

Jeanette Krause and William Connick, Program Chairs

WEDNESDAY MORNING

Northern Kentucky Convention Center

Room 9

Analysis of Dietary Supplements

S. Kern, Organizer, Presiding

8:00 1. Elemental analysis and speciation of dietary supplements. **K. Kubachka**

8:25 2. Thermal profiling and in-source fragment ions for rapid characterization of supplements: Tools for using a compact DART-MS system for quality control and contamination detection. **B. Musselman**, R. Goguen, F. Li

9:10 3. Identification of a purported dietary supplement ingredient using a multi-pronged analysis approach. **V. Toomey**, A. Lanzarotta, L. Lorenz

9:35 Intermission.

10:05 4. Analysis of dietary supplements containing phosphodiesterase type-5 (PDE-5) inhibitors. **B. Hanson**, R. Flurer, S. Kern, E. Nickum, V. Toomey, S. Voelker

10:30 5. Simplifying 2D-LC, 2D-LC/MS automated workflows fast and efficient multi-dimension LC & LC/MS method development. **B. Giuffre**

11:15 6. Non-targeted mass spectrometric analysis of dietary supplements. **T. Falconer**

**Northern Kentucky Convention Center
Room 4
Assessment of Community, Environmental &
Occupational Exposures to Chemicals related to the
Unconventional Oil & Gas Industry
J. Snawder, *Organizer, Presiding***

8:00 Introductory Remarks.

8:15 7. Engaging community in air quality research near unconventional oil and gas extraction sites. **E. Haynes**, L. Kincl, D. Rohlman, B. Paulik, K.A. Anderson

8:40 8. Potential worker exposures to hydrocarbon gas and vapors when opening oil and gas production tanks. **J. Snawder**, M. Alexander-Scott, M. Breitenstein, B. Johnson, **C.A. Striley**, J. Toseski

9:05 9. Stable isotopic constraints on methane migration into groundwater and emissions to the atmosphere from unconventional natural gas extraction: Examples from Ohio, Colorado, and Texas. **A. Townsend-Small**

9:30 10. Hydrocarbon gas and vapor exposure of upstream oil and gas workers during completion and production activities and factors affecting these exposures. **M. Breitenstein**, J. Snawder, M. Alexander-Scott, B. Johnson, C.A. Striley

9:55 Intermission.

10:10 11. Assessment of oil and gas worker exposures to volatile organic compounds using evacuated glass bottle samplers with analysis by gc-time of flight mass spectroscopy. **C.A. Striley**, M. Alexander-Scott, M. Breitenstein, B. Johnson, J. Snawder

10:35 12. Rapid measurement of urinary PAH and benzene metabolites by ELISA. **D. Sammons**, J. Smith, S. Robertson, C.A. Striley, M. Alexander-Scott, J. Snawder

11:00 13. Diesel particulate matter exposures in oil and gas workers: A preliminary study. **M. Alexander-Scott**, J. Snawder, M. Breitenstein

11:25 14. Cardiovascular toxicology of particle matter collected during hydraulic fracturing. **T. Knuckles**, M. Nye, A. Dzomba, M. McCawley

Northern Kentucky Convention Center

Ballroom A

Bioinspired Chemistry

Financially supported by Procter & Gamble Company

B. Isfort, Z. Khambatta, *Organizers, Presiding*

8:00 Introductory Remarks.

8:15 15. Biomimicry: Sustainable solutions inspired by nature.
J. Lim

9:00 16. Bioinspired chemistry in the air, on land, and in the seas. **J.J. Wilker**

9:45 Intermission.

10:00 17. Animal tracks: Do living organisms leave behind chemical clues to adhesive success? **A.Y. Stark**

10:30 18. Hierarchical assembly of virus-based nanoreactors.
T. Douglas

11:00 Panel Discussion.

Northern Kentucky Convention Center
Room 2
Catalysis in Natural Product Synthesis
M. K. Brown, A. E. Mattson, *Organizers, Presiding*

8:00 19. Iron-catalyzed carbonyl olefin metathesis. **C. Schindler**

8:25 20. Chemical synthesis methods via cooperative catalysis. **T.N. Snaddon**

8:50 21. Chiral spiro-borates and chiral boroxinates in asymmetric catalysis. **W. Wulff**, Y. Zhou, A.K. Gupta, M. Mukherjee, G. Hu, L. Huang, W. Zhao, X. Yin, W. Osminski, R. Huang, Y. Dai, A.A. Desai

9:25 22. Cascade processes using N–O bond rearrangements for the synthesis of *N*-heterocycles. **L.L. Anderson**

10:00 Intermission.

10:15 23. A unified strategy to access protoilludane sesquiterpenoids through carbene catalysis. **K. Scheidt**

10:50 24. Natural Product directed lead generation: Enhancing success of early stage discovery programs in crop protection. **M.R. Loso**, V.B. Hegde, J.E. Hunter, T.C. Sparks

11:25 25. Asymmetric hydrovinylation reactions in natural product synthesis. **T. RajanBabu**

Northern Kentucky Convention Center
Ballroom E
Frontiers in Nucleic Acids Chemistry
N. Leontis, *Organizer*
R. M. Wilson, *Organizer, Presiding*

8:00 26. Oxidation of purine bases. **R.M. Wilson**

8:30 27. Early events in the photochemistry of nucleic acid bases. **C.E. Crespo-Hernández**

9:00 28. The role of the electron in radiation damage to DNA.
M.D. Sevilla, A. Kumar, A. Adhikary, L. Shamoun

9:30 29. A ROS-activated DNA damaging agent that targets leukemias. **E.J. Merino**

10:00 Intermission.

10:30 30. Watching the bypass of a major oxidative lesion by a human DNA polymerase. **Z. Suo**

11:00 31. RNA evolution in a highly oxidizing environment: The case of the mammalian mitochondrial ribosome. **P. ROY, M. Hosseini, M. Sissler, E. Westhof, N. Leontis**

11:30 32. Dynamics and mechanism of DNA-repair by photolyases. **D. Zhong**

Northern Kentucky Convention Center
Room 5
Inorganic Chemistry, Organometallics & Sensors-
Inorganic Chemistry & Sensors
J. A. Krause, *Organizer*
W. B. Connick, *Organizer, Presiding*

8:00 33. A dinuclear nickel catalyst for cycloaddition reactions: Alkyne cyclotrimerization and reductive methylene cyclopropanation. **S. Pal, C. Uyeda**

8:30 34. Cationic dirhodium(II,II) complexes as dual action electrocatalysts for H⁺ and CO₂ reduction. **S. Witt, C. Turro**

9:00 35. Development of new cobalt pincer complexes for catalytic applications. **Y. Li**

9:30 36. Compromised catalysis vs mechanistic insight: Using a sterically hindered iron catalyst to produce and characterize high-valent iron species in water and organic solvents. **M.R. Mills, A.D. Ryabov, T.J. Collins**

10:00 Intermission.

10:20 37. Colorimetric and optical sensing of anions. **A. Hossain**

10:50 38. Reconstructive 3D ToF-SIMS imaging of perovskite films in controlled D₂O humidity. **W. Lin, H. Chang, J. Shyue, C. Burda**

11:20 39. Pseudohalogen- and fluorine-based water-stable perovskite solar cells. **N. Lu, H. Kuo, J. Huang, R. Wei, C. Kung, Y. Lu**

Northern Kentucky Convention Center
Room 7
Inorganic Materials, Nanomaterials & Solid-State
Chemistry: Synthesis, Properties & Applications
J. E. Goldberger, Organizer, Presiding

8:00 40. Colloidal syntheses of anisotropic lead-salt nanostructures using chloroalkanes. **L. Sun**, Z. Jiang, S. Premathilaka, S. Chiluwal, S. Kandel, A. Antu, Y. Tang, S. Khan

8:25 41. Linking the forward and reverse vapor-liquid-solid mechanisms in metal oxide nanostructures. B.M. Hudak, L. Yu, Y. Chang, M. Park, **B.S. Guiton**

8:50 42. Halide double perovskites: A new class of compound semiconductors. **P. Woodward**, E. McClure

9:15 43. Diamond-like semiconductors: Toward improved infrared nonlinear optical materials. **J.A. Aitken**

9:40 Intermission.

10:00 44. NIR-to-visible light upconversion in lanthanide-doped alkaline-earth fluorohalide nanocrystals. K. Dissanayake, **F. Rabuffetti**

10:25 45. Tailoring magnetism and electronic transport in MPn_2Se_4 semiconductors. **P.F. Poudeu Poudeu**

10:50 46. Topochemical synthesis and properties of organic-terminated (SnR)P/As/Sb graphane derivatives. **M. Arguilla**, W.D. McCulloch, K. Krymowski, N.D. Cultrara, S. Jiang, W. Windl, Y. Wu, J.E. Goldberger

11:10 47. Hydrothermal synthesis of non-centrosymmetric lead oxide carboxylates. **C. Oertel**, N. Fellah, E. Liu, M. Zeller

11:35 48. Colloidal nitride semiconductor nanomaterials: New molecular precursors and mechanisms. Y. Chen, N.S. Karan, Z. Liu, **R. Beaulac**

Northern Kentucky Convention Center

Room 1

Mass Spec Methods for Analysis of Radioisotopes in Environmental & Nuclear Forensic Applications

Cosponsored by NUCL

J. L. Steeb, E. Widom, *Organizers, Presiding*

8:00 49. Mass spectrometry for nuclear forensics. **R.W. Williams**

9:00 50. Actinide analysis of lichen by TIMS: Identifying anthropogenic contamination in the environment. **E. Widom, K. McHugh, D. Kuentz**

9:20 51. Uranium isotope constraints on radioactive contaminant sources in tree bark. **E.R. Conte, E. Widom, D. Kuentz**

9:40 52. Uranium mobility across annual growth rings in multiple tree species. **K. McHugh, E. Widom, G. Sam**

10:00 Intermission.

10:30 53. Developing Argonne's two-parameter (non-linearity and weighted mass bias) model for high precision ICP-QMS isotope ratio measurements: Results from Inter-laboratory round robin. **J.L. Steeb, D.G. Graczyk, Y. Tsai, M. Snow, C.R. Hexel**

10:50 54. Development of a new uraninite reference material for nuclear forensic analysis at high spatial resolution. **C. Dorais, T.L. Spano, E. Balboni, A. Simonetti, A.E. Hixon, P.C. Burns**

11:10 55. Trace element signatures of uranium ore concentrates: Source attribution and proof of concept. **T.L. Spano**, E. Balboni, C. Dorais, A. Simonetti, P.C. Burns

11:30 56. High purification of Ta and W from Hf and complex matrix constituents. **M. Snow**, M.R. Finck, K.P. Carney

Northern Kentucky Convention Center

Room 6

Nanoscience & Biotechnology

Cosponsored by BIOT

L. Esfandiari, H. Kumari, *Organizers, Presiding*

8:30 57. Molecular dynamics investigation of the binding of P1 peptide and mutants on graphitic surfaces. **E. Helton**, S. Barr, G.M. Leuty, R.J. Berry

9:05 58. Degradation of 1,1,1-trichloroethane by nanoscale zero valent iron (NZVI) supported on powdered activated carbon (PAC). **M. Chowdhury**

9:40 59. Role of fiber length on phagocytosis and inflammatory response by alveolar macrophages. T. Padmore, C. Stark, **L. Turkevich**, J. Champion

10:15 Intermission.

10:30 60. Tuning of size and shape of RNA nanoparticles for applications in nanotechnology. **P. Guo**

11:05 61. Dimensional control of chemical interfaces using polymerizable amphiphiles. **S.A. Claridge**

**Northern Kentucky Convention Center
Room 10
Physical Chemistry/Computational Chemistry
W. B. Connick, J. A. Krause, *Organizers*
B. S. Ault, *Presiding***

8:30 62. Photochemistry of aqueous pyruvic acid under model atmospheric conditions. **A.J. Eugene**, S. Xia, M.I. Guzman

9:00 63. Ozonolysis of catechol at the gas-solid interface. **E.A. Pillar-Little**, M.I. Guzman

9:30 64. Reusable mineral ZnS for photocatalytic reduction of fumarate to succinate. **R. Zhou**, M.I. Guzman

10:00 Intermission.

10:15 65. Measuring thermal processes of methylammonium lead iodide ($\text{CH}_3\text{NH}_3\text{PbI}_3$) perovskite. **A. Kovalsky**, L. Wang, G. Marek, J. Dyck, C. Burda

10:45 66. Monitoring charge separation and injection processes of semiconductor perovskite thin films. **C. McCleese**, L. Wang, Y. Zhao, C. Burda

11:15 67. Photochemical reduction of CHCl_3 initiated by SPEEK systems using solutions and swollen films. **M. Islam**

**Northern Kentucky Convention Center
Room 3
Responsive & Functional Polymeric (Nano)Materials
N. Ayres, D. Konkolewicz, *Organizers, Presiding***

8:30 68. Introducing functionality to poly(arylene ether)s via sulfonamide activated nucleophilic aromatic substitution polycondensations. **E. Fossum**

9:00 69. Synthesis and polymerizability of 1-functionalized vinylbenzocyclobutenes with controlled curing temperatures. **C.R. Pugh**, W.K. Storms, J.S. Baker, A.R. Amrutkar

9:30 70. Kinetic study of amine catalyzed photo-initiated RAFT polymerization. **M. Allegrezza**

10:00 Intermission.

10:30 71. Utilizing assembly of graphene oxide at the oil-water interface to access tailored structures. B. Rodier, P. Wei, Q. Luo, E. Mosher, S. Burton, **E. Pentzer**

11:00 72. Building a theoretical perspective on how chemical structure determines the performance of polymer-based electronic devices. **C. Risko**

Northern Kentucky Convention Center

Room 8

**Innovations & Initiatives in K-16 Chemical Education-
Online Learning: Expanding the Classroom**

**Financially supported by PCS Administration-Potash
Corp**

J. Breiner, *Organizer*

A. Vonderheide, D. Waddell, *Organizers, Presiding*

9:00 73. Incorporating recorded video lectures into organic chemistry course content: Student survey and standardized exam results. **C.G. Gulgas**

9:30 74. Advancing technology and its impact on internet enhanced teaching. **R.K. Gilpin**, C.S. Gilpin

10:00 Intermission.

