M. Yazdanparast**, E.J. McLaurin

8:40 319. Physical and chemical applications of photodoping in electrodeposited cuprous oxide thin films. **R. Coridan**, J.M. Lowe

9:00 320. Significance of inserting an oxidative ring-fusion aromatization step at the early stages of pyrolytic carbonization of polybenzoxazines and other phenolic resins. **H. Majedifar**, S. Donthula, S. Mahadik, T. Yazdeli, M. Adnan Saeed, N. Leventis, C. Sotiriou-Leventis

9:20 321. Synthesis and first MRI results of mesoporous silica-stabilized very small iron oxide contrast agents. **J. Covarrubias**, H. Wang, T.B. Shrestha, D.L. Troyer, S.H. Bossmann

9:40 Intermission.

9:50 322. Scalable synthesis of block functionalized carbon nanotubes. **L. Barrett**, B.P. Grady, S. Crossley

10:10 323. Withdrawn

10:30 324. Solid-state landscape of a class of activated halogen bond donors. **B. Sandhu**, A. Sinha, C.B. Aakeroy

10:50 325. Dynamic crosslinks through the reversible thia-Michael addition reaction. **P. Getty**, K. Greenman, S.J. Rowan

11:10 326. Synthetic strategies for versatile functionalization of cavitands. **N. Sarkar**, C.B. Aakeroy, A. Sinha

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Organic & Medicinal Chemistry

R. A. Altman, H. Malinakova, *Organizers*
J. L. Markley, *Presiding*

8:00 327. Synthesis of dibenzothiophene sulfoxide derivatives and their potential for site-selective oxidation of nucleic acids. **J.C. Throgmorton**, A. Eischen, L. Zhong, D.A. Baum, R.D. McCulla

8:20 328. Synthesis of endophenazines and analogues and their antimicrobial evaluation. **K. Maddeboina**, N. Rodrigues de Almeida, V.R. Udumula, M.M. Conda-Sheridan

8:40 329. Synthesis of fluorescently labelled analogs of cyclophostin and cyclipostin. **G.R. Gnawali**, B. Martin, C.D. Spilling

9:00 330. Synthesis and evaluation of tricyclic pyrone derivatives for the treatment of Alzheimer's disease. **M. Zhang**, I. Maezawa, B. Zou, S. Weerasekara, B. Hao, M.L. Weber, W.S. Cao, C. Pascual, X.S. Xie, L. Jin, D.H. Hua

9:20 331. Development of pot-economical strategies for the synthesis of (-)-13-Desmethyl-lyngbouilloside and novel electrophilic macrocycles. **A. Ganguly**, S. Javed, G.C. Dissanayake, D. Vithanage, P.R. Hanson

9:40 Intermission.

9:50 332. Syntheses of substituted 6-(Dimethylamino)-2-phenylisoindolin-1-ones for the inhibition of luciferase. M.J. Gunaratna, M. Nakagomi, A. Ito, B. Hao, **K. Apley**, D.H. Hua

10:10 333. Synthesis of 1,3-anti diol containing bioactive natural products and analogs via modular, pot-economical and library amenable protocols. **S. Javed**, A. Ganguly, G.C. Dissanayake, D. Vithanage, P.R. Hanson

10:30 334. Synthesis of phostone and furanose phosphonates. **R.R. Paudel**, J.N. Ridenour, S. Dawadi, C.D. Spilling

10:50 335. One-pot sequential strategies for the synthesis of polyol fragments: Applications in natural product synthesis. **C.N. Ndi**, P.R. Hanson

11:10 336. Stream-lined synthesis of 3-Hydroxy- β -lactams: Norrish-Yang type II photocyclizations of β -ketoformamides. **J.L. Markley**, T. Morse, N.P. Rath, T.A. Wencewicz

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Organic Synthesis & Catalysis

M. D. Clift, *Organizer*

J. A. Tunge, *Organizer, Presiding*

8:00 337. Highly selective preparation of heteroleptic Zn(II)-methylene bis(imidazoline) complexes through a chirality driven self-assembly, and its applications toward building multi-functional dendrimer catalysts. **S.A. Moteki**

8:30 338. Intra- and intermolecular functionalization of alkenes via transition metal-catalyzed activation of amide C-N bonds. **L.M. Stanley**

9:00 339. Direct functionalization of alcohols using cobalt photocatalysis. **D.B. Martin**, D. Chambers, E. Sodagar

9:30 340. Progress toward a tunable terpenoid synthesis strategy. **A.J. Grenning**

10:00 341. Cofactors as a source of inspiration for discovering new modes of catalytic activation. **M.D. Clift**

10:30 342. Stereoselective strategies for the synthesis of chiral amines with imine and enamine umpolung reagents. **S. Malcolmson**, K. Li, P. Daniel, X. Shao, A. Weber, L. Tseng

11:00 343. New methods for chemical screening library construction and applications: Overcoming complex barrier. **R. Rafferty**

KS Union
Divine 9

Physical Chemistry

M. Caricato, *Organizer*

X. Chen, *Presiding*

8:00 344. Diffusion of benzene and alkylbenzenes in nonpolar solvents. **B.A. Kowert**

8:30 345. Real-time TDDFT investigation of plasmon resonances in gold nanowires. **R.D. Senanayake**, D. Lingerfelt, X. Li, C.M. Aikens

8:45 346. Enhancing the sensitivity of solid-state NMR for characterization of organolead halide perovskites. **M. Hanrahan**, L. Men, B. Rosales, J. Vela , A.J. Rossini

9:00 Intermission.