10:30 75. Development and implementation of an online general chemistry course. **Y. Law**

11:00 76. Development of an online college-level general chemistry preparatory program. **J. Roach**

11:30 77. Assessing the effectiveness of an adaptive-based online homework program for general chemistry preparation. **D. Turner**, K. Trick, M. Masthay, D.W. Johnson

WEDNESDAY AFTERNOON

**Northern Kentucky Convention Center
Room 3**

**Bioconjugates for a Changing World
Cosponsored by PMSE**

**D. Konkolewicz, R. C. Page, *Organizers*
J. Berberich, *Organizer, Presiding***

1:30 78. Protein modification via ring-opening metathesis polymerization. S.A. Isarov, P. Lee, J.D. Wallat, **J.K. Pokorski**

2:05 79. Opioid polymer biohybrids. **S. Averick**, S. Li, D. Cohen-Karni, D. Whiting

2:40 80. Functional polymers to tune the activity and stability of protein-polymer conjugates. **M. Lucius**, D. Konkolewicz, J. Berberich, R.C. Page

3:00 81. Synthesis of well-defined protein-polymer conjugates using ligase-mediated site-specific modification. **J.D. Stapleton**, R. Falatach, J. Plaks, R.C. Page, D. Konkolewicz, J. Kaar, J. Berberich

3:20 Intermission.

3:50 82. Chemoenzymatic labeling methods for bioorthogonal protein conjugation applications. M. Parasa, A. Saleh, A. Witten, J. Fraseur, **T. Kinzer-Ursem**

4:25 83. Materials at the beach: Characterizing and mimicking shellfish adhesives. **J.J. Wilker**

5:00 84. Development of horseradish peroxidase as a RAFT-initiator. **D. Konkolewicz**, R.C. Page, J. Berberich, M. Lucius, A. Danielson, J. Bornstein, D. Bailey-Van Kuren, K. Makaroff, C. Williams

Northern Kentucky Convention Center

Ballroom A

Bioinspired Chemistry

Financially supported by Procter & Gamble Company

B. Isfort, Z. Khambatta, *Organizers, Presiding*

1:30 Introductory Remarks.

1:45 85. Micro-architectures and interfaces in biological and synthetic materials. **F. Barthelat**

2:30 86. Self-organization and other biomimetic properties of nanoparticles. **N. Kotov**

3:15 Intermission.

3:30 87. Bioinspired chelates for light-responsive control of transition metal availability. **M.J. Baldwin**

4:00 88. Bioinspired strategies for enhancing function in degradable polymers. **M. Becker**

4:30 Panel Discussion.

5:15 Concluding Remarks.

**Northern Kentucky Convention Center
Ballroom E
Frontiers in Nucleic Acids Chemistry
R. M. Wilson, *Organizer*,
N. Leontis, *Organizer, Presiding***

1:30 89. RNA nanostructures for biomedical applications. **P. Guo**

2:00 90. Fabrication of nanometer scale functional polygons utilizing RNA 3WJ motif. **E. Khisamutdinov**

2:30 91. The pluses of DNA-seeking porphyrins. **D.R. McMillin, S. Ghimire**

3:00 Intermission.

3:30 92. RNA drug discovery: A paradigm shift for targeting cis regulatory RNA. **J.V. Hines**

4:00 93. Backbone-branched and mini-lariat RNA: Synthesis and debranching-dependent RNA interference. **S.R. Das**

4:30 94. NMR based profiling of pancreatic cancer, type 1 diabetes, and acute kidney injury. **M.A. Kennedy**

**Northern Kentucky Convention Center
Room 8
Innovations & Initiatives in K-16 Chemical Education-
Innovative Teaching Strategies
Financially supported by PCS Administration-Potash
Corp
J. Breiner, *Organizer*
A. Vonderheide, D. Waddell, *Organizers, Presiding***

1:30 95. Implementation of computer simulations in general chemistry labs: Student perspectives and instructional implications. **T.M. Clark**

2:00 96. POGIL vs. lecture in an organic chemistry classroom: Does it make a difference in student performance? **M.P. Dematteo**, M.L. Greer

2:30 97. Blended learning in chemistry courses: A conversation. **C.A. Currie**, A. Donnell

3:00 Intermission.

3:30 98. A one-semester chemistry survey course for nursing majors taught concurrently in three formats: face-to-face, flipped classroom, and on-line. **S.S. Preston**

4:00 99. Moving from pure science research to science education research: The initial strides from a graduate student perspective. **E.G. Westbrook**, **J. Breiner**

4:30 100. Using Google forms and Google sheets in AP chemistry lab. **T. Pinyayev**

**Northern Kentucky Convention Center
Room 5**

**Inorganic Chemistry, Organometallics & Sensors-
Inorganic/Organometallics & Catalysis**

W. B. Connick, J. A. Krause, *Organizers*

R. Muvirimi, *Presiding*

1:30 101. Insight into the dinuclear intermediates of the Pauson–Khand reaction. **D.R. Hartline**, C. Uyeda

2:00 102. Near-IR fluorescent probes based on zinc phthalocyanines and their subphthalocyanine intermediates. B.A. Corbin, L. Sejdarasi, M.A. Kaster, **E.R. Trivedi**

2:30 103. Diverse reactivity of azides with a dinuclear nickel complex: H-atom abstraction, N–N coupling, and C–H amination. **I. Powers**, C. Uyeda

3:00 Intermission.

3:30 104. Wet-chemical synthesis of iron dichalcogenide marcasite FeSe₂ and FeTe₂ nanocrystals. **E. Bastola**, K.P. Bhandari, N. Shrestha, R.J. Ellingson

4:00 105. Correlation of structure of square-planar metal complexes with pendant nucleophiles. **J. Ringo**, T.W. Green, J.A. Krause, W.B. Connick

4:30 106. SCrALS: Providing a straightforward solution to challenging samples. **A.G. Oliver**, J.A. Krause

Northern Kentucky Convention Center

Room 1

Mass Spectrometry

P. A. Limbach, *Organizer, Presiding*

1:30 107. Yin and Yang in mass spectrometry: Research-level mass spectrometry in industry. **L. Sallans**

1:50 108. Coupling electrochemistry with probe electrospray ionization mass spectrometry (PESI-MS). **Y. Cai**, H. Chen

2:10 109. Charge detection mass spectrometry for monitoring virus assembly in real time. **C. Lutomski**, K. Zhao, A. Zlotnick, M. Jarrold

2:30 110. Accessing alternative ionization chemistries with a flowing atmospheric-pressure afterglow (FAPA) ambient desorption/ionization (ADI) source. **S.P. Badal**, S.D. Michalak, Y. You, J.T. Shelley

2:50 111. A new thiol derivatization reactions with 2,1,3-benzotelluradiazole studied by mass spectrometry. **C. Xu, Q. Zheng, K. Xu, B. Tang**

3:10 112. Analysis of native electrospray of ubiquitin, cytochrome c and bovine serum albumin studied by IMS-IMS-MS. **A. Jacobs, D.E. Clemmer**

3:30 Intermission.

3:50 113. Confirmation of subunit-subunit connectivity and topology of computationally designed protein complexes using surface induced dissociation/ion mobility. **A. Sahasrabudde, Y. Hsia, F. Busch, D. Baker, V.H. Wysocki**

4:10 114. Salivary protein changes in medical residents performing stressful clinical simulations. **R. Marvin, M.B. Saepoo, S. Ye, D. White, K. Hensley, P. Rega, V. Kazan, D. Giovannucci, D. Isailovic**

4:30 115. Perturbation of the phosphoproteome of colony stimulating factor 3 receptor (CSF3R) in normal myeloid development, myeloid leukemia and neutrophilic leukemia. **P. Dwivedi, D. Muench, M. Azam, H.L. Grimes, K.D. Greis**

4:50 116. Targeted metabolic profiling for qualitative and quantitative measurement of bacterial metabolites and their response to antibiotic exposure. **K. Schelli, J. Rutowski, J. Zhu**

5:10 117. Differential mass spectrometry analysis of transfer RNA by stable isotope labelling. **M. Paulines**

**Northern Kentucky Convention Center
Room 4
Methods & Applications of Analytical Chemistry in
Occupational Health
Cosponsored by NUCL
R. Streicher, *Organizer, Presiding***

1:30 118. Introducing the 5th edition of the NIOSH manual of analytical methods. **P. O'Connor**

1:50 119. Biomonitoring emphasis in the 5th edition of the NIOSH manual of analytical methods. **D. Shoemaker**

2:10 120. Manganese speciation in workplace samples: Method development and validation. **R.N. Andrews, K. Hanley, H. Feng, K. Ashley**

2:30 121. Optical molecular fluorescence determination of ultra-trace beryllium in occupational and environmental samples using highly alkaline conditions. **K. Ashley, L. Adams, A. Agrawal, J. Cronin**

2:50 Intermission.

3:20 122. Measurement of diacetyl and 2,3-pentanedione in powdered flavorings by headspace SPME and GC-MS. **F. Nourian, R.P. Streicher**

3:40 123. Use of the DAN (1,8-diaminonaphthalene) method for assessment of isocyanate hazards related to application of spray foam insulation. **R. Streicher, D. Bello, F. Nourian, M.K. Ernst, J.E. Arnold, M.A. Steinmetz, T. Scott, J.R. Pretty**

4:00 124. Characterization of micronized/nanoscale copper particles in wood dust by electron microscopy. **C. Wang, C. Qi, A.S. Echt, A.K. Dozier, J.E. Fernback, M.E. Birch**

4:20 125. The application of analytical electron microscopy to the study of nanoparticles in tissue samples. **A.K. Dozier**, U.M. Graham, G. Oberdoerster, C. Wang, J.E. Fernback, M. Birch, B.H. Davis

Northern Kentucky Convention Center

Room 6

Nanoscience & Biotechnology

Cosponsored by BIOT

L. Esfandiari, H. Kumari, *Organizers, Presiding*

1:30 126. Pyrogallol[4]arene capsules seamed together by potassium, rubidium, and magnesium ions. C. Zhang, R.S. Patil, P.H. Atwood, C.L. Barnes, **J.L. Atwood**

2:05 127. Current challenges and approaches for improved localized surface plasmon resonance biosensing. D. Jana, J. He, I. Bruzas, **L. Litosh Sagle**

2:40 128. Encapsulation of xenon in the context of materials and ^{129}Xe NMR-based sensors. **K.T. Holman**

3:15 Intermission.

3:30 129. Membrane-active, synthetic amphiphiles that mediate antibiotic resistance reversal. **G.W. Gokel**

4:05 130. Optically transparent carbon nanotube film electrode for thin layer spectroelectrochemistry. **D. Zhao**, T. Wang, N. Alvarez, V.N. Shanov, W.R. Heineman

4:40 131. Porous materials for clean energy applications. **P.K. Thallapally**

Northern Kentucky Convention Center
Room 2
Organic Synthesis of Bioactive Molecules
Cosponsored by MEDI
M. DAI, Organizer, Presiding

1:30 132. Alkaloid synthesis based on cyclopropanols. **J.K. Cha**

2:00 133. Exploring chemoselectivity through natural product total synthesis. **S.A. Snyder**

2:30 134. Dearomative functionalization with arenophiles. **D. Sarlah**

3:00 135. 2-chloro-4-[[*(1R,2R)*-2-hydroxy-2-methylcyclopentyl]amino]-3-methyl-benzonitrile: Discovery and synthesis of transdermal selective androgen receptor modulators (SARM) for muscle atrophy. **A. Saeed**

3:30 Intermission.

3:45 136. Rh(I)-catalyzed cycloadditions and cycloisomerizations in natural product synthesis and drug discovery. **W. Tang**

4:15 137. Natural products as a fountainhead for chemical innovation. **P.E. Floreancig**

4:45 138. Preparation and electrocyclization of *N*-alkenylnitrones for the synthesis of novel oxazine heterocycles. **L.L. Anderson**

5:15 139. Recent advances in the total synthesis of biologically active natural products. **C.J. Forsyth**

**Northern Kentucky Convention Center
Ballroom D
What is Happening Down on the Pharm
Financially supported by Aerpio Therapeutics
D. J. McLoughlin, *Organizer, Presiding***

1:30 140. Setting a course for biomedical innovation in the 21st century. **G. Zhu**

2:15 141. Novel medicines, high-risk new mechanisms, high reward. **J. Gardner**

3:00 Intermission.

3:15 142. The on-demand synthesis economy: Complexity, diversity, and immediacy in chemical synthesis. **J.N. Johnston**

4:00 143. Late phase development of abemaciclib. **D.P. Kjell,** J. Merritt, K. Sullivan, M.A. Pietz, M. Andiappan, N.A. Furr

4:45 144. Therapeutic targeting of oncogenic protein tyrosine phosphatases. **Z. Zhang**

**Northern Kentucky Convention Center
Room 7
Controlled Assembly of Functional Supramolecular
Materials
J. K. Klosterman, *Organizer, Presiding***

2:00 145. Design and synthesis of dehydrobenzoannulene based 2D covalent organic frameworks. **J.W. Crowe,** P. McGrier

2:20 146. Metal organic frameworks: A retrosynthetic approach. **D. Genna**

2:50 147. Assembly of laminar metal-organic frameworks using a supramolecular building block strategy. **J.K. Klosterman**

3:20 Intermission.