9:15 347. Electronic coupling for donor-bridge-acceptor systems with a bridge-overlap approach: A benchmark study. **A. Biancardi**, M. Caricato

9:35 348. Graphene field effect transistors as a high-throughput platform for measuring exciton dissociation dynamics at organic interfaces. **B. Kattel**, T. Kafle, L. Qin, W. Chan

9:50 349. Residue based contributions to the thermodynamic properties of ubiquitin. **N. Kariyawasam Manachchige**, E.A. Ploetz, P.E. Smith

10:05 Intermission.

10:20 350. Cu-oxo complexes supported in MOR zeolites as active sites for methane-to-methanol conversion. **J. Xu**, B. Liu

10:35 351. Investigation of solvation effects on optical rotatory dispersion using the polarizable continuum model. **T. Aharon**, P. Lemler, P.H. Vaccaro, M. Caricato

10:50 352. Ultrafast relaxation dynamics of *trans*-stilbene derivatives in confined organic capsules. **C.J. Otolski**, A.M. Raj, V. Ramamurthy, C.G. Elles

KS Union
Malott

Theory of Interfaces

B. B. Laird, W. H. Thompson, *Organizers*
J. P. Palafox - Hernandez, *Presiding*

8:00 353. Surface potentials, surface spectroscopy, and solvation: A theoretical perspective. **C.J. Mundy**, M.D. Baer

8:40 354. Understanding liquid structure and dynamics near amorphous SiO₂ through simulations of sum frequency generation spectra. **P.N. Wimalasiri**, P.C. Burris, J. Harvey, W.H. Thompson

9:00 Intermission.

9:15 355. Heterogeneous hydration dynamics around *Candida Antarctica* lipase B: Relationships with protein dynamics and water structure. J.N. Dahanayake, **K.R. Mitchell-Koch**

9:55 356. Atomistic insights into nitrogen-cycle electrochemistry: NO electrochemical reduction on Pt surfaces from first principles calculations. H. Chun, **A.Z. Clayborne**, V. Apaja, K. Honkala, J.P. Greeley

10:15 Intermission.

10:30 357. Accelerated nucleation and polymorph selection with trace additives: theory and simulation. **B. Peters**

11:10 358. Removing the barrier to the calculation of activation energies and volumes: Diffusion and reorientation in water. **E.A. Piskulich**, O. Mesele, W.H. Thompson

Spectroscopy Applied to Structure, Dynamics, & Imaging

C. G. Elles, C. K. Johnson, *Organizers, Presiding*

8:10 359. Resolving interfacial protein dynamics by Super Temporal-Resolved Microscopy (STReM). **C.F. Landes**

8:40 360. *In Situ* biomolecular structural elucidation by super-resolution microscopy with single particle averaging. **J. Unruh**

9:10 361. Methods of analyzing sparse data sets from time-correlated, single-photon counting experiments: Application of the maximum likelihood and related methods to mixtures of rose bengal and rhodamine B. **K. Santra**, E.A. Smith, J.W. Petrich, X. Song

9:30 Intermission.

9:50 362. Oscillatory enzyme dynamics and their role in enzyme-catalyzed reactions. **C.M. Cheatum**

10:20 363. Split-GFP assay to survey proteins, interactions, and dynamics of the inner nuclear envelope in live cells. **B.D. Slaughter**

10:50 364. Spectroscopic imaging studies of micropolarity in plasmid DNA using a solvatochromic dye and chemically graded surfaces. **Z. Li**, R. Kumarasinghe, D.A. Higgins

11:10 365. Energy landscape of the FMO antenna from *C. tepidum* and its L122Q and Y16F mutants: Low temperature high resolution spectroscopic and modeling studies. **A. Khmelnitskiy**, R. Saer, R.E. Blankenship, R. Jankowiak