3:40 148. STM study of supramolecular nanostructures at electrode/electrolyte interfaces. **Z. Li**

4:10 149. Tuning mechanical properties in metallo-supramolecular polymers with ligands and light. A. Razgoniaev, **A. Ostrowski**

4:30 150. Sumanene as new material for supramolecular aggregates. **A.Y. Rogachev**

WEDNESDAY EVENING

Northern Kentucky Convention Center

Ballroom B-C

ACS Sponsored Posters

J. A. Krause, *Organizer*

5:30 - 7:30

Get involved with the ACS division of chemical education. **D. Zimmerman.**

SCHB experience helps you meet the challenges in the chemical sciences sector. **J. Sabol.**

ACS Small Chemical Businesses Division membership: A valuable tool for the entrepreneur. **J. Sabol.**

Northern Kentucky Convention Center

Ballroom B-C

Analytical Chemistry/Instrumentation

J. A. Krause, Organizer

5:30 - 7:30

151. Development and validation of a new method to measure activity of the Na⁺, K⁺ ATPase using ICP-MS QQQ. **C.A. Stiner**, J. Landero, T. Radzyukevich, J. Heiny

152. Workplace monitoring of airborne carbon nanomaterials by HRTEM. **M.E. Birch**, C. Wang, J.E. Fernback, H. Feng, Q. Birch, A.K. Dozier

153. Development of an electrochemical biosensor for arsenic. **S. Minderlein**, J. Berberich, J.P. Scaffidi

154. A pH and surface charge study of the adsorption behavior of silver nanoparticles to corundum mineral. **K.A. O'Neil**, J. Sikon, D.P. Foose, S.W. Brittle, S.R. Higgins, I.E. Pavel Sizemore

155. Synthesis and characterization of Nafion-ionic liquid polymer composite membranes. **L.A. Zook-Gerdau**, C. Daley, R. Holman

156. Comparison of boron-doped diamond and nitrogen-incorporated tetrahedral amorphous carbon thin-film electrodes for the detection of estrogenic compounds by HPLC-EC. **A. Castiaux**, J. Qiu, G.M. Swain

157. The electrochemical behavior of boron-doped diamond and nitrogen-incorporated tetrahedral amorphous carbon thin-film electrodes in ionic liquids. **R. Jarosova**

158. Analysis of a series of dietary supplements via energy dispersive X-ray fluorescence spectroscopy (EDXRF). **W. Bair**, S. Maurice, M.A. Benvenuto

159. Classification of key ororants in coffee by headspace solid phase microextraction and gas chromatography-mass spectrometry. **J. Kyle**, E.A. Baldauff

160. Does temperature affect confirmatory analysis of blood, cell morphology of red blood cells and DNA degradation? **B.K. Bosley**, F. Musko, M. Wright

161. Comparison of metal partition coefficients for soils determined by x-ray fluorescence and atomic absorption. **C. Lupse**, J. Allison, P.B. Nolibos

162. Selection of aptamers for microcystin-LR using quantum dots and capillary electrophoresis. **M. Brito**, **C. Rousseau**, **J. Guthrie**

163. Water quality studies of contributing streams to the Huron River in southeast Michigan. **O. Hajihassani**, **J. Powers**, J. Vites

Northern Kentucky Convention Center

Ballroom B-C

Biochemistry/Medicinal Chemistry

J. A. Krause, *Organizer*

5:30 - 7:30

164. Enzyme immobilized microfiltration membrane for environmental bioremediation. **R. Sarma**, D. Bhattacharyya

165. Design and synthesis of new allosteric HIV-1 integrase inhibitors.. **Y. Mansour**, P. Koneru, M. Kobe, A. Hoyte, M.S. Mohamed, M. Kvaratskhelia, J. Fuchs

166. The morphology dependent *in vivo* behaviour of self-assembling peptide amphiphiles. **C.J. Buettner**, A.J. Wallace, M. Williams, E. Paradis, A. Manos, H. Ding, A. Bratasz, K. Kumar, M.F. Tweedle, J.E. Goldberger

167. Analogues of the natural product ethyl *N*-(2-phenethyl) as potent biofilm inhibitors of methicillin resistant *staphylococcus aureus*. **M. Stephens**, N. Yodsanit, C. Melander

168. Functionalization of Indole scaffold as allosteric HIV-1 integrase inhibitors. **J. Antwi**, P. Koneru, M. Kobe, M. Kvaratskhelia, J. Fuchs

169. Optimization of cytidine-specific cleavage mediated by recombinant cusativin for detecting modifications in RNA. **P. Thakur**, B. Addepalli, . Limbach, V. Short

170. The effects of PEGylation on the self-assembling properties of a peptide amphiphilic imaging agent. **A.J. Wallace**, C.J. Buettner, A. Manos, E. Paradis, M.F. Tweedle, J.E. Goldberger

171. A modified ribonuclease assay for *E. coli* clones secreting RNase U₂. **B. Solivio**, **A. Beiersdorfer**, **B. Addepalli**, **P. Limbach**

172. Inhibition of Ras-Raf interaction by bicyclic peptides. **W.A. Bedewy**, N.A. Abou Taleb, T.M. Nasr, S.F. Hammad, D. Pei

173. Deoxygenation of sugars leads the way to sustainable chemical production. **M. Morrow**, J. Brantley , A. Samant , D. Toste

174. An investigation into the components of little bluestem seed exudate and its ability to degrade bisphenol A. **K. Parson**, C. Nyland, L.J. Putman

175. Synthesis and reactivity study of alpha substituted chalcones. I. Janser, **J. Wotring**, A. Fried

Northern Kentucky Convention Center

Ballroom B-C

Chemical Education

J. A. Krause, *Organizer*

5:30 - 7:30

- 176.** Introducing non-science majors to science through an environmental chemistry course. **V.C. Ezeh**
- 177.** Primary literature in a foundations of inorganic chemistry course. **V.C. Ezeh**
- 178.** Development and characterization of a teaching constant current coulometry instrument for a multifunctional chemical analysis (MCA) system. E.M. Coombs, J.P. De Jesus, **N.D. Danielson**
- 179.** Development and characterization of a teaching sequential flow Injection analysis instrument for a multifunctional chemical analysis (MCA) system. S.R. Vogelsong, A. Ali, **N.D. Danielson**
- 180.** Student friendly science labs utilizing IPADS and videos. **S. Ladogana**, J. Green, P.D. Voegel

Northern Kentucky Convention Center

Ballroom B-C

Inorganic Chemistry/Organometallic Chemistry/Catalysis

J. A. Krause, *Organizer*

5:30 - 7:30

- 181.** Phosphate removal and recovery using drinking water plant waste residuals. **G. Varshney**, E. Martin, S. Chae, N. Kesav, M. Nadagouda
- 182.** Photovalic properties of silver doped nickel tungstate. **A. Riley**, Z. Li, S. Hosseini

- 183.** Coordination of 1,3-bis(diphenylphosphinomethyl)benzene and 1,3-bis(ditertbutylphosphinomethyl)benzene ligand to uranyl nitrate. **M. Alotaibi**
- 184.** Boron subphthalocyanines as fluorescent probes and synthetic intermediates for low-symmetry phthalocyanines. **B.A. Corbin**, L. Sejdarasi, E.R. Trivedi
- 185.** Fluorinated zinc phthalocyanines as imaging probes: Balancing fluorescence with amphiphilicity. **M.A. Kaster**, E.R. Trivedi
- 186.** Catalysis kinetics of two generations of supramolecular Co(III)-salen catalysts and the influence of varying electron-donor aromatic compounds. **D.R. Blechschmidt**, M. Woodhouse, Y. Liu
- 187.** Palladium-catalyzed transfer hydrogenation by substituted-hydrogensilanes. Z. Clarke, **C.I. Onyeagusi**, I.H. Bonck, **B.J. Duke**, J. Fotie
- 188.** Boracarboxylation of vinyl arenes. **E.J. McClain**, T.W. Butcher, **T.G. Hamilton**, B.V. Popp
- 189.** A study of two [Pt(typ)Cl]BF polymorphs: Red vs. green. **J. Reifsteck**, A. Norton, M. Karimi Abdolmaleki, J.A. Krause, W. Connick
- 190.** A facile method for the hydrolysis of a nickel schiff base complex useful for synthesis of side-chain protected unnatural amino acids. **C. Bontrager**, **T. Geibel**, G. Lengyel

Northern Kentucky Convention Center
Ballroom B-C
Materials Chemistry/Nanomaterials/Sensors
J. A. Krause, Organizer
5:30 - 7:30

- 191.** Biolabeling through the use of water-soluble colloidal quantum dots. **Y. Tang**, D.M. Dimick, C.A. Stombaugh, L. Sun
- 192.** The role of acetic acid and water in the synthesis of colloidal PbS nanosheets. **S. Premathilaka**, Z. Jiang, A. Antu, L. Sun
- 193.** Sorption of noble metal nanoparticles from the water column by periphytic algal turf communities. **H. Faraj, J.B. Miller**
- 194.** Photocontrollable visible range absorbing rhodamine spiro lactams for super resolution imaging. **P. Rai**
- 195.** Ultrathin colloidal PbS/CdS core/shell nanosheets. **Z. Jiang**, K. Simeen, S. Premathilka, J. Hu, A. Voevodin, P. Roland, R.J. Ellingson, L. Sun
- 196.** Understanding the mechanism of formation of PbSe NR. **S. Chiluwal**, S. Kandel, Z. Jiang, L. Sun
- 197.** Understanding octahedral tilting in n=2 Ruddlesden popper phases. **A. Sharits**, P. Woodward, N. Benedek
- 198.** Controlled Spacing of emissive phenylene diacrylic acids in Pillared Metal Organic Frameworks. **S. Puri**, J.K. Klosterman
- 199.** Cs₂AgBiX₆ (X = Br, Cl) — New visible light absorbing, lead-free halide perovskite semiconductors. **E. McClure**, P. Woodward

200. Synthesis and characterization of $Al_xSc_{2-x}Mo_3O_{12}$ using non-hydrolytic sol-gel methods. **L. Lovings**, D. Blum, A. El-Amin, C. Lind-Kovacs

201. Synthesis of 5-Arylethynylisophthalic acids for directed aggregation of interdigitated aromatics. **V. Singh**, J.K. Klosterman

202. Towards Donor-substituted phenylene isophthalic acids for non-interpenetrated MOFs with tailored emissive behavior. **M.J. Ayodele**, J.K. Klosterman

203. Correlating structural properties to biosorption capacity. Z. Kelper, T. Robaska, K. Villegas, **D.J. Schauer**

Northern Kentucky Convention Center

Ballroom B-C

Organic Chemistry/Green Chemistry/Catalysis

J. A. Krause, *Organizer*

5:30 - 7:30

204. Towards the optimization of the allylation of phenols and alcohols *via* oxypyridinium salts. **A. Jacobs**, P.A. Albinia

205. Tetrazolones: From supramolecular synthons to anion recognition. **H. Zhou**, S. Rayat

206. 1,3-dipolar cycloaddition of nitrile oxides containing quinoline-5,8-dione. **R. Ravanfar**, J. Nguyen, R.E. Sammelson

207. Hyperbranched poly(ester)s as platforms for the controlled delivery of drugs. G. Greene, **B.A. Howell**

208. Gallic acrylates as a base for the development of nontoxic flame retardants. J. Bahry, **B.A. Howell**

- 209.** Phosphorus esters of gallic acid. K. Oberdorfer, **B.A. Howell**
- 210.** Generation of phosphorus flame retardants for textiles and plastics from itaconic acid. V. Hill, Y. Daniel, **B.A. Howell**
- 211.** Brominated phosphorus compounds from alkynols. A. Gudbrandson, **B.A. Howell**
- 212.** Phosphorus derivatives of biophenol as flame retardants for polymeric materials. C. Schmaltz, **B.A. Howell**
- 213.** The 1,8-diaminonaphthalene phytic acid salt as a biobased flame retardant. A. Dembski, Y. Daniel, **B.A. Howell**
- 214.** Exploring the reactivity of oxypyridinium salt derivatives with oxygen nucleophiles. **C. Culy**, P.A. Albiniak
- 215.** Synthesis of a series of long-chain molecules for use as possible water remediation chelators. **G. Nguyen**, J. Pothoof, S. Tinawi, M.A. Benvenuto
- 216.** Production of a series of multi-dentate podand ligands and incorporation into plastics for use as potential metal chelators. M.A. Benvenuto, **J. Payne**
- 217.** Synthesis of a series of bis-bi-dentate ligands for metal complexation trials. **S. Anderson**, S. Makki, M.A. Benvenuto
- 218.** Evaluation of the reactivity of *N*-Alkylmaleimides and Diels-Alder adducts of anthracene as potential paper sizing agents. **I.H. Bonck**, **B.N. Michel**, J. Fotie
- 219.** Electronic substituent effects on the reactivity of 2-benzyloxy-1-methylpyridinium triflate derivatives. **S.A. Harry**, P.A. Albiniak

220. Formation of the synthons 4,4'-dipyridil diketone and 1,3-di(4-pyridinyl)acetone. **B.D. Coleman, J.C. Martinez,** M.P. Castellani

**Northern Kentucky Convention Center
Ballroom B-C
Physical Chemistry/Computational Chemistry
J. A. Krause, Organizer
5:30 - 7:30**

221. Using metal nanostructures to enhance the intrinsic fluorescence of hemoglobin. **H. Sekhon,** C. Whitcher, M. Cheng, J.S. Biteen

222. Light-sensitive reaction-diffusion waves in a checkerboard-like illumination system. **S. Kirn,** N. Manz

223. *Ab initio* and semi-empirical quantum chemistry calculations of DMPO and DMPO-OH - water clusters. P. Campbell, **S.J. Kirkby**

224. *Ab initio* and semi-empirical calculations of cyanoligated rhodium dimer complexes. Y. Asiri, **S.J. Kirkby**

225. Quantum chemistry calculations of glucan building blocks. U.P. Patel, **S.J. Kirkby**

226. Computational study of the energetics of binding and folding of the pH (Low) insertion peptide (pHLIP). **A. Clark,** **Z. Bonham,** N. Graziano, B. Mertz

Northern Kentucky Convention Center
Ballroom B-C
Polymer Chemistry
J. A. Krause, *Organizer*
5:30 - 7:30

227. Synthesis and properties of bisimidazolium-containing Michael addition polyester networks. **J.A. Dippie**, K.M. Miller

228. Post-polymerization modification of branched polyglycidol with *N*-hydroxyphthalimide to give ratio-controlled amino-oxy functionalized species for biomedical applications. **D.B. Beezer**, E. Harth

THURSDAY MORNING

Northern Kentucky Convention Center
Ballroom D
Electroanalytical Chemistry in the Central Region
Cosponsored by ANYL
A. F. Bange, *Organizer, Presiding*

8:00 229. Electrochemically modulated delivery of nitric oxide (NO) for biomedical applications: From improved intravascular catheters and chemical sensors to inhaled NO therapy. **H. Ren**, A. Hunt, N. Lehnert, M.E. Meyerhoff

8:40 230. Applications of diamond electrodes in electroanalysis and spectroelectrochemistry. **G.M. Swain**

9:20 231. A calibration-free anodic stripping detection system for truly remote sensing of heavy metals via anodic stripping coulometry. **R. Baldwin**, M.M. Marei, T. Roussel, R. Keynton

10:00 Intermission.

10:20 232. Ultrafast electron-transfer kinetics of graphene as revealed by nanogap voltammetry. **S. Amemiya**

11:00 233. Electrochemical imaging with ion channel probes.
L.A. Baker

Northern Kentucky Convention Center

Room 2

**Functional Porous & Polymeric Materials: Synthesis,
Properties & Applications**

Cosponsored by POLY

P. McGrier, *Organizer, Presiding*

8:00 234. Siloxane functionalized polynorbornenes via vinyl-addition polymerization for CO₂ separation membranes. **B.K. Long**, K. Gmernicki, E. Hong, C. Maroon, T. Saito

8:35 235. Laser-driven nanopore formation using magnetically guided nanochisels. **N. Kadasala**, M. Saei, G. Cheng, A. Wei

8:55 236. Patternable conjugated polymers with latent hydrogen-bonding on the main chain. **Y. Zhu**

9:25 237. Fluorinated porous materials: From metal-organic frameworks to molecular crystals. **O. Miljanic**

10:00 Intermission.