Analytical Chemistry

Y. Zeng, *Organizer*

10:10 - 12:10

- 366.** Development and validation of high performance liquid chromatography method for quantitative determination of 4-hydroxybenzoate and related renal cell carcinoma biomarkers in human urine. **S. Gamagedara**, T. An-Yen, K.S. Dahal, N.T. Perera, B.K. Lavine
- 367.** Development of a hydrogen exchange-mass spectrometry method to predict aggregation propensity of protein therapeutics. **J.P. Rincon**, G. Meric, C. Calero-Rubio, C. O'Brien, H. Shahfar, A.S. Robinson, C.J. Roberts, D.D. Weis
- 368.** Rapid prediction of deamidation rates of proteins to assess their long-term stability using hydrogen exchange mass spectrometry (HX-MS). **C.L. Demalgiriya Gamage**, D.D. Weis
- 369.** Sparse representation for hydrogen exchange mass spectrometry (HX-MS) data by using LASSO optimization. **Y. Shi**, D.D. Weis
- 370.** Hydrogen exchange mass spectrometry can reliably detect small fractions of destabilized protein in comparability studies. **T. Hageman**, J. Arora, D.D. Weis
- 371.** Identification of individual phenolic metabolites in American elderberry pomace extract utilizing high performance liquid chromatography tandem mass spectrometry. **R. Krueger**, A.L. Thomas, C.M. Greenlief
- 372.** High-throughput microfluidic separation of plasma from whole blood for downstream biomarker detection. **E.M. Mohr**, C. Campos, S.A. Soper
- 373.** Microfluidic affinity purification of cancer-specific extracellular vesicles. **J.M. Jackson**, M.A. Witek, S. Pullagurla, D. Park, K. Herrera, M. Murphy, S.A. Soper
- 374.** Label-free enumeration of Circulating Tumor Cells (CTCs) using μ -Coulter counter. **C. Kong**, M. Hu, M.L. Hupert, S.A. Soper
- 375.** Nano-coulter counter for the quantification of extracellular vesicles. **J.D. Conner**, S. Pullagurla, B. Gross, S.A. Soper
- 376.** Evaluation of minimal residual disease in acute leukemia using microfluidics and spectral time-delayed integration multi-parameter flow cytometry. **W. Hu**, M. Jackson, M.A. Witek, S.A. Soper
- 377.** Automated sealing system for digitalizing multiplexed biomarkers in femtoliter compartments. **D. Lella**, Y. Zeng
- 378.** Microfluidic-based exponential rolling circle amplification for exosomal microRNA detection. **H. Cao**, Y. Zeng

379. Connecting land use and water quality: Agricultural and restored prairie outputs. **A. Miller**, A. Dere, C. Jackson

380. Detection of metal ions by organic dyes on paper-based analytical devices. **K. Yoshimatsu**

381. Fabrication of polymer microneedle implants using an atomized spray process for controlled drug delivery. **M. Kim**, S. Choi

382. Analysis of drug-protein interactions during diabetes by high-performance affinity chromatography. **P. Tao**, Z. Li, R.E. Matsuda, D.S. Hage

383. Analysis of free drug fractions by high performance affinity chromatography: Interactions of sulfonylurea drugs with human serum albumin. **B. Yang**, X. Zheng, D.S. Hage

384. Controlled drug release from solution blow spun core-shell nanofibers with blended shell. **S. Park**, S. Choi

385. Soxhlet extraction of avocado endocarp and trituration of avocado mesocarp for biodiesel production. **A.J. Cruz**, D. Kostner, I. Oraemesi, B. Maricle

386. Nanoscale solid-phase enzymatic reactor for biopolymer (DNA/RNA) disassembly. **U.S. Athapattu**, S.A. Soper

387. Nanoparticle composition and reactivity contribute to the bacterial toxicity of nanoscale metal phosphates. **P.L. Clement**, J.E. Kuether, J.R. Borgatta, T.A. Qiu, V. Feng, R.J. Hamers, C.L. Haynes

388. Ligands binded paramagnetic nanoparticles applied in enzyme activity studies. **S. Jia**, C.T. Culbertson

389. Vapor phase plotting of organotrichlorosilane sub-monolayer gradients. **J. Bautista**, J. Austin, A. Forzano, M.M. Collinson, D.A. Higgins

390. Hydrogen peroxide detection in chemotherapy treated wistar rats. **K.J. Garcia**, R. Gehringer, A.I. Bandara, M.A. Johnson

391. Evaluation of cyclic olefin copolymer as a new material for fabrication of microchip electrophoresis devices for online monitoring of amino acids in brain dialysate. **G.A. Bulgakova**, N.J. Oborny, S.M. Lunte

392. Comparison of CE-UV and CE-MS as analysis methods for dynorphin peptides. **E.A. Kurfman**, A.M. Al-Hossaini, M.B. Wijesinghe, S.M. Lunte

393. Entrapment of proteins in high-performance affinity columns for chromatographic studies of solute-protein interactions. **S. Poddar**, E.L. Rodriguez, S. Azaria, D.S. Hage

394. On-column preconcentration of adenine nucleotides for analysis of brain tissues by CE. **E. Buyuktuncel**, S. Gunawarhana UngawelDurayalage, S.M. Lunte

395. Single-cell analysis of nitric oxide production in stimulated RAW 264.7 macrophages by microchip electrophoresis coupled with laser Induced fluorescence detection. **J. Sibbitts**, D.E. Patabadige, C.T. Culbertson