10:30 238. Contorted aromatics and polymers from cyclopenta-fused polycyclic aromatic hydrocarbons. **K.N. Plunkett**

11:05 239. Design of triblock polymers and their implementation as high-performance nanostructured membranes and high capacity metal ion adsorbent systems.
B.W. Boudouris, R.A. Mulvenna, J.L. Weidman, Y. Zhang, W.A. Phillip

11:40 240. 2-isopropenyl-2-oxazoline: a versatile monomer for precise synthesis of “dumb-bell” shaped polymer brush via living ionic polymerization. **H. Feng**, J. Zhu, K. Hong, J.W. Mays, N. Kang

Northern Kentucky Convention Center

Room 7

Sensors & Their Applications in Environmental & Occupational Health

Financially supported by Spectroscopy Society of Pittsburgh

D. DeBord, M. Hoover, *Organizers, Presiding*

8:00 241. When & where: Wearable IoT direct-reading exposure assessment and location sensors. **K. Brown**, K.R. Mead, P.B. Shaw, R.J. Kovein, R.T. Voorhees, A.R. Brandes

8:30 242. Applicability of commercially available sensor for volatile detection in the aerospace environment. **G. Slusher**, J. Martin, C.C. Grigsby, D. Ott, B.A. Geier

9:00 243. Portable spectrometer for near real-time measurement of elemental concentration of aerosols. **P. Kulkarni**, L. Zheng, M. Birch

9:30 Intermission.

10:00 244. Portable ultrafine particle counter sampling in ground and aerospace environment. **C.M. Grabinski**, G.M. Slusher, J. Martin, C.C. Grigsby, D. Ott

10:30 245. Personal ultrafine ($\geq 4.5\text{nm}$) real-time particle counters utilizing innovative and versatile water-based CPC technology. **J. Lockey**, S. Son, G. LeMasters, P. Ryan

11:00 Panel Discussion.

**Northern Kentucky Convention Center
Ballroom E
Frontiers in Nucleic Acids Chemistry
B. Addepalli, M. Lemaitre, *Organizers, Presiding***

8:30 246. Rapid synthesis of challenging oligonucleotides for research and pre-clinic studies. **H. Zhu**

9:00 247. Development of allele-specific stereopure antisense oligonucleotides (ASOs). **M. M**

9:30 248. 5'- triphosphate oligonucleotides synthesis: From research scale to up to 40 g batch. **S. Jiang**, E. Paredes, H. Cramer, K. Ackley

10:00 Intermission.

10:30 249. A transcription factor aids in noncoding RNA-templated replication by DNA-dependent RNA polymerase II. **J. Qu**, Y. Wang, A. Tanimoto, S. Ji, A.J. Wallace , T. Chen, J. Wu, Y. Li, V.H. Wysocki, V. Gopalan, B. Ding

11:00 250. Mechanisms and applications of 3'-5' RNA polymerases: Substrate recognition by non-canonical polymerases. **K. Patel**, P. Yourik, J.E. Jackman

11:30 251. DNA in tight spaces: Linking structure, stability and protection in cation packaged DNA. **J.E. Derouchey**

**Northern Kentucky Convention Center
Room 4
Frontiers in Organometallic Chemistry
H. Guan, *Organizer, Presiding***

8:30 252. Pincer-templated ruthenium hydrides for catalytic hydrogen transfer reactions. **N.K. Szymczak**

9:05 253. Ligand influences on base metals for two-electron transformations. **A.R. Fout**

9:40 254. Half-sandwich iron(II) scorpionate complexes as nitrene transfer catalysts. **M.P. Jensen**, C.M. Anderson, S. Liang

10:15 Intermission.

10:35 255. Catalysis at metal-metal bonds. **C. Uyeda**

11:10 256. Pyrrole-based PNP pincer complexes with late transition metals. **V.M. Iluc**, J.A. Kessler

**Northern Kentucky Convention Center
Room 8**

**Innovations & Initiatives in K-16 Chemical Education
Pupils to Pedagogy & Everything In Between**
Financially supported by PCS Administration-Potash Corp

A. Vonderheide, *Organizer*

J. Breiner, D. Waddell, *Organizers, Presiding*

9:00 257. More complex models for the acid-base equilibria of monoprotic acids. **W. Hensel**, R.K. Gilpin

9:30 259. One discovery leads to another: An interactive chemical sensing workshop. **J. McElveen**, A.E. Norton, J. Ringo, W. Connick

10:00 Intermission.

10:30 260. Student understanding of chemistry concepts related to climate science: A survey for use in chemistry and liberal arts courses. **A. Zabih**, A. Versprille, T. Holme, P.G. Mahaffy, B. Martin, L.C. McKenzie, M.H. Towns

11:00 261. Utilizing 3D printing to enhance introductory chemistry lectures and labs. **J.D. Mendez**

11:30 262. Internationalizing undergraduate chemistry research. **I.L. Lagadic**, S. Gauthier, A. Maicaneanu, C. Zambrano

12:00 258. 187 years of working stoichiometry problems. **W. Jensen WITHDRAWN**

Northern Kentucky Convention Center

Room 1

Materials Chemistry & Application: Environment, Energy & Biology

Financially supported by Shepherd Chemical Company

N. A. Eckert, R. Hart, S. Taylor, *Organizers, Presiding*

8:30 263. Levitating liquids. **C. Benmore**

9:15 264. Composition/property relationships in optical glass. **J.W. Zwanziger**

10:00 265. Theoretical framework for understanding the role of solution phase conditions within successful hydrothermal synthesis of metal organic frameworks. **A.E. Clark**, C. Wang, X. Yang

10:30 Intermission.

11:00 266. Living on the edge: Chemistry at the interfaces. **M. Dolgos**

11:30 267. The chemistry of self-healing materials. **K. Hart**

Northern Kentucky Convention Center

Room 9

Molecular Modeling of Energy Storage Devices & Biomolecular Complexes

T. L. Beck, R. I. Dima, G. Stan, *Organizers, Presiding*

8:30 268. Structural and morphological aspects of polymeric electrolytes. **S.J. Paddison**

9:00 269. Deciphering structural dynamic mechanisms in molecular motors and switches. **B. Grant**

9:30 270. Revisiting the TA^+/TB^- hypothesis: quasichemical partitioning of single-ion solvation free energies from simulation reveals hidden contribution from interfacial potentials. **T.P. Pollard**, T.L. Beck

9:50 271. Density-functional study of the $La_2Zr_2O_7$ low-index faces. **Y. Mantz**, Y. Duan

10:10 Intermission.

10:25 272. The role of allostery and conformational dynamics in protein evolution. **S. Ozkan**

10:55 273. Eigenstate-specific canonical and microcanonical temperatures in two-level paramagnetic spin lattices. **M. Masthay**, C. Eads, A. Johnson, R. Keil, P. Miller, R.E. Jones, J. Mashburn, H. Fannin

11:15 274. Modeling heterogeneity in protein and RNA complexes under tension. **M. Hinczewski**, D. Thirumalai

11:45 275. Coarse-grained simulations of mechanical threading of Immunoglobulin domains through non-allosteric ClpY ATPase pore. **A. Javidialesaadi**, G. Stan

Northern Kentucky Convention Center

Room 5

Nanomaterials & Nanotechnology for Analytical & Spectroscopy-Based Applications

Financially supported by PITTCO

P. Zhang, Organizer, Presiding

8:30 276. Single-molecule super-resolution microscopy study of the distance-dependent interaction between a fluorescent molecule and a nano-antenna. **B. Fu**, J.D. Flynn, B. Isaacoff, H. Tuson, J.S. Biteen

9:00 277. Quantitative SERS measurement for halogenated organic compounds in environmental water. **Z. Yu**, Y. Zhou, P. Zhang

9:30 278. Utilizing analytical- and microscopy-based methods to examine ADMES of silver nanoparticles (AgNPs) in vero 76 cells. **S.A. Paluri**, J.D. Ryan, N. Lam, I.E. Pavel Sizemore

10:00 Intermission.

10:30 279. Towards the development of reproducible, flexible, and highly effective SERS substrates with an incorporated internal reference. **M.E. Smith**, Z. Yu, D. Collini, Y. Zhou, P. Zhang

11:00 280. Photodynamic inactivation of *staphylococcus aureus* using amphiphilic block copolymer stabilized gold nanoparticles. **N. Wijesiri**, T. Ozkaya Ahmadov, p. Wang, P. Zhang

11:30 281. Reaction of oxide based mesoporous nanoparticles: An *in situ* FT-IR study. D.K. Paul

Northern Kentucky Convention Center

Room 3

Organic Chemistry & Catalysis

M. Dai, Organizer, Presiding

9:00 282. Tuning the optoelectronic properties of coresubstituted naphthalene diimides by the selective conversion of imides to monothioimides. **F.S. Etheridge**, R. Fernando, J. Golen, A.L. Rheingold, G. Sauve

9:20 283. Synthesis of oxaspirolactones via palladium-catalyzed cyclopropanol ring opening carbonylative spirocyclization: Total synthesis of levantenolides. **D. Davis**, K. Walker, C. Hu, R.N. Zare, R.M. Waymouth, M. Dai

9:40 284. Alkylation of heteroarene bases via deoxygenation of alcohols. **J.M. Lear**, A. Mustafa, K. Pan, D. Nagib

10:00 285. Developing a novel, tunable carbene scaffold for small molecule activation and catalysis. **J.P. Moerdyk**

10:20 Intermission.

10:40 286. A novel directing group strategy for the ²-amination of alcohols. **K. Nakafuku**, A. Vanitcha, M. Bekkaye, D. Nagib

11:00 287. Copper-catalyzed cyclopropanol cross coupling: An umpolung strategy to access beta-substituted carbonyls. **K.E. Gettys**, M. Dai

11:20 288. A triiodide-mediated ¹C-H amination. **E. Wappes**, S. Fosu, T. Chopko, D. Nagib

11:40 289. Bis-corannulenoanthracene (C₅₀H₂₂): A versatile precursor for benzocorannulene molecular receptors with polar tethers. **K.R. Kumarasinghe**, F.R. Fronczek, H.U. Valle, A. Sygula

THURSDAY AFTERNOON

**Northern Kentucky Convention Center
Ballroom D**

**Electroanalytical Chemistry in the Central Region
Cosponsored by ANYL
A. F. Bange, *Organizer, Presiding***

1:30 290. Does science drive technology or vice versa? The special case of electroanalytical chemistry over the past fifty years. **P.T. Kissinger**

2:10 291. Size-dependent electrooxidation and electrophoretic deposition of gold nanoparticles. **F.P. Zamborini**, S. Allen, R. Masitas Castillo

2:50 292. Recent advances in in situ spectroscopy and on line spectrometry. **D.A. Scherson**

3:30 Intermission.

3:50 293. Voltammetry at catalytic size-exclusion electrodes. **J.A. Cox**, M. Ciabocco, M. Berrettoni, S. Zamponi

4:30 294. Electrochemistry at 800°C and no reference electrode. **H.O. Finklea**

Northern Kentucky Convention Center

Ballroom E

Frontiers in Nucleic Acids Chemistry

B. Addepalli, M. Lemaitre, *Organizers, Presiding*

1:30 295. Tuning Cas9 activity with CRISPR RNA modification. **K.T. Gagnon**, Z.J. Kartje, K. Rohilla, C.L. Barkau

2:00 296. Gamma peptide nucleic acids: Chemistry and applications. **A. Fraley**

2:30 297. Translation control using ³PNA probes. **T. Canady**

3:00 Intermission.

3:30 298. Use of chemical modification and mass spectrometry to identify substrate-contacting sites in

proteinaceous RNase P, a tRNA processing enzyme. **T. Chen**,
A. Tanimoto, V.H. Wysocki, V. Gopalan

4:00 299. Efficient gene editing in *Neurospora crassa* with
CRISPR technology. **T. Matsu-ura**, M. Baek, J. Kwon, C.
Hong

4:30 300. Clinical trials with oligonucleotide therapeutics. **M.**
Lemaitre

Northern Kentucky Convention Center

Room 4

Frontiers in Organometallic Chemistry

H. Guan, Organizer, Presiding

1:30 301. Insights into the inverse trans influence as illustrated
by uranium-nitrogen multiple bonds. **S.C. Bart**, N. Anderson,
M. Zeller, P. Fanwick

2:05 302. Mild carboxylation strategies with base metal
catalysts. **B.V. Popp**

2:40 303. Iron-catalyzed hydrogenation and dehydrogenation
reactions. H. Dai, J.A. Krause, **H. Guan**

3:15 Intermission.

3:35 304. N-N and C-N bond formation reactions catalyzed by
3d metal centers in bis(alkoxide) ligand environments. **S.**
Groysman, J. Bellow, M. Yousif, R.L. Lord

4:10 305. Multifunctional ligand design towards green
chemical catalysis. **K.G. Caulton**

**Northern Kentucky Convention Center
Room 8
Innovations & Initiatives in K-16 Chemical Education-
New Lessons in the Laboratory
Financially supported by PCS Administration-Potash
Corp
A. Vonderheide, *Organizer*
J. Breiner, D. Waddell, *Organizers, Presiding***

1:30 306. Solar cells as a model for integrated laboratory experiences. **P. Tandler**

2:00 307. Thin layer chromatography for detection of neonatal respiratory distress. **M.O. Garcia**, G. Clark

2:30 308. Labs that relate chemistry to healthcare using MORE. **G. Clark**

3:00 Intermission.

3:30 309. Using digital badges to improve student hands-on skills in the undergraduate laboratory. **S. Hensiek**, C. Harwood, K. O'Shea, J. Fish, M.H. Towns

4:00 310. Cigarette smoke and cancer cells: An interdisciplinary, collaborative, research-based laboratory initiative. **D.K. Hoover**, J. Fornsaglio

**Northern Kentucky Convention Center
Room 3
Materials & Polymer Chemistry
D. Konkolewicz, *Organizer, Presiding***

1:30 311. Stabilization of general purpose poly(styrene) by hydrogen-atom transfer. S. Lazar, **B.A. Howell**

2:00 312. Imidazolium-containing thiol-ene polymer networks and gels: Synthesis and properties. **K.M. Miller**

2:30 313. The synthesis and tribological performance of phosphonium/phosphate based ionic liquids as friction reducing engine oil additives. **M. Welmers**, M. Mueller

3:00 Intermission.