- 396.** Simultaneous detection and quantification of nitric oxide and superoxide using microchip electrophoresis coupled with laser-induced fluorescence. **D.B. Weerasekara**, G. Caruso, C. Fresta, J. Siegel, M.B. Wijesinghe, S.M. Lunte
- 397.** Single-molecule tracking studies of charge-dependent translational and orientational dye motions within surfactant- and solvent-filled silica mesopores. **R. Kumarasinghe**, D.A. Higgins, T. Ito
- 398.** Impact of perturbing the BfrB:Bfd interaction on *Pseudomonas aeruginosa* biofilms. **A. Soldano**, M.E. Rivera
- 399.** Thermal characterization of lignin residue after high-temperature hydrotreatment. **R. Roy**, D.E. Raynie
- 400.** Depolymerization of alkali lignin in the presence of subcritical water and Ni-G catalyst. **B. Jadhav**, D.E. Raynie
- 401.** Thermoplastic nanofluidic sensor for the fluorescence detection of chemotherapeutically induced damage in genomic Dna. **S. Vaidyanathan**, K. Weerakoon-Ratnayake, S.A. Soper, D. Kaufman
- 402.** Microfluidic platform for isolation of extracellular vesicles: Potential stroke biomarkers. **S. Pullagurla**, M.A. Witek, J.M. Jackson, A. Baird, S.A. Soper
- 403.** Effective identification of benzaldehyde product in oxidation reactions using Co(II)/TEMPO Catalytic system. B. Sweetman, L. Handin, **Y. Liu**
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FRIDAY AFTERNOON

KS Union
Alderson

Analytical Applications of Microfluidics

Cosponsored by ANYL

Financially supported by Center for Molecular Analysis of Disease Pathways; Adams Institute for Bioanalytical Chemistry

S. M. Lunte, *Organizer, Presiding*

12:30 Introductory Remarks.

12:35 404. Using microchip electrophoresis and electrochemical detection to investigate cellular communication. **R.S. Martin**

1:15 405. Microfluidic paper-based analytical devices for forensic applications. T. Cardoso, P. Garcia, R. Channon, J. Adkins, C. Henry, **W. Coltro**

1:55 406. Enhancing the information content of single cell analysis on microfluidic devices using optical fiber bridge. **C.T. Culbertson**, J. Sibitts

2:35 Intermission.

2:45 407. Expanding the paper-microfluidics toolbox. **E. Verpoorte**, G.I. Salentijn, N.N. Hamidon, Y. Hong

3:25 408. Microfluidics for isolation of orthogonal populations of circulating tumor cells. **M.A. Witek**

4:05 Concluding Remarks.

KS Union
Big 12

Chemical Biology of Microbial Processes

M. E. Rivera, *Organizer*
R. De Guzman, *Presiding*

12:30 409. Biliverdin IX β a signaling molecule for extracellular heme uptake by the opportunistic pathogen *Pseudomonas aeruginosa*. **A. Wilks**

1:05 410. Biosynthetic mechanisms for antibiotics from the emerging biocontrol agents *Lysobacter*. **L. Du**

1:40 411. Using archaea for what they do best: Redirecting carbon and energy towards isoprene as an anaerobic respiration/fermentation product. J. Aldridge, S. Carr, K.A. Weber, **N.R. Buan**

2:15 Intermission.

2:35 412. Unraveling the MSTery. **A.L. Lamb**

3:10 413. Mechanistic insights into bacterial dye-decolorizing peroxidases. **P. Li**, R. Shrestha, G. Huang, B.V. Geisbrecht

3:45 414. Inhibiting the bacterioferritin (BfrB):bacterioferritin associated ferredoxin (Bfd) interaction in *P. aeruginosa* causes iron homeostasis dysregulation. **M.E. Rivera**, H. Yao, A. Punchi Hewage, A. Soldano, S. Lovell

KS Union
Jayhawk

Inorganic Chemistry

J. D. Blakemore, *Organizer, Presiding*

12:30 Introductory Remarks.

12:45 415. Preparation of transition metal cluster complexes containing NHC ligands. **L.F. Szczepura**, W. Wilson, D.N. Huh

1:00 416. Assembly and characterization of heterobimetallic complexes of nickel with trivalent redox-inactive cations. **A. Kumar**, J.D. Blakemore

1:15 417. Structural landscape assessment: N-heterocycle containing tritopic acceptors. **S.N. Andree**, A. Sinha, M. Dakovic, C.B. Aakeroy

1:30 418. Halide-bridged coordination polymers from mono-picolyli biimidazoles and cadmium(II). **C.A. Gunawardana**, A. Sinha, C.B. Aakeroy

1:45 Intermission.

2:00 419. Assessing the chemical variations in thorium, uranium, and neptunium bonding reactivity through macrocyclic ligand encapsulation. **M.C. Basile**, E. Cole, A. Blanes, T. Forbes

2:15 420. Surface immobilization of molecular complexes of the f-elements. **K.J. Cannon**, D. Lionetti, J.D. Blakemore

2:30 421. O-O bond activation by a series of Mn complexes supported by amide-containing ligands. **J. Parham**, T.A. Jackson

2:45 422. Photodecomposition mechanisms of manganese tricarbonyl complexes. **W.C. Henke**, C.J. Otolski, W. Moore, K.V. Prather, C.G. Elles, J.D. Blakemore

3:00 Intermission.

3:15 423. Noncovalent immobilization of a manganese electrocatalyst for CO₂ reduction. **K. Prather**, J.D. Blakemore

3:30 424. Morphology inheritance from hollow metal-organic frameworks to hollow carbon polyherons in preparing electrocatalysts. **Y. Pei**, Z. Qi, W. Huang

3:45 425. Development of new media for electrochemical CO₂ conversion. **T. Kerr**, C. Shaughnessy, H. Lee, D.J. Sconyers, B. Subramaniam, K.C. Leonard, J.D. Blakemore

KS Union
Pine

Materials Chemistry

F. Tao, *Organizer, Presiding*

12:30 426. Sorption kinetics and structural features of water confined in a 1-D metal organic nanotube. **T. Forbes**, J. Leddy

12:50 427. Positron interactions with asymmetric materials. **J. Van Horn**, Y. Jean

1:10 428. Electrode wettability influences on the deep discharge capacity of Li–O₂ batteries. **F. Wang**, X. Li

1:30 429. Organometallic self-assembled monolayer films of linear azulenic and biazulenic p-linkers featuring asymmetric anchoring. **M.K. Okeowo**, J. Applegate, C.L. Berrie, M.V. Barybin

1:50 430. Epitaxial lift-off of electrodeposited single-crystal gold foils for flexible electronics. **N. Mahenderkar**, Q. Chen, Y. Liu, A.R. Duchild, S. Hofheins, E. Chason, J.A. Switzer

2:10 Intermission.

2:20 431. Molecular structure of silicon nanocrystal surfaces characterized by multidimensional solid-state NMR spectroscopy. **M. Hanrahan**, E. Fought, T.L. Windus, L. Wheeler, N. Anderson, N.R. Neale, A.J. Rossini

2:40 432. Study of soy protein isolate as a functional modifier for polymer materials. **Z. Zheng**, B. Li

3:00 433. Characterization of energy-rich hydrochars from microwave-assisted hydrothermal carbonization of coconut shell. **S. Elaigwu**, G. Greenway

3:20 434. K-Index: a quantitative tool that describes complex soft-matter nanomorphology and correlates it to synthetic conditions. **T. Yazdelli**, S. Donthula, C. Sotiriou-Leventis, N. Leventis

3:40 435. Fighting the world's most dangerous villain: Multidrug resistant bacteria. **L. Chlebanowski**, O. Covarrubias-Zambrano, S. Barrett, D.L. Troyer, F. Wolschendorf, S.H. Bossmann

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KS Union
Kansas

New Directions in Chemistry Education

D. D. Weis, *Organizer, Presiding*

12:30 Introductory Remarks.

12:35 436. Ripped from the headlines: Analytical chemistry in the news. **C.T. Culbertson**

1:05 437. Preliminary investigation of students' beliefs about their academic ability and how those beliefs affect performance. **L.M. Wojcinski**

1:35 438. Enhancing learning by assessing process skills in STEM courses. **R.S. Cole, J. Lantz, S.M. Ruder, J.A. Schmidt-McCormack, G. Reynders**

2:05 Intermission.

2:15 439. Infusing systems thinking in the general chemistry curriculum. **T. Holme**

2:45 440. Leveraging the Learner-Centered Teaching rubric to characterize instructional practices in undergraduate chemistry courses. **M.N. Stains, Z. Nelson, R.M. Erdmann**

3:15 441. Promoting change where change is hard: Tales of a teaching postdoc. **A.A. Vartia**

3:45 Discussion.

3:55 Concluding Remarks.

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Organic & Medicinal Chemistry

H. Malinakova, *Organizer*
R. A. Altman, *Organizer, Presiding*

12:30 442. Resorufamines as fluorescent probes of the endoplasmic reticulum. **S. Phaniraj**, Z. Gao, D. Rane, B.R. Peterson

12:50 443. Liquid biopsy for early stage pancreatic cancer detection. **O. Covarrubias-Zambrano**, M. Kalubowilage, A.P. Malalasekera, D.N. Udukala, H. Wang, S.O. Wendel, D.L. Troyer, S.H. Bossmann

1:10 444. Pacific blue-taxoids: New fluorescent probes of the anticancer properties of taxol. **Z. Gao**, M. Lee, B.R. Peterson

1:30 445. Nanobiosensor for the arginase detection. **M. Kalubowilage**, A.P. Malalasekera, O. Covarrubias-Zambrano, F. Rahman, H. Wang, D.L. Troyer, S.H. Bossmann

1:50 446. Molecular modeling of membrane glucose transporter (GLUT1) as target for anticancer drugs. **S. Almamoud**, X. Wang, J.L. Vennerstrom, H.A. Zhong

2:10 Intermission.