3:30 314. Electrochemical platforms for point-of-care micronutrient sensing applied to the quantification of potassium ion. I.A. Taylor, **F. Deiss**

4:00 315. Unexpected variables in P3HT synthesis. **J. Gadiant**, C. Lind-Kovacs

4:30 316. Molecular architecture of electrospun fibers of poly (ϵ -caprolactone) / aminopropyl isobutyl polyhedral oligomeric silsesquioxane (AMPOSS)- blends. **Z.B. Grim**, A.J. Bauer, B. Li

Northern Kentucky Convention Center

Room 1

Materials Chemistry & Application: Environment, Energy & Biology

Financially supported by Shepherd Chemical Company

N. A. Eckert, R. Hart, S. Taylor, *Organizers, Presiding*

1:30 317. Biofiltration through co-metabolism for the controlled removal of gaseous chloroform. **K. Palanisamy**, B. Mezgebe, G. Sorial, E. Sahle-Demessie

2:00 318. Antimicrobial activity of unfunctionalized silver nanoparticles against water quality indicator organisms. **M. Markopoulos**, S.A. Paluri, I.E. Pavel Sizemore

2:30 319. Sustainability challenges in the complex inorganic colored pigment market. **G.T. Peake**

3:00 Intermission.

3:30 320. Alternative electron acceptors for bulk heterojunction organic solar cells. **G. Sauve**

4:00 321. A monomeric chromium(III) carboxylate. **O.L. Sydora**, R. Hart, N.A. Eckert, C. Benmore

4:30 322. Innovation at the intersections of mature catalytic processes. **E.G. Rightor**

Northern Kentucky Convention Center

Room 9

Molecular Modeling of Energy Storage Devices & Biomolecular Complexes

T. L. Beck, R. I. Dima, G. Stan, *Organizers, Presiding*

1:30 323. Understanding transport and packing of ionic liquids during electrode charging. **B. Sumpter**, Y. He, J. Huang, R. Qiao

2:00 324. A kinetic model for the stepping dynamics of myosin VI. **R. Tehver**

2:30 325. Investigation of inhibitory potency of BHQ derivatives as SERCA inhibitors to use as potential drugs as well as tools to study the SERCA function: Binding free energy computation using FEP/MD. **M. Jayasinghe**, Q. Wang, A. Schirmer, G. Stan, S. Paula

2:50 326. A Power Flex in Hsp70: The nucleotides' impact on the actin-like ATPase domain. **D.R. Merz**, R.I. Dima

3:10 Intermission.

3:25 327. Computational modeling of various types of protein complexes. **D. Kihara**

3:55 328. Structure and dynamics of electrolytes confined in MXene-based supercapacitors. **L. Vlcek**, H. Wang, N. Osti, E. Mamontov

4:25 329. Modeling the molecular mechanics of hearing. **M. Sotomayor**

Northern Kentucky Convention Center

Room 5

Nanomaterials & Medicine

Financially supported by Fisher Scientific

L. Sagle, A. S. Samia, *Organizers, Presiding*

1:30 330. Small nanoparticle alloys. **J. Millstone**

2:05 331. Synthesis of high-index faceted iron oxide nanoparticles for magnetic resonance imaging applications. **S. Wickramasinghe**, S.F. Situ, A.S. Samia

2:25 332. Gd@C-dots as a safe and effective T1 contrast agent. **J. Xie**

3:00 Intermission.

3:15 333. Green synthesis of magnetic gold nanoclusters. **L. Lin**, N. Kadasala, A. Wei

3:35 334. Nanoscale temperature measurement and thermal imaging with Er³⁺ based nanothermometry. **S. Baral**, H. Richardson, A. Aulamic, A. Rafiei Miandashti

4:10 335. Optimizing iron oxide nanoparticles for magnetic particle imaging: Guided hyperthermia (hMPI). **S.F. Situ**, L.M. Bauer, M.A. Griswold, A.S. Samia

4:30 336. Ligand-mediated “turn on,” high quantum yield near-infrared emission in small gold nanoparticles. **S.E. Crawford**, C.M. Andolina, A. Smith, L. Marbella, K. Johnston, P. Straney, M.J. Hartmann, J. Millstone

Northern Kentucky Convention Center

Room 6

Organic Chemistry & Chemical Biology: Their Impact on Human Health

Cosponsored by MEDI

R. Viswanathan, Organizer, Presiding

1:30 337. New Reactions and Reagents to Molecularly Edit Therapeutics and Natural Products with Fluorine. J.N. Johnston, B.A. Vara, S.V. Tsukanov, K. Schwieter

2:15 338. Design, synthesis and biological evaluation of novel largazole analogues as histone deacetylase inhibitors. **A. Al-Hamashi**, J. Almaliti, L. Tillekeratne

2:40 339. Parameters that predict potential cardiovascular side effects of drugs. **G.X. Wang**, C. Kordik

3:05 340. Uncovering cryptic secondary metabolites from *Aspergillus nidulans* with HDAC inhibition. **M.T. Henke**, A.A. Soukup, R.A. McClure, A.W. Goering, R.J. Thomson, N.P. Keller, N.L. Kelleher

3:30 Intermission.

3:45 341. Discovery and characterization of aryl isonitriles as a new class of compounds versus methicillin- and vancomycin-resistant *Staphylococcus aureus*. D. Davis, H. Mohammad, **K. Kyei-Baffour**, W. Younis, M. Seleem, M. Dai

4:10 342. Polymorphism: Changing active pharmaceuticals by surface modification. **N. Searls**, R. Quiñones

4:35 343. Structural and thermodynamic insights into cap-independent translation in enterovirus 71. **M. Tolbert**, C.E. Morgan, B.S. Tolbert

5:00 344. Non-nucleoside inhibitors of human ribonucleotide reductases. **R. Viswanathan**, **S. Huff**, C.G. Dealwis

Northern Kentucky Convention Center

Room 2

Organic Chemistry-Design of Functional Macromolecules

J. R. Parquette, *Organizer, Presiding*

1:30 345. Controlling molecular encapsulation with amphiphilic and bolaamphiphilic baskets in water. **J. Badjic**

1:50 346. Catechol-based coatings inspired by melanin as colorimetric metal-ion sensors. **J.M. Belitsky**

2:10 347. Stimuli-responsive calixarene-capped azobenzene dimers: Synthesis, switching, and supramolecular chemistry. **P.A. Bonvallet**, A. Steiger, C.M. VanDenburgh, A.J. Darling, P. Evans

2:30 348. Fluorinated azadipyrrromethene ligands and chelates as electron acceptors in organic photovoltaics. **F.S. Etheridge**, S. Pejic, R. Fernando, G. Sauve

2:50 349. Immobilization of biocatalyst with self-assembled nanostructures for CO₂ conversion. **Y. Sun**, S. Satagopan, F.R. Tabita, J.R. Parquette

3:10 Intermission.

3:30 350. Dynamic oligomers and stereoisomers controlled by Cucurbiturils. **E. Masson**

3:50 351. Synthesis & design of benzoxazole-linked covalent organic frameworks. **P. McGrier**

4:10 352. Energy-transfer in self-assembled chromophores.
D.A. Modarelli

4:30 353. Design of narrow band-gap benzobisoxazole-containing polymers for organic photovoltaic cells. **J.J. Intemann**

4:50 354. Solution behavior of metal-organic lantern cages.
J.K. Klosterman

5:10 355. Dendritic polymers and crosslinked hydrogel sealants and dressing: Bench to clinic to bench to **M.W. Grinstaff**

Northern Kentucky Convention Center

Room 7

Sensors & Their Applications in Environmental & Occupational Health

Financially supported by Spectroscopy Society of Pittsburgh

D. DeBord, M. Hoover, *Organizers, Presiding*

1:30 356. Bio-nano interface study to build electronic biomarker sensing platform. **S.S. Kim**, Y.H. Ngo, Z. Kuang, J.A. Hagen, B.L. Farmer, R.R. Naik

2:00 357. Development of a lab-on-a-chip for on-site biomonitoring of workers exposed to respirable silica aerosol. A. Chakraborty, **B. Ku**, C.H. Ahn

2:30 358. Evaluation of portable technologies for field sampling applications: HAPSITE field sampling study. **J. Martin**, J. Kwak, C.M. Grabinski, S.W. Harshman, K.L. Chan, M. Fan, B.A. Geier, C.C. Grigsby, D. Ott

3:00 Intermission.

3:30 359. Near real-time detection of surface contamination by hazardous drugs. **J. Smith**, D. Sammons, J. Pretty, K. Kurtz, S. Robertson, D. DeBord, T. Connor, J. Snawder

4:00 Panel Discussion.

THURSDAY EVENING

**Northern Kentucky Convention Center
Ballroom B-C**

ACS Sponsored Posters

J. A. Krause, *Organizer*

5:30 - 7:30

Get involved with the ACS division of chemical education. **D. Zimmerman.**

SCHB experience helps you meet the challenges in the chemical sciences sector. **J. Sabol.**

ACS Small Chemical Businesses Division membership: A valuable tool for the entrepreneur. **J. Sabol.**

**Northern Kentucky Convention Center
Ballroom B-C**

Analytical Chemistry/Instrumentation

J. A. Krause, *Organizer*

5:30 - 7:30

360. One-dimensional transport of colloidal silver nanoparticles in a saturated porous media: A laboratory experiment for chemistry and engineering students. **S.W. Brittle**, S.R. Kanel, J. Dagher, A.J. Meyerhoefer, I.E. Pavel Sizemore

361. Determination of Orexin A by electrochemical impedance spectroscopy. **D. Zhao**, X. Wang, W.R. Heineman, I. Papautsky

- 362.** Enhanced chemistry learning through instrument access and personalized secondary educator training (ECLIPSE): A high school chemistry teacher workshop. **T.M. Perrine**, C. Bowers, B. Wile, C.E. Spiese
- 363.** Composting in a bioreactor lab as part of an environmental chemistry course. **A.M. Reinsel**
- 364.** Probing the UV-induced effects on RNA and RNA-modifications by LC-MS. **C. Sun**, B. Addepalli
- 365.** The need for speed: Efficiency gains of UHPLC vs. high performance column technology. **J.E. Clark**, J. Canty
- 366.** Pyrolysis-gas chromatography of alkyl-modified silica and alkyl-siloxanes: A comparative study. M.E. Gangoda, L. Maurer, **J.H. Murphy**
- 367.** Hazardous byproducts of improperly managed electronic waste. **J. Dietrich**, E. Sahle-Demessie, T. Richardson, J.A. Glaser, C. Lee
- 368.** Rapid evaluation of flame retardants using coated wooden samples. **Y. Li**, T. Deans, D.A. Schiraldi
- 369.** Determination of manganese using cathodic stripping voltammetry and lead using anodic stripping voltammetry. **L. Stegner**, W. Kang, E. Haynes, W.R. Heineman, I. Papautsky
- 370.** Electroanalytical characterization of selected polyphenolic compounds utilizing linear sweep voltammetry (LSV) and DC potential amperometry (DCPA). **K.J. Kubelsky**, N.J. Ronkainen
- 371.** A method development column chromatographic separation of methanol extracts and determination of the chemical profile from Yellow – Striped Oakworm. **J. Howell**,

R. Patel, R. Posey, J. Ellenburg, M. Melnychuk, A. Thomas,
P.B. Nolibos, T. Howell

Northern Kentucky Convention Center
Ballroom B-C
Biochemistry/Medicinal Chemistry
J. A. Krause, Organizer
5:30 - 7:30

372. Examination of the disordered C-terminal domain of a host regulator of HIV-1 splicing. **J.D. Levengood**, C.E. Morgan, B.S. Tolbert

373. The anticancer effects of the antimicrobial peptide CDT and analogs on A549 lung cancer cells. **M. Jujjavarapu**, D. Heyl-Clegg, H. Evans, J. Guthrie

374. NMR studying for conformational selection of hnRNP H on mRNA splicing regulation. **L. Chiu**, S. Penumutthu, B.S. Tolbert

375. Investigating the binding affinity of the peptide humanin and its analogs to amyloid beta. **D. Eस्कilsen**, H. Evans, M. Milletti, J. Guthrie, H. Holmes, D. Heyl-Clegg

376. Biophysical insights into hnRNP A1 recognition of enterovirus 71 stem loop VI IRES domain. **N. Wells**, M. Tolbert, B.S. Tolbert

377. Exploiting kinase-catalyzed labeling to unravel the cellular phosphorylation network. **P.M. Dedigama Arachchige**, M. Pflum

378. Disruption of the dopamine D1/D2 heteromer using synthetic peptides. **M. Champion**, H. Evans, D. Heyl-Clegg, N. Jaber, Z. Alsheemary

379. Inhibition of mushroom tyrosinase by picloram. **K. Alberts**

380. Small-scale modeling of post-synthetic N-acetylgalactosamine (GalNAc) conjugation to oligonucleotide for over 1 kg scale manufacture. **T. Ratterman**, A. Nielander, E. Paredes, H. Cramer, K. Ackley

381. Plasmonic nanoparticle-based hybrid photosensitizers with broadened excitation profile for photodynamic therapy against cancer cells. **P. Wang**, P. Zhang

382. Synthesis and biological activity of aniline-derived diarylisoxazoline insecticides. **J.D. Eckelbarger**, W.C. Lo, R. Hunter, N.M. Niyaz, J.M. Renga, F.E. Tisdell, G. Whiteker

383. Molecular devices for novel drug delivery systems via photoisomerization. D.H. Federman, K. Ratnayake, W. Karunaratne, **J.L. Payton**

384. Structural characterization of the ACCH domain of angiomin family members. **P. Virtanen**

385. The effects of ethylene glycol versus glycerol on lipid production in *Chlorella vulgaris*. **P.E. Adkins**, **A.T. Holland**, A. Stephenson, B. Woodworth, D. Kolling

Northern Kentucky Convention Center

Ballroom B-C

Chemical Education

J. A. Krause, *Organizer*

5:30 - 7:30

386. Effectiveness of the 2015 active learning in organic chemistry mini-workshop. **M. Miller**, J. Houseknecht

387. Comparison of methods to determine the absence of copper from solution: With and without an ammonia test. **M.O. Byrd**, C.J. Ohrenberg

388. Water quality testing as a portion of a service learning experience in the Dominican Republic. C. Daniels, **E. Cady**, **M. Brubaker**

389. Utilizing recycled materials to create a novel product while teaching real-world applications. **L. Gerlinger**, S.K. Lunsford

390. Analysis of functional groups through urinalysis. **J. Domingo**

Northern Kentucky Convention Center

Ballroom B-C

Inorganic Chemistry/Organometallic Chemistry/Catalysis

J. A. Krause, *Organizer*

5:30 - 7:30

391. Photoactive uranyl complexes of salicylidene- \pm -hydroxy acid chelates. **M.A. Chrisman**, J.A. Krause, M.J. Baldwin

392. Luminescence response to capsaicin in an EDTA *bis*-methylamide Tb³⁺ chelate compared to [Tb(EDTA)]⁻. **C.G. Gulgas**, Z. Siddiqui

393. Small ring-openings using a bimetallic nickel catalyst. **H. Schoonover**, C. Uyeda

394. Storage and release of drug molecules in metal-organic frameworks. **P.S. Szalay**

395. Synthesis and characterization of late transition metal complexes with P–N heterobidentate ligands. **N.N. Baughman**, J.L. Petersen, B.V. Popp

396. Four-membered metallacycles arising from an ambiphilic ligand: Synthesis and characterization of Group IX complexes. **R.N. Pickens**, V. Vajpayee, B.R. Nichols, J.L. Petersen, N. Ahkmedov, B.V. Popp

397. In situ infrared spectroscopy study of iron-catalyzed hydromagnesiation of styrene derivatives. **J.A. Rogers**, B.V. Popp

398. Synthesis and investigation of novel water stable lanthanide (III) complexes. I. Janser, **B. Buzrukov**

Northern Kentucky Convention Center

Ballroom B-C

Materials Chemistry/Nanomaterials/Sensors

J. A. Krause, Organizer

5:30 - 7:30

399. Role of structural parameters on constructing ultrasensitive plasmonic-based cardiac Troponin-T sensors. **T.U. Habarakada Liyanage**

400. The growth mechanism and phosphorus doping of MnAs nanoparticles: optimizing properties for magnetic refrigeration. **S.R. Pimmachcharige**, S. Brock

401. Fluorescence imaging of methicillin-resistant staphylococcus aureus with carboxylic acid edging planar surface graphene quantum dots. **S. Begum**, S.R. Chavva, A. Pramanik, P.C. Ray

402. Shape and size tuning of zinc-doped iron oxide nanoparticles for antibacterial applications. **M. Navarreto Lugo**, S. Situ, A. Samia

403. Study of magnetic ordering in cubic-phase double perovskites. **P. Tran**, P. Woodward

- 404.** In-situ liquid cell observation of cysteine-mediated gold nanorod chain assembly. **Y. Chang**, R. Unocic, N. Merrill, M.R. Knecht, B.S. Guiton
- 405.** Rational synthesis of dimensionally reduced TiS₂ phases. **R.A. Morasse**, T. Li, Z. Baum, J.E. Goldberger
- 406.** Inverted linear Halbach array: A novel analytical approach to separate mixed phase magnetic iron oxide nanoparticles. **E.C. Abenojar**, J. Heitler-Klevans, Y. Ijiri, A.S. Samia
- 407.** Structural determination and thermal properties of germanane. **N.D. Cultrara**, M. Arguilla, S. Jiang, B. He, J.E. Goldberger, J. Heremans
- 408.** Rational design and synthesis and covalent postsynthetic modification of *pcu* MOFs based on rare earth M₄(μ₃-OH)₄ clusters. **T. Luo**, S.V. Eliseeva, C. Liu, P. Muldoon, S. Petoud, N.L. Rosi
- 409.** Photo-controlled assembly/disassembly of gold nanoparticles from disordered states to organized states. **Y. Zhou**, N.L. Rosi
- 410.** Low temperature FT-IR studies of adsorption of aldehyde on GaInTiO₂: Role of acid-base sites. **D.K. Paul**, S. Mahhub
- 411.** Development of a multiplexed plasmonic nanoparticle-based assay to identify inhibitors of HuR protein-RNA binding. **G. Yoshida**, J. He, L. Sagle, M. Tranter, A. Gabanic
- 412.** Dioxyalkylene PEEK polymers containing vanillin subunits. **J. Herbort**, **N. Yahna**, W.A. Feld
- 413.** Ultrathin Silica film formation for LSPR based membrane protein biosensing. **I. Bruzas**, S. Unser, S. Yazdi, E. Ringe, L. Sagle

414. Quantitative evaluation of ligand co-loading for gold nanoparticle functionalization. **A. Smith**, K. Johnston, L. Marbella, J. Millstone

415. Modification of Nitinol Nanoparticles with Phosphonic Acid Films. **S. Garretson**, R. Quiñones

**Northern Kentucky Convention Center
Ballroom B-C
Organic Chemistry/Green Chemistry/Catalysis
J. A. Krause, Organizer
5:30 - 7:30**

416. Synthesis of bis(2,2,2-trifluoroethyl) phosphonoesters. **J.A. Zaluski**, J.A. Jackson

417. TLC Dyes. **X. Sun**

418. An epoxidation with possibilities for inquiry-based organic lab. **E. Treadwell**, X. Xiao

419. Large-scale diastereoselective syntheses of cycloheptadienylsulfones and stereotetrads: Application towards the total synthesis of the scarce marine macrolide aplyronine A. **M. Noshi**, S. Abdelmawla, P.L. Fuchs

420. Dearomative dihydroxylation with arenophiles. **E.H. Southgate**, J. Pospech, J. Fu, D.R. Holycross, D. Sarlah

421. Asymmetric synthesis of ³-lactones from vinyl sulfoxonium salts. **S. Kaster**, N. Peraino, N. Kerrigan

422. Dinuclear nickel complex and catalysis. **Y. Zhou**, C. Uyeda

423. A dehydrogenative pictet–spengler-type cyclization using a platinized TiO₂ photocatalyst. **C.M. Adolph**, J. Werth, C. Uyeda

- 424.** Acidity trends under high speed ball milling. **L.N. Trankina**, J. Mack
- 425.** Preparation of cinnamaldehyde *N*-phenylsemicarbazones and dicinnamaldehyde carbazones to explore their photochromicity. **B. Hull**, E. Treadwell
- 426.** Synthesis and investigation of novel chalcone derivatives as chemotherapeutics. I. Janser, **A. Fried**, J. Wotring
- 427.** Developing a sugar-based carboxylic acid hardener for thermoset epoxy resins. **M. Molenda**, Q. Zhang, T.M. Reineke
- 428.** Quantification of weak non-covalent bonding interactions through molecular torsion balances: Alkyl Chlorine. **B. Bloom**
- 429.** Imidazolium-containing thiol-ene polymer networks: Thermal, mechanical and conductive properties. **T. Rhoades**, R.D. Johnson, K.M. Miller
- 430.** Carbon-hydrogen bond activation utilizing monodentate ligands: Synthesis of substituted 2-benzylpyridine ligands and palladium complexes. **M. Straub**, C. Munro-Leighton

Northern Kentucky Convention Center

Ballroom B-C

Physical Chemistry/Computational Chemistry

J. A. Krause, *Organizer*

5:30 - 7:30

- 431.** The surface structure of PEG (polyethylene glycol) hydrogels and peptide functionalized hydrogels as examined by VSFG spectroscopy. **M.R. Watry**, J. McGee, R. Asawa, H. Baca, D. Schmitt, D. Doroski

432. Molecular dynamics simulations of HTLV-1 protease catalyzed reactions. N. Petrillo, K. Vogt, C. VanNess, **S. Ma**

433. Predicting reaction mechanisms and potentials in acid and base from self-consistent quantum theory: H(ads) and OH(ads) deposition on the Pt(111) electrode. **M. Zhao**, A.B. Anderson

434. Molecular dynamics investigation of detergent micelle properties. **B. Bonnett, A. Hoffmaster**, S. Faramarzi, D. Grodi, B. Mertz, E.L. Harvey

Northern Kentucky Convention Center

Ballroom B-C

Polymer Chemistry

J. A. Krause, Organizer

5:30 - 7:30

435. Post-synthetic metallation of 3D dehydrobenzoannulene COFs to enhance adsorption properties. **L.A. Baldwin**, J.W. Crowe, P. McGrier

436. Photo-responsive monomer for light mediated ring opening metathesis polymerization. **I. Fursule**, Q. Zhou, B. Berron, M. Beck

FRIDAY MORNING

Northern Kentucky Convention Center

Room 5

Chemistry & Energy Conversion at Interfaces

L. Baker, Organizer, Presiding

8:00 437. Iron oxide influences the performance of catalysts in the methanol synthesis from syngas. N. Baird, N. Kuchkina, A. Torozova, E. Serkova, Z. Shifrina, M.E. Grigoriev, A. Sidorov, E. Sulman, D.G. Morgan, Y. Losovyj, **L. Bronstein**

8:40 438. Dehydrocyclization of peripheral alkyl groups in porphyrins on copper and silver surfaces. **C.G. Williams**, M. Wang, C. Tempas, D. Skomski, L. Kesmodel, S.L. Tait

9:10 439. Determining the active site for highly selective c=o bond hydrogenation: Understanding the role of the pt–support interface. **Y. Mueannern**

9:40 Intermission.

10:10 440. Recently developed theory and applications to understanding mechanisms in electrocatalysis. **A.B. Anderson**

10:50 441. Improving the stability and selectivity for OER of WO₃ photoanodes with an FeOOH oxygen evolution catalyst. **C.R. Lhermitte**, J.G. Verwer, B.M. Bartlett

11:20 442. Reduction of CO₂ catalyzed by nickel pincer complexes. **H. Guan**

Northern Kentucky Convention Center

Room 9

Entrepreneurship in the Chemical Community

Cosponsored by SCHB

E. Picos, Organizer

J. E. Sabol, Organizer, Presiding

8:00 443. The scientist as an entrepreneur. **E. Picos**

8:30 444. Sources of funding for your business start-up. **S. Jacobs**

9:00 445. Evidence based entrepreneurship. **R. D'Souza**

9:30 446. Starting an analytical testing laboratory in Ohio: Some unanticipated and often amusing problems. **C.S. Gilpin**, R.K. Gilpin

10:00 Intermission.

10:30 447. ACS Entrepreneurial Resources Center: Looking back and looking forward. **D.G. Schmidt**

11:00 448. How the state of Ohio enable and attract business start-ups. **N. Clarke**

11:30 449. Novel ribonucleases for sequencing chemical modifications in RNA. **B. Addepalli**

Northern Kentucky Convention Center

Room 1

Materials Chemistry & Application: Environment, Energy & Biology

Financially supported by Shepherd Chemical Company

N. A. Eckert, R. Hart, S. Taylor, *Organizers, Presiding*

8:00 450. Synthesis of new Mg-rich phases in RE-TM-Mg (RE = rare-earth, T = transition metal) systems: Application for hydrogen storage and much more.... **J. Bobet, E. Guadin**

8:30 451. Cr(III) and Cr(VI) distribution in a Zr/Cr(III) conversion coating on aluminum alloy. **B. Whitman, R. Estrada, G.M. Swain**

9:00 452. Structural and quantitative characterization of CIGS solar cells with different conversion efficiencies. **J. Lee, M. Kim, Y. Lee**

9:30 453. The electrochemical and material properties of a Zr/Cr(III) conversion coating on aluminum alloy 7075. **C. Munson, G.M. Swain**

10:00 Intermission.

10:30 454. Controlled growth of $\text{CH}_3\text{NH}_3\text{PbBr}_3$ nanostructures. **M. Teunis, R. Sardar, P. Dutta**

11:00 455. Effects of metal ions on the antimicrobial properties of silver nanoparticles. **C.D. Bonner**, F.H. Moore, S.O. Obare

11:30 456. Covalently linking anthracene acceptors and the effect on triplet-triplet annihilation upconversion quantum yield. **E.G. Westbrook**, A. Alazemi, P. Zhang

Northern Kentucky Convention Center

Ballroom E

Organic Chemistry & Chemical Biology: Their Impact on Human Health

Cosponsored by MEDI

R. Viswanathan, Organizer, Presiding

8:00 457. Design, synthesis and optimization of 3-phenylchroman-4-one (isoflavanone) aromatase inhibitors. **L. Ma**, K. Bonfield, E. Amato, A.P. Bankemper, A.M. McCallum, T.D. Do, A.J. Onate, F.S. Thowfeik, E.J. Merino, S.F. Paula

8:40 458. Melanin-inspired chemistry. **J.M. Belitsky**

9:15 459. Targeting human ribonucleotide reductase for cancer chemotherapy. **R. Viswanathan**, C.G. Dealwis

9:45 460. Target-inspired innovation in the synthesis of alkaloid natural products. **D.R. Williams**

10:30 Intermission.

10:45 461. Optimization of epithelial-mesenchymal transition inhibitors and a computational analysis of their binding pocket interactions. **R.B. Lettan**, D. Krishnan Achary, N. Werwie, S. Strellec, D. Basu, M. Reyes-Mugica, N. Myshakina, A. Rebbaa

11:15 462. Targeting anti-apoptotic Bcl-2 proteins with re-engineered scorpion toxins. **J.M. Holub**

Northern Kentucky Convention Center

Room 7

Responsive & Functional Polymeric (Nano)Materials

N. Ayres, D. Konkolewicz, *Organizers, Presiding*

8:00 463. The effect of the extent of cross-linking on healing rates of self-healing polymers. **P. Tandler, A. Ellfritz**

8:30 464. Dynamic crosslinked materials using both supramolecular and dynamic covalent linkages. **B. Zhang, Z. Digby, J. Flum, E. Foster, D. Konkolewicz, J. Sparks**

9:00 465. Shape memory polymer heparin-mimicking biomaterials. **Q. Chai, Y. Huang, N. Ayres**

9:30 Intermission.

10:00 466. Synthesis of heparin-mimicking polymers. **N. Ayres, Y. Huang, Q. Chai**

10:30 467. Peptidomimetic polyesters: A modular biomaterials platform with diverse applications. **J.P. Swanson, S.R. Govindarajan, S. Mankoci, T. Jain, A. Joy**

11:00 468. Lactose-containing hydrogels for papain stabilization. **Y. Huang, Q. Chai, M. Warmin, N. Ayres**

Northern Kentucky Convention Center

Room 3

Science at the EPA

S. Willison, *Organizer, Presiding*

8:00 469. Approaches to the development of material flow analysis for used and recycled electronic materials. **J.A.**

Glaser, E. Sahle-Demessie, T. Richardson, C. Lee, S.R. Al-Abed

8:30 470. Advanced oxidation of perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) by ozone and ozone/hydrogen peroxide. **K.M. Finan**, M. Mills, A. Agrawal

9:00 471. Impact of harmful algal blooms on several Lake Erie drinking water treatment facilities and methodology considerations. **H. Mash**

9:30 472. Method development and monitoring of cyanotoxins in water. **J.A. Shoemaker**, D.R. Tettenhorst, W.L. Dietrich, A. de la Cruz, H.J. Allen

10:00 Intermission.