2:20 447. Peptide-nanosponges for advanced drug delivery. **A.S. Yapa**, M. Kalubowilage, H. Wang, P. Thapa, T.B. Shrestha, J. Yu, O. Covarrubias-Zambrano, M. Pyle, D.L. Troyer, S.H. Bossmann

2:40 448. Design, synthesis and antimicrobial properties of self-assembled cationic amphiphilic peptides. **N. Rodrigues de Almeida**, M. Samad, M.M. Conda-Sheridan

3:00 449. Developing potent and broad spectrum analogues of the antimicrobial peptide Citropin 1.1. **M. Samad**, M. Conda-Sheridan

3:20 450. Synthesis of novel copper-activatable drugs against MRSA. **A. Delpe Acharige**, T. Shrestha, M. Zhang, A.P. Malalasekera, H. Wang, M. Kalubowilage, F. Wolschendorf, S.H. Bossmann

3:40 451. Preparation and characterization of family of charged ammonium pocket with para-substituted multi-functional receptors that target to anionic phospholipid found in bacterial membrane. **M. Alsuri**

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Physical Chemistry

M. Caricato, *Organizer*

12:30 - 2:30

452. Electronic structure, geometric properties, and catalytic performance of the multishell Au-nanoparticle $\text{Au}_{70}\text{S}_{20}[\text{P}(\text{Ph}_3)]_{12}$. **A. Frojd**, S. Kenzler, H. Hakkinen, A. Schnepf, A.Z. Clayborne

453. Infrared studies of crystalline thiocyanate hydrates: Evidence of solid phase simultaneous vibrational transitions. **H.R. Krueger**

454. Measurement of one-bond $^1\text{H}-^{17}\text{O}$ scalar couplings in organic solids and inorganic materials. **S.L. Carnahan**, B. Lampkin, P. Naik, M. Hanrahan, I.I. Slowing, B. VanVeller, A.J. Rossini

455. Vapor-liquid equilibria: Ammonia and 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide. **T. Turnaoglu**, M. Shiflett

456. Clathrate hydrate formation using fluorocarbons. **A. Rocha**, M. Shiflett

457. Simulations of ammonia adsorption for the characterization of acid sites in metal-doped amorphous silicates. **A. Jystad**, A. Biancardi, M. Caricato

458. Structure determination of boron carbide thin films using solid state NMR spectroscopy. **A. Alnafisah**, N.A. Oyler, T. Nguyen, M. Paquette

459. Analysis of the effect of glycine on the hygroscopic properties of sodium chloride aerosols. **D. Birge**, S. Gottuso, A. Kanley, J.P. Darr

460. Electronic properties of [n]cyclacene series versus Möbius[n]cyclacene series. **J.R. Dias**

461. Solubility of vinyl fluoride in aqueous lithium bis(trifluoromethylsulfonyl)imide solutions. **D.L. Minnick**, W.J. Gilbert, A. Rocha, M. Shiflett

462. Understanding catalytic bifunctionality of Cu/ZSM5 and Cu/Y zeolites for biomass conversions. **J. Xu**, Q. Zheng, K.L. Hohn, B. Liu

463. Computational studies of $\text{Si}_3\text{N}_3\text{H}_x$ ($x = 0 - 9$) clusters. **K. Suh**, G. Guirgis, C. Metz, A.Z. Clayborne

464. Infrared spectra of phosphoenolpyruvate in aqueous solutions: Vibrational frequency shifts of functional groups due to presence of metal ions. **R.E. Brenner**, C.J. Wurrey, A. Fenton

465. Ultrafast interlayer electron transfer in incommensurate transition metal dichalcogenide homobilayers. **Y. Li**, Q. Cui, F. Ceballos, S. Lane, Z. Qi, H. Zhao

466. Characterizing the structural overpotentials induced by bubble evolution during water electrolysis on spatially-distributed electrocatalyst-semiconductor interfaces. **Z. Schichtl**, R. Coridan

- 467.** Carrier dynamics in phosphorene and multilayer black phosphorous. **P. Zereshki**, F. Ceballos, M. Bellus, S. Pan, H. Zhao
- 468.** Using bulk-heterojunction and selective electron trapping to enhance the responsivity of perovskite-graphene photodetector. **L. Qin**, B. Kattel, W. Chan
- 469.** Understanding the dynamics of the resorcin[4]arene hexameric supramolecular assembly. **A. Katiyar**, W.H. Thompson
- 470.** Modeling the permeation of aromatic dipeptides across lipid bilayers. **B. Lee**, K. Kuczera
- 471.** Stability of gold thiolate and gold chloride nanoclusters. **G. Kuda Singappulige**, C.M. Aikens
- 472.** Disrupting protein-protein interactions to modulate the integrity of the blood brain barrier. **J. He**, T.J. Siahaan, K. Kuczera
- 473.** Electron and nuclear dynamics in $[Au_{24}Ag(SH)_{18}]^{-1}$ and $[Au_{13}Ag_{12}(SH)_{18}]^{-1}$ nanoparticles. **P. Pandeya**, C.M. Aikens
- 474.** Measuring accurate absolute Two-Photon Absorption cross sections using stimulated Raman scattering as an internal standard. **D.A. Stierwalt**, A.L. Houk, C.G. Elles
- 475.** Computational study of the interactions of hydrogen peroxide and water with reduced ceria surfaces. N. Shao, N. Al-Aqtash, K. Tarawneh, **C.L. Cheung**, W. Mei, R. Sabirianov
- 476.** Novel reaction cell design for simultaneous in situ diffuse reflectance UV-visible and FTIR spectroscopies: Application to CO oxidation on gold catalysts. **P.D. Srinivasan**, J.J. Bravo-Suarez
- 477.** Cavity-mediated catalysis via metal-organic supercontainers. **Z. Wang**, Y. Qiao, P. Jampani

KS Union
Malott

Physical Chemistry

M. Caricato, *Organizer*
B. A. Kowert, *Presiding*

12:30 478. Hydrogenated TiO₂ nanomaterials for microwave absorption. **X. Chen**

1:00 479. Exploiting CO₂-expanded liquids in hydroformylation: A molecular simulation approach. **C.H. Mendis**, J.P. Palafox - Hernandez, B.B. Laird, W.H. Thompson

1:15 480. Reanalysis of the $a\ ^4\Sigma^- - X\ ^2\Pi_{1/2}$ transition of GeH using intracavity laser spectroscopy. J. Harms, **L.C. O'Brien**, J.J. O'Brien

1:30 Intermission.

1:45 481. Evaluating cations' competitive interactions with water-soluble anionic polyelectrolytes using an ion exchange model. **M. Chen**, K. Shafer-Peltier, E.S. Albertson, S. Randtke, E.F. Peltier

2:05 482. An EOM-CCSD-PCM benchmark for electronic excitation energies of solvated molecules. **S. Ren**, M. Caricato

2:20 483. Development of gold nanostructures using AFM based nanopatterning of self-assembled monolayers on silicon to study gold binding peptide tagged proteins. **N.J. Kamathewatta**, D.O. Deay, M.L. Richter, C.L. Berrie

2:35 484. Phase equilibria, transport properties, and structure of CO₂-expanded ethylene oxide and methanol. **E.A. Piskulich**, B.B. Laird, W.H. Thompson

2:50 Intermission.

3:05 485. Effects of water and pH on electrocatalytic conversion of carbon dioxide in ionic liquid media. **A. Hailu**, S.K. Shaw

3:20 486. Electronic coupling in diazulenic molecular rectifiers: A theoretical approach. **T.C. Balduf**, A. Biancardi, M. Caricato

3:35 487. Positron interactions with natural and synthetic chiral quartz crystals in non-z orientations. **F. Wu**, J. Van Horn, Y. Jean

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J. A. Tunge, *Organizer*

M. D. Clift, *Organizer, Presiding*

1:00 488. Development of a long term manufacturing route to HCV NS5b inhibitor, MK-3682. **J. Limanto**

1:30 489. Inter- and intramolecular aryl insertion reactions of borylnitrenes. **F.J. Williams**

2:00 490. Radical chemistry of the Breslow intermediate. **M. McIntosh**

2:30 491. New approaches to allylic fluorination and radiofluorination. **H.M. Nguyen**

3:00 492. Take a CA_HB direct to chiral boronic esters, but don't interrupt? **J.M. Takacs**

3:30 493. Stereoselective synthesis of saturated heterocycles via copper-catalyzed alkene difunctionalizations. **S.R. Chemler**

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Inorganic Chemistry

J. D. Blakemore, *Organizer*

2:40 - 4:40

494. Nano-particles for water treatment synthesized from conjugated linoleic acid (CLA). **M. Chen**, C.T. Jafvert

495. Early detection of non-small-lung cancer in liquid biopsies by ultrasensitive protease-activity analysis. **M. Kalubowilage**, D.N. Udukala, A.P. Malalasekera, S.O. Wendel, H. Wang, A.S. Yapa, D.L. Troyer, S.H. Bossmann

496. Benzalkonium-derived Mesoporous Silica Nanoparticles Against *Micrococcus luteus*. **S. Barrett**, L. Chlebanowski, O. Covarrubias-Zambrano, D.L. Troyer, S.H. Bossmann

497. Catalyst for conversion of methyl ethyl ketone to butenes. **Z. Alauda**, H. Alatabi, Q. Zheng, K.L. Hohn

498. Simultaneous upgrading of furanics and phenolics via hydroxyalkylation/aldol condensation reactions. **T.V. Bui**, T. Sooknoi, D. Resasco

499. Synthesis of novel rhenium selenide clusters containing isonitrile ligands. **C.P. Chin**, W. Wilson, D.N. Huh, L.F. Szczepura

500. Photopatterned noble metal functional surfaces via galvanic replacement reactions on Cu₂O thin films. **J.M. Lowe**, R. Coridan

501. Hierarchical nano-on-microsized copper crystals on nickel foam for highly efficient electro-oxidation of hydrazine. **X. Yan**, Y. Liu, K. Scheel, Y. Li, Y. Yu, X. Yang, Z. Peng

502. Supramolecular and coordination chemistry: search for new classes of carboxamide pincers. **S. Pramanik**, S. Kaur, V.W. Day, K. Bowman-James