10:30 473. Critical infrastructure resilience: Applied research to respond and recover from contamination of drinking water and infrastructure. **M. Magnuson**, R. Phillips

11:00 474. EPA's selected analytical methods for environmental remediation and recovery. **R. Campisano**

11:30 475. U.S. environmental protection agency's efforts to enhance US radiochemistry capacity and capability in support of a large scale radiological response. **K. Hall**

Northern Kentucky Convention Center

Room 6

Green Chemistry

J. Mack, Organizer, Presiding

9:00 476. The impact of the presence of bromine on the effectiveness of a biobased phosphorus flame retardant. E. Ostrander, **B.A. Howell**

9:25 477. A recyclable surface catalyst for cyclopropenation under mechanochemical conditions. **L. Chen**

9:50 478. Water and nickel: A green combination for reducing carbonyl compounds. **R.A. Haley**, A.A. Fertig, H. Guan, J. Mack

10:15 Intermission.

10:45 479. Green processes for the degradation of organic pesticides. **S.O. Obare**, H.A. Al- Zubaidi, T. Saeed

11:10 480. The synthesis of polyaromatic hydrocarbons via mechanochemistry. **C. Wang**, J. Mack

11:35 481. Making carbon-carbon bonds in tight place. **H. Hopgood**, J. Mack

**Northern Kentucky Convention Center
Room 4**

Nanomaterials & Medicine

Financially supported by ThermoFisher Scientific

L. Sagle, A. S. Samia, *Organizers, Presiding*

9:00 482. Controlling the shape of iron oxide nanoparticles using lyotropic liquid crystal templates. **T. Hegmann**

9:35 483. Plasmon-resonant nanorods and nanostars: Multifunctional agents for nanomedicine. **A. Wei**

10:10 484. Novel nanoparticle development for controlled drug release with ultrasound imaging monitoring. **Z. Zhang**, M. Taylor, C. Collins, X. He

10:30 Intermission.

10:50 485. Nanoparticle delivery of PDT drugs: Covalent versus non-covalent drug loading. **C. Burda**

11:25 486. Targeting membrane receptors with plasmonic nanostructures. **Z.D. Schultz**

FRIDAY AFTERNOON

Northern Kentucky Convention Center

Ballroom B-C

ACS Sponsored Posters

J. A. Krause, *Organizer*

12:00 - 2:00

Get involved with the ACS division of chemical education. **D. Zimmerman.**

SCHB experience helps you meet the challenges in the chemical sciences sector. **J. Sabol.**

ACS Small Chemical Businesses Division membership: A valuable tool for the entrepreneur. **J. Sabol.**

Northern Kentucky Convention Center

Ballroom B-C

Analytical Chemistry/Instrumentation

J. A. Krause, *Organizer*

12:00 - 2:00

487. Optimum experimental conditions for the determination of total polyphenols using the peroxidase-based amperometric biosensor. **Y. Kong**

488. Electrochemical behavior of 1,2-dihydroxybenzenes in the presence of common intereferent with cnt-P3HT electrode. **J. Lee, D. Dodson, L. Zhai, S.K. Lunsford**

489. Aldehyde detection in electronic cigarette aerosols. **M. Ogunwale, M. Li, M. Ramakrishnam Raju, M.H. Nantz, D. Conklin, X. Fu**

490. Mercury in an aquaponics system: Effects of diet supplementation on Nile tilapia reared in a closed recirculating aquaculture system (RAS). **M. Schmale**, S. Smith, M. Wang, J.A. Landero, J.A. Caruso

491. Gold nanoprisms for plasmon-enhanced single-molecule fluorescence in live bacteria. **S.A. Lee**, J.D. Flynn, J.S. Biteen

492. Mathematical strategies for the analysis of human cremated remains. **C.A. Farwick**, K.L. Sparks, W.C. Wetzel, C.A. Currie

493. Effect of water on the chemical residue from combusted accelerants. **K.L. Hood**, W.C. Wetzel

494. A pluronic gel phase for electrophoresis of peptides. E.M. Leonard, A.E. Richardson, **N.D. Danielson**

495. Initial synthesis and characterization of acrylate and methacrylate porous polymer monoliths. **B. Cecil**, K. Ries, J. Ziebro, C. Daniels

496. Analysis of ground spices with a handheld x-ray fluorescence analyzer. M.Y. Wu, S. Baghaie, S. Thomas, M.A. Benvenuto, **E. Roberts-Kirchhoff**

497. Energy and water sustainability: A University of Cincinnati and University of Bordeaux collaboration. **A. Kelsey**, **S. Braley**, **G. Bown**, **G. Buckey**, **J. Burke**, **V. Chamard**, **X. Chudeau**, **M. Dottor**, **E. Ferguson**, **V. Fericelli**, **G. Roudier**, **A. Negri**, **I. Perez**, **M. Sarama**, **C. Soule**, **M. Thomas**, J. Bobet, H. Guan, W.B. Connick

Northern Kentucky Convention Center
Ballroom B-C
Biochemistry/Medicinal Chemistry
J. A. Krause, *Organizer*
12:00 - 2:00

498. Beta-lactones formed via ketoketene dimerization inhibit carboxylesterases but not by covalent mechanisms. **K. McAuliffe**, N. Kerrigan, A.W. Bull

499. Impact of as-synthesized ligands and low-oxygen conditions on silver nanoparticle surface functionalization. **K. Johnston**, A. Smith, L. Marbella, J. Millstone

500. Investigation of RNA oxidation via selective generation of a C5'-uridinyl radical. **M. Ellis**, A.C. Bryant-Friedrich

501. Structural and inhibitor screening studies of fungal forms of aspartate semialdehyde dehydrogenase. **G.P. Dahal**, R.E. Viola

502. Synthesis of 2'-C-methyl pseudouridines for the inhibition of HCV RNA-Polymerase. **I. Sappy**, J. Nunnari

503. Fate of A 5'-aldehyde derived from C5'-oxidation in single-stranded oligonucleotides. **S.H. Cho**, S.A. Audat, A.C. Bryant-Friedrich

504. Preliminary characterization of human aspartate *N*-acetyltransferase. **Q. Wang**, M. Zhao, G.G. Parungao, R.E. Viola

505. Single molecule protein patterning using hole mask colloidal lithography. **W. Lum**, M. Vieweger, I. Bruzas, P. Guo, L.B. Sagle

506. Investigating host-guest interactions of avobenzone with *tert*.-butylcalix[8]arene. **A. Eisenhart**, M. Mirzamani, F. Heinrich, A.D. Gudmundsdottir, T.L. Beck, H. Kumari

507. Identification of urine metabolic biomarkers for mouse ischemic acute kidney injury. **T. Chihanga**

508. Synthesis and DNA binding activity of Pt(II)-DMSO and Ru(I)-bipyridine complexes of N-3-pyridylmethylthymidine. **K.M. Church**, J. Chen, K. Li, S. Swavey

509. Synthesis of penicillin-G derivatives. **K. Burrige**, D.T. Esterline

510. Progress towards a plant expression system for copper amine oxidases. **V. Doss**, S.A. Mills

511. Structure-guided development of antibiotics targeting metallo-beta-lactamases using protein X-ray crystallography. **C. Williams**, M. Aitha, R. Bonomo, D.L. Tierney, M.W. Crowder, S. Cohen, W. Fast, R.C. Page

Northern Kentucky Convention Center

Ballroom B-C

Chemical Education

J. A. Krause, *Organizer*

12:00 - 2:00

512. How the ACS bylaw for director-at-large elections was changed. **W.L. Dilling**

513. “Chemical-free” gardens, produce, crop storage bags, pest control materials, weed killers, and food. **W.L. Dilling**

Northern Kentucky Convention Center

Ballroom B-C

Inorganic Chemistry/Organometallic Chemistry/Catalysis

J. A. Krause, *Organizer*

12:00 - 2:00

514. Bioinspired \pm -hydroxy acid containing tripodal amine chelates, derivatives and photoactivity of their metal complexes. **J.E. Vernia**, M.J. Baldwin

515. Nickel complexes of deprotonated $\text{HN}(\text{CH}_2\text{CH}_2\text{P}^i\text{Pr}_2)_2$ and their reactivity. **N.P. Nambukara Wellala**, J. Luebking, H. Guan

516. Nickel-catalyzed hydroamination of allenes utilizing novel [(Iminophosphine)nickel(allyl)][OTf] catalyst. **H. Tafazolian**, J.A. Schmidt

517. Preparation of cooperative multi-electron reagents. **S. Hendrickson**

518. Stoichiometric delivery of chlorine to substrates. **A. Stastny**, A.E. Norton, J.A. Krause, W.B. Connick

519. Formation of new transition metal complexes containing two \pm -hydroxy acid moieties. **A. Elshewy**, M.J. Baldwin

520. Synthesis and spectroscopy of two benzil-based diimine ligands and their complexation to palladium(II) and platinum(II). **J.M. Justice**, T.W. Green

Northern Kentucky Convention Center

Ballroom B-C

Materials Chemistry/Nanomaterials/Sensors

J. A. Krause, Organizer

12:00 - 2:00

521. Kinetic studies of vapochromic platinum(II) complexes. **M. Karimi Abdolmaleki**, A.E. Norton, S. Taylor, W.B. Connick

522. Detection of lead by anodic stripping voltammetry using vertically aligned carbon nanofibers. **J. Robinson**, L. Sagle, W.R. Heineman, M. Meyyappan, J. Koehne

523. Investigating the effect of surfactant ethoxylation on the aqueous solubility of calixarene-based nanocapsules. **C. Ade-Browne**, H. Kumari

524. Investigating host-guest interactions of Curcumin with *p*-*tert*-butylcalix[n]arenes. **M. Mirzamani, H. Kumari**

525. Water-soluble porphyrins as supramolecular biosensors. **A. Mammana, S. Thorpe**

526. Biosensors development for monitoring cyanotoxins in water environment systems. **V. Voghazi, L. Zhang, D. Zhao, N. Alvarez, S. Chae, L. Sagle, W.R. Heineman, V.N. Shanov, D.D. Dionysiou, I. Papautsky**

527. One-pot in-situ synthesis of polypyrrole composites with inorganic fillers. **V. Livingstone, C. Lind-Kovacs**

528. A solution-phase route towards transition metal carbido clusters. **Z. Baum, J.E. Goldberger**

529. ²-galactosidase langmuir monolayer at air/subphase interface. **S.K. Sharma, R.M. Leblanc**

530. Microwave-assisted synthesis of polystyrene-organoclay nanocomposites by surface-initiated polymerization from thiol-functionalized organoclays. **J. Becker, T. Schuyler, M. Coeurdray, K. Mbow, I.L. Lagadic**

531. Spectroscopic analysis of tunable, stimuli responsive polymeric materials. **A. Gasper, J. Church, C. Daniels**

Northern Kentucky Convention Center

Ballroom B-C

Organic Chemistry/Green Chemistry/Catalysis

J. A. Krause, Organizer

12:00 - 2:00

532. Developing a novel, electronically diverse and persistent carbene. **D.J. Martin, J. Wardale, B. Mayro, Z. Herman, J.P. Moerdyk**

- 533.** A Chemical Indirect Quantification Method of 5-HydroxymethylcytosinA chemical indirect quantification method of 5-hydroxymethylcytosine. **G. Premnauth**
- 534.** Stability of nitrene radical intermediate in solid state and solution phase, Photochemistry of 3-azido-3-phenylphthalide. **K.R. Thenna Hewa, A. Gudmundsdottir**
- 535.** Alkyl nitrene formation from diazido derivate in solution and cryogenic matrices. **D.M. Sriyarthne, A. Gudmundsdottir**
- 536.** Cationic palladium catalyzed acylation of alcohols and carbohydrate-derived polyols with highly hindered acid anhydrides. **E. Mensah, M. Eichholtz, F. Reyes**
- 537.** Chemo-selective transfer hydrogenation of nitroarenes by highly dispersed Ni-Co BMNPs. **C. Chun**
- 538.** Impact of incorporation of \pm -alkylated amino acids on 2 -hairpin peptide folded stability. **S.L. Schettler, M. Karnes, G. Lengyel**
- 539.** Wavelength Dependent Matrix Isolation of Vinyl Azides. **O. Osisioma, B. Ault, A. Gudmundsdottir**
- 540.** Solid state photochemistry of diazide naphthaquinones: A tale of dancing crystals. **D. Shields, S.K. Sarkar, A.D. Gudmundsdottir, J.A. Krause**
- 541.** Transition metal oxide catalysts for photoelectrochemical CO₂ reduction and water oxidation. **E. Fugate, X. Yang, J. Husek, L. Baker**
- 542.** Light as a reagent: 3 -azido aryl carbonyls in photochemical synthesis. **D.M. Gatlin, A. Perry, A.D. Gudmundsdottir**

543. Effects of *para*-Substitution in Imine Synthesis. **E. Hruska**, B. Knettle

544. Organic chemistry lab development: Enantiomeric resolution using \pm -amino acids. **A.E. Brown, M. Tate**, J.L. Marshall, S.S. Marine

545. Reductions of carbonyl compounds in high speed ball mill. **A.A. Fertig**, R.A. Haley, J. Mack, H. Guan

546. Heteroarene alkylation using alcohols. **D.N. Mustafa**, J.M. Lear, K. Pan, D. Nagib

547. Degradation of β -carotene in the presence of Photogenerated 1 $^\circ$, 2 $^\circ$, and 3 $^\circ$ alkyl radicals. **P. Dugan**, A. Johnson, K. Arnold, S. Dubay, R. Poston, M. Duniyakh, M. Masthay

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Ballroom B-C

Physical Chemistry/Computational Chemistry

J. A. Krause, *Organizer*

12:00 - 2:00

548. Molecular dynamics simulations of protein unfolding and translocation by the ClpY ATPase in the protein degradation pathway. **Y. Shih**, G. Stan

549. ClpB-mediated unfolding mechanisms of GFP: Two different pathways breakdown and the effect of force directionality. **R. Jiang**, A. Kravats, G. Stan

550. Light scattering contributions to the absorption and circular dichroism spectra of the laser-induced blue state of bacteriorhodopsin. **C. McGrath**, A. Rudraraju, A. Mammana, **M. Hufnagle**, M. Masthay

551. Structural modeling of modularly designed coiled-coil based supramolecular polymers. **N.A. Tavenor**, M. Lawless, M. Murnin, S.K. Saxena, W.S. Horne

552. Normal mode analysis of conformational changes in the ClpP peptidase. **Q. Wang**, G. Stan

553. Investigating the role of lattice defects in the severing of microtubules using large scale simulations. **N. Jiangu**, R.I. Dima

554. DFT modeling of the antioxidant properties of thione and selone ligands coordinated to iron(II). **M.I. Brewer**, C.A. Bayse

Northern Kentucky Convention Center

Room 2

Bio-Analytical Chemistry from Instrumentation to Regulation

J. A. Landero, *Organizer, Presiding*

1:30 555. A zinc regulatory nexus programs the M2 macrophage phenotype and promotes pathogen survival. **K. Subramanian Vignesh**, J.A. Landero, A. Porollo, S. Divanovic, J.A. Caruso, G.S. Deepe Jr.