503. Preparation and investigation of the pKa of [Mn^{II}(H₂O)(dpaq^{2Me})]⁺ and the characterization of a one electron oxidized version of [Mn^{III}(OH)(dpaq^{2Me})]⁺. **A.A. Munasinghe**, J. Parham, D. Rice, T.A. Jackson

504. Investigation of bis(μ-oxo)dimanganese(III,IV) and oxomanganese(IV) complexes: Comparison of structure and reactivity. **Y. Lee**, A.A. Massie, T.A. Jackson

505. Bidentate ligands modulate hydrogen generation by [Cp^{*}Rh] complexes. **E.A. Boyd**, K. Prather, D. Lionetti, J.D. Blakemore

506. Investigation of actinide reactivity by synthesis with crown ethers. **E. Cole**, M.C. Basile, A. Blanes, T. Forbes

Materials Chemistry

F. Tao, *Organizer*

2:40 - 4:40

- 507.** Binder free approach to synthesize nanostructured nickel compounds for energy storage applications. **N. Albeladi, C. Zhang, S.D. Bhoyate, K.S. Siam, P.K. Kahol, R. Gupta**
- 508.** Tea leaves derived carbon for high temperature energy storage devices. **S.D. Bhoyate, C. Ranaweera, C. Zhang, M. Hyatt, P.K. Kahol, R. Gupta**
- 509.** Orange peel derived highly flame retardant rigid polyurethane foam. **C. Zhang, S.D. Bhoyate, M. Ionescu, P.K. Kahol, R. Gupta**
- 510.** Hierarchically structured electrodes prepared from selective atomic layer deposition in self-assembled, composite colloidal films. **M.A. Norman, W. Perez, R. Coridan**
- 511.** Progress towards a large-scale synthesis of hollow Mn₃O₄ nanoparticles from the galvanic reaction between MnO nanocrystals and Cu²⁺. **B. Onserio, S. Varapragasam, J.D. Hoefelmeyer**
- 512.** Withdrawn
- 513.** Development of high-load, hybrid ROMP reagents and scavengers immobilized on silica and Co/C magnetic nano-particles for their application in sequestration and parallel synthesis. **S. Faisal, J. Jun, T.A. Klein, Q. Zang, P. Maity, P.C. Kearney, D. Stoianova, P.R. Hanson**
- 514.** Highly porous SiC & Si₃N₄ monoliths via carbothermal reduction of polymer-crosslinked sol-gel silica powder compacts. **P.M. Rewatkar, T. Taghvaeae, M. Adnan Saeed, S. Donthula, T. Leventis, J. Schisler, C. Sotiriou-Leventis, N. Leventis**
- 515.** Selective hydrogenation of citral over supported Pt catalysts: Insights into support effects. **X. Wang, X. Liang**
- 516.** Supported nickel nanoparticle catalysts synthesized by atomic layer deposition for dry reforming of methane. **Z. Shang, X. Liang**
- 517.** The role of surface-wettability in electrochemical reactions involving gas-phase reactants or products. **H. Mehrabi, R. Coridan**
- 518.** Electropolymerization of perfluoroalkylated thiophene- and aniline-based aromatic compounds for high-performance batteries. **E.L. Moen, J.C. Lawrence, S. Mao, J.H. Kramer, M.O. BaniKhaled, H. Sun**

519. Evaluating the functional similarity of hydrogen and halogen bonding. **A.M. Abeysekera**, C.B. Aakeroy, A. Sinha

520. SERS detection of toxins via substrates with anchored polymeric chains. **R.S. Rodriguez**, V.M. Szlag, S. Jung, S. Bryson, M. Bourgeois, G.C. Schatz, T.M. Reineke, C.L. Haynes

521. Effect of nanostructure morphology and C=charge on esterase-release of ketoprofen from supramolecular nanostructures. **V.R. Udumula**, M.M. Conda-Sheridan

522. Dielectric properties of soy protein isolate and its nanocomposites. **M. Cox**, Z. Zheng, B. Li

523. Effect of surface passivation on photothermal effect of gold nanorod. **R. Marasini**, A. Pitchaimani, T. Nguyen, S. Aryal

524. Structural reorganization of silica wet-gels upon drying: Why aerogels shrink? **C. Mandal**, S. Donthula, C. Sotiriou-Leventis, N. Leventis

525. Multiscale hierarchical nanoporous polyurethane aerogels based on α - and β -Cyclodextrin for CO₂ sequestration, water vapor uptake and cationic dye separation. **P.M. Rewatkar**, M. Adnan Saeed, S. Donthula, H. Majedifar, N. Leventis, C. Sotiriou-Leventis

526. One-step synthesis and characterization of “click-able” polymers for biomedical applications. **W. Alqahtani**, S. Santra, R.A. Gross

527. Systematic route for heterobifunctionalization of polypropylene glycol polymers and poly(propyleneglycol)-block-poly(ethyleneglycol) copolymers. **J. Blankenship**, K. Yoshimatsu

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