1:55 556. Methodologies for the characterization of trace elemental impurities in FDA regulated products. **T.A. Hanley**, K. Kubachka, R.A. Wilson, M. Mantha, J. Urban, K. Niehaus, R. Saadawi, E. Yanes-Santos, N. Shockey

2:20 557. Investigation of the mechanism of lead biosorption by cilantro. **T.B. Robertson**, D.J. Schauer

2:45 558. HPLC separation & detection of PAHs in hookah tobacco smoke via C-18 SPME. **A.A. Clutterbuck**, J.A. Caruso, J.A. Landero

3:10 Intermission.

3:30 559. Interactive effects of arsenic and selenium in aquaponic systems by HPLC and ICP-MS. **S. Smith, M. Schmale, J.A. Landero, J.A. Caruso**

3:55 560. Metal ion transport in biological tissues measured by ICP-MS. **J. Heiny, J.A. Landero, C.A. Stiner, T. Radzyukevich**

4:20 561. Subtle omega end group functionalization drives drastic depletion from polymer surfaces observed by emerging mass spectrometry technique. **J. Hill, K. Endres, Q. He, M.D. Foster, C. Wesdemiotis**

4:45 562. Unique atmospheric-pressure plasmas as sources of atomic, molecular, and biomolecular ions for mass spectrometry. **J.T. Shelley, A. Schwartz, S.P. Badal, K.L. Williams, C.L. Walton, G.M. Hieftje**

5:10 563. Essential approaches to characterization of lignin hydrotreatment products. **A. Artemyeva, J. Kreft, K. Voeller, J. Bilek, A. Dostalkova, E.I. Kozliak, A. Kubatova**

Northern Kentucky Convention Center

Room 7

Biochemical & Biophysical Approaches to Tackling Disease

R. C. Page, *Organizer, Presiding*

1:30 564. The biophysics behind bacterial biofilms: how metal-dependent protein assembly leads to recurrent Staph infections. **A.B. Herr**

2:10 565. Structural basis for phospholipase C regulation. **A. Lyon**

2:40 566. Structural insights of ZIP4 extracellular domain critical for optimal zinc transport. **J. Hu**

3:10 567. Two-photon induced fluorescence resonance energy transfer (2P-iFRET) to monitor molecule-DNA interactions and DNA melting. **S.H. Al-Otaibi**, R. Guda

3:35 Intermission.

3:55 568. Integrated biophysical approaches to reveal mechanisms that control HIV genome splicing. **B.S. Tolbert**

4:25 569. New frontiers in lipidomics: tools for understanding how an emerging class of biological lipids, lipoamines, play novel roles in cellular communication. **H. Bradshaw**

4:55 570. Perilipin 5: A regulator of neutral lipid storage in oxidative tissues. **J.T. Tansey**

Northern Kentucky Convention Center

Room 5

Chemistry & Energy Conversion at Interfaces

L. Baker, Organizer, Presiding

1:30 571. Structural conformation of methacrylate-based functionalized monomers and polymer thin films at the air-monomer, and air-polymer thin films interfaces. **K.A. Cimat**, S.C. Chan, U. Premadasa, N.M. Adhikari

2:10 572. Extracting electrons out of colloidal quantum dots: Challenges and new perspectives. P. Dutta, C. Mi, M. Saniepay, J.W. Sayen, **R. Beaulac**

2:50 573. Synthesis of $\text{Cu}_x\text{Ni}_{1-x}\text{WO}_4$ and application in energy conversion. **S. Hosseini**, Z. Li, H. Farsi

3:20 Intermission.

3:50 574. CO₂ hydration enhancement using homogenous catalysts in primary amine solution. **M. Sarma**, C. Lippert, L. Widger, K. Liu

4:30 575. Synthesis, photophysical properties and water oxidation studies of a series of novel photosensitizer-catalyst dyads. **N. Nair**, R. Zhou, R.P. Thummel

5:00 576. Thermodynamics of POCOP pincer nickel hydride and formate complexes. **N.A. Eberhardt**, J.A. Krause, H. Guan

Northern Kentucky Convention Center

Ballroom D

**Electroanalytical Chemistry in the Central Region-
Special Symposium Honoring the Career of William
Heineman**

Cosponsored by ANYL

A. F. Bange, Organizer, Presiding

1:30 577. Microfluidic platforms and technologies for neurotransmitter measurement with capillary electrophoresis. **M. Gong**

2:00 578. Flow injection based analysis: Flexible framework for new approaches in chemical and biochemical analysis. **S. Kradtap**

2:30 579. Modified thin-film spectroelectrochemical sensor for the detection of technetium. **S.D. Branch**, J. Bello, S.A. Bryan, W.R. Heineman

3:00 580. Determination of manganese using cathodic stripping voltammetry. **A.F. Bange**, C.A. Rusinek, W. Kang, W.R. Heineman, I. Papautsky

3:30 Intermission.

4:00 581. The personal impact of chemistry graduate school training, research and mentoring on industrial researchers and their impacts on industrial R&D. **P. Schofield**, K. Wehmeyer, M.J. Doyle

4:30 582. Developing new electrode materials through analytical chemistry. **E.S. De Castro**

5:00 583. The critical role cheminformatics plays in defining the future of toxicology: A new basis for chemical/product risk assessment. **M.J. Doyle**, S. Wu

Northern Kentucky Convention Center

Room 9

Entrepreneurship in the Chemical Community

Cosponsored by SCHB

J. E. Sabol, *Organizer*

E. Picos, *Organizer, Presiding*

1:30 584. From scientist to entrepreneur: How I started and where i am now: A panel discussion session. **J.E. Sabol, R. Takigiku, R. Ford, L.K. Tennant**, Y. Hsieh

1:45 Panel Discussion.

Northern Kentucky Convention Center

Room 6

Green Chemistry

J. Mack, *Organizer, Presiding*

1:30 585. Sustainability education by the Midland, MI kids and chemistry group. **R.M. Malczewski**, M.L. Rivard

1:55 586. Two decades of the presidential green chemistry challenge awards provide powerful illustrations of green chemistry for greening the chemistry curriculum, to educate the public, and for industries to emulate. **M.C. Cann**

2:20 587. From the minds of graduate students: an online green chemistry course. **H. Hopgood**, A. Das, K. Leahy, R.A. Haley, J. Ringo, D. Waddell

2:45 588. Greening the curriculum at the University of Toledo School of Green Chemistry and Engineering. **M.R. Mason**

3:10 Intermission.

3:40 589. A mechanochemical TEMPO/Oxone system for the oxidation of primary alcohols. **K. Leahy**, P. Carr, J. Mack

4:05 590. Renewable biosources for the generation of effective flame retardants for polymeric materials. **B.A. Howell**

4:30 591. Understanding the mechanochemistry energetics in an 8000M mixer/mill. **J.M. Andersen**, J. Mack

4:55 592. Flame retardant polymers for multilayered systems. **T. Deans**, Y. Li, D.A. Schiraldi

Northern Kentucky Convention Center

Room 1

Inorganic Chemistry, Organometallics & Sensors-Bioinorganic & Catalysis

W. B. Connick, J. A. Krause, *Organizers*

M. J. Baldwin, *Presiding*

1:30 593. Silver(I)-promoted oxidative cross-dehydrogenative coupling of phenols and aniline derivatives. **J. Fotie**, S. Berkessa, Z. Clarke

2:00 594. Ferrocene containing n-heterocyclic carbene based gold anticancer agents. **K. Arumugam**, K. Sidoran, R.E. McCall, J.F. Arambula

2:30 595. Ferrioxamine microarrays for the rapid detection and discrimination of pathogenic bacteria. **N. Arora**, A. Wei

3:00 Intermission.

3:15 596. Solid-state thermochromic and spin equilibria of $\text{Ni}(\text{detu})_4\text{Cl}_2$. **M.P. Jensen**, I.A. Alfurayj, V.G. Young

3:45 597. Substrate activation and catalysis at an intact metal-metal bond. **T. Steiman**, C. Uyeda

4:15 598. Electrocatalytic effects induced by adsorbed halides: The reduction of hexaaquairon (III) in aqueous solutions. **N. Georgescu**, A.J. Jebaraj, D.A. Scherson

4:45 599. Peptide-directed synthesis of single helical gold nanoparticle superstructures. **A. Merg**, G. Zhao, A. Mandal, J. Boatz, X. Wang, P. Van Der Wel, P. Zhang, N.L. Rosi

Northern Kentucky Convention Center

Room 8

Methods & Applications of Radioanalytical Chemistry for Nuclear Forensics & Health

S. Glover, H. Spitz, *Organizers, Presiding*

1:30 600. Implications to Nuclear Forensics of Early Manhattan Project Facilities and Processes. **S. Glover**, H. Spitz, S. LaMont

2:10 601. Analysis of post-detonation actinide-rich particles found in Bikini Atoll soil. **K. Hoffman**, G. Sam, W. Connick, H. Spitz

2:40 Intermission.

3:00 602. Analysis of strontium-90 and cesium-137 in samples of calcium-rich soil from the Marshall Islands. **S. Herman**, S. Glover, W.B. Connick, H. Spitz

3:30 603. Radiation effects on Li-ion battery electrolyte. **C. Tan**, D.J. Lyons, Y.F. Zheng, A. Co, L.R. Cao

Northern Kentucky Convention Center

Room 4

Nanomaterials & Medicine

Financially supported by ThermoFisher Scientific

L. Sagle, A. S. Samia, Organizers, Presiding

1:30 604. Biocompatible liquid crystal elastomers with porous morphology for spatial cell scaffolds. **E. Hegmann**, T. Mori, A. Sharma, R.J. Clements, E.J. Freeman, J.A. McDonough, L.T. Korley, T. Hegmann

2:05 605. Controlling the diverse interactions of collagen for plasmonic biosensing applications. **S. Unser**, L. Sagle

2:25 606. Surface-enhanced raman spectroscopy study of the interaction between colloidal silver nanoparticles and *dengue virus* virions: Unsupervised automated peak detection and quantification using a newly released spectroscopic imaging software. **D.P. Foose**, A.A. Paluri, K.J. Williams, C. Anders, K.M. Dorney, N.J. Bigley, I.E. Pavel Sizemore

2:45 607. Near-Infrared Photothermal Therapy *In-Vitro* Utilizing Iron Oxide Nanoparticles. **A. Dunn**, D. Shi, Y. Zhang

3:05 Intermission.

3:25 608. Nanoplasmonic-based microRNA assay in patients plasma: From benchtop to bedside. T. Liyanage, M. Korc, **R. Sardar**

4:00 609. Microfluidic and multiplexed LSPR substrates for DNA detection. **J. He**, C. Bulach, M. Boegli, L.B. Sagle

**Northern Kentucky Convention Center
Room 3
New Frontiers in Organic Chemistry
D. Nagib, *Organizer, Presiding***

1:30 610. Development of new catalytic methods for the synthesis of natural products. **P. Nagorny**

2:05 611. Total synthesis of complex natural product via carbonylation strategy. **M. Dai**

2:40 612. A radical chaperone strategy for directed C-H functionalization. **D. Nagib**

3:15 Intermission.

3:30 613. Catalytic transformations that utilize bimetallic cooperation. **N.P. Mankad**

4:05 614. Transition metal-catalyzed direct functionalization of unactivated sp^3 CH bonds. **H. Ge**

4:40 615. New developments in catalytic carbocyclization reactions. **C. Schindler**

**Northern Kentucky Convention Center
Ballroom E
Organic Chemistry & Chemical Biology: Their Impact on Human Health
Cosponsored by MEDI
R. Viswanathan, *Organizer, Presiding***

1:30 616. Microbial natural products discovery and diversification. **J.S. Thorson**

2:15 617. Structures and mechanisms of nicotinate catabolizing enzymes: A model system for investigating

bacterial *N*-heterocyclic aromatic compound degradation and for undergraduate education. **M.J. Snider**

3:00 Intermission.

3:15 618. Biochemical characterization of *E. coli* periplasmic beta-glucosidase BglX. **N.V. Stourman**, L. Sui, L. Ngo, J. Weimer, T. Pickens

3:55 619. The Discovery of Novel Antifungal Compounds using a Multidisciplinary Undergraduate Training Pipeline. **R. McLane**, A. Cox, S. Reid, L. Edelen, Y. Daher, A. Grau, H. Otte, K. Wesley, S. Anderson, **A.J. Onorato**, J. Carmen

4:30 620. Unusual mechanisms in alkaloid natural product biosynthesis. **R. Viswanathan**

SATURDAY MORNING

Northern Kentucky Convention Center

Room 2

K-12 Teachers Program & Workshop

Cosponsored by CHED

Financially supported by ACS Midland Section

L. Ford, L. Hogue, *Organizers, Presiding*

8:15 Introductory Remarks.

8:30 621. Teaching climate change at the pre-college level. **A.D. Jorgensen**

9:45 622. Greening your laboratory program. **L. Ford**

10:30 623. Argument-based inquiry. **L. Hogue**

Logan Hall, Xavier University
Room 204
K-12 Teachers Program & Workshop
Cosponsored by CHED
Financially supported by ACS Midland Section
L. Ford, L. Hogue, *Organizers*
R. M. Malczewski, *Presiding*

8:15 Introductory Remarks.

8:30 624. Sci tech next generation: A hands-on science workshop for elementary and middle school teachers. **R.M. Malczewski**

SATURDAY AFTERNOON

Northern Kentucky Convention Center
Room 2
K-12 Teachers Program & Workshop
Cosponsored by CHED
Financially supported by ACS Midland Section
L. Ford, L. Hogue, *Organizers, Presiding*

1:15 625. Teaching the delicious chemistry of food. **J.L. Marshall**

2:45 626. Enriching high school chemistry teaching through POGIL. **P.W. Butler**