NSF-supported Peer Reviewed Publications: (Undergraduate co-authors are underlined)


NSF-supported Manuscripts in Peer-Review: (Undergraduate co-authors are underlined)


4. Morales, A. C.; Cooper, N. C.; Reisner, B. A.; DeVore, T. C. Enthalpy of formation of $K_2M(SO_4)_2 \cdot 6 \text{H}_2\text{O}$ (M = Mg, Co, Ni, Cu, Zn). *J. Therm Ana., Calor,* submitted. [REU CHE-1461175, MRI CHE-0320245, and IMR DMR-0315345]


7. Walton, L. R.; Knight, S. E.; Herold, S. K.; Olsonowski, K. J.; Amenta, D. S.; Gilje, J. W.; Yap, G. P. A. The reactions of $\text{RuCl}_3(\text{NO})(\text{PPPh}_3)_2$ and $\text{RuCl}_3(\text{NO})\text{H}_2\text{O}$ with $\text{Ph}_2\text{P(\text{CH}_2)_n(\text{O})Ph}_2$, $n = 1, 2, \text{or} 3$: Crystal structures of ruthenium nitrosyl complexes containing monodentate and chelating $\text{Ph}_2\text{P(\text{CH}_2)_n(\text{O})Ph}_2$ ligands. *Polyhedron*, submitted. [REU CHE-1062629 and REU CHE-1461175]

NSF-supported non-JMU presentations:

Amenta/Gilje


5. Jackson, C. E.; Amenta, D. S.; Gilje, J. W. The synthesis of propanamide derivatives of 1H-1,2,3-triazole and their reaction with palladium complexes. Presented at the 19th Undergraduate Research Symposium, Baltimore, MD October 22, 2016. REU CHE-1461175

Boardman


8. Boardman, B. M.; Reeves, B. J.; Shircliff, D. M.; Shott, J. L. Synthesis, characterization, and investigation of cobalt chalcogenide clusters with thienyl phosphate ligands as new acceptor materials for P3HT. Presented at 249th American Chemical Society National Meeting & Exposition, Denver, CO, March 22-26, 2015; INORG-909, Cottrell College Science Award, 22628, REU CHE-1062629


14. Corbin, D. A.; Shircliff, D. M.; Reeves, B. J.; Boardman, B. M. The synthesis and characterization of polymerized cobalt selenide clusters with photovoltaic applications. Presented at University of Baltimore Maryland County, Baltimore, MD, October 3, 2015. Won 2nd place poster in chemical sciences Cottrell College Science Award 22628, REU CHE-1461175


17. Corbin, D. A.; Boardman, B. M. Solid state characterization of hybrid copolymers with photovoltaic applications. Presented at University of Baltimore Maryland County Undergraduate Research Symposium, Baltimore, MD, October 22, 2016. Won 2nd place in Chemical Sciences. Cottrell College Science Award 22628, REU CHE-1461175


21. Corbin, D. A.; Boardman, B. M. Recent advances in the optical and structural characterization of organic-inorganic copolymers with photovoltaic applications. Presented at ACS Local Section Meeting, University of Virginia, Charlottesville, VA, April 14, 2017. Cottrell College Science Award 22628, REU CHE-1461175

Caran


24. Walsh, B.; Thompson, K.; Marafino, J. N.; Damiano, L.; McKenna, K.; Gallagher, T.; Seifert, K.; Caran, K. L. Synthesis and study of novel amphiphiles as potent antiseptics. Presented at the 17th Annual Undergraduate Research Symposium in the Chemical and Biological Sciences, University of Maryland, Baltimore County, October 25, 2014; poster presentation. *Brenna and Kirstie won first prize in their section for their presentation of this poster. RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521


Antiseptics and Novel Colloids: Exploring Structure Activity Relationships. Presented at the 18th Annual Undergraduate Research Symposium in the Chemical and Biological Sciences at the University of Maryland, Baltimore County (UMBC), Baltimore, MD, October 3, 2015; poster presentation. *Brenna won first prize in her section for her presentation of this poster. RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521

29. Rister, A.; Marafino, J.; Rogers, E.; Caran, K.; Seifert, K. Colloidal and Biological Properties of M-E. Presented at the 18th Annual Undergraduate Research Symposium in the Chemical and Biological Sciences at the University of Maryland, Baltimore County (UMBC), Baltimore, MD, October 3, 2015; poster presentation. RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521

30. Thompson, K.; Rogers, E.; Seifert, K.; Caran, K. L. The Effect of Hofmeister Series Counterions on the Colloidal and Antimicrobial Properties of a Triple-Headed Single-Tailed Amphiphile. Presented at the 18th Annual Undergraduate Research Symposium in the Chemical and Biological Sciences at the University of Maryland, Baltimore County (UMBC), Baltimore, MD, October 3, 2015; poster presentation. *Kirstie won first prize in her section for her presentation of this poster. RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521


33. Ashamole, B.; Rogers, E.; Ogunjirin, E.; Seifert, K.; Caran, K. L. Antimicrobial and Colloidal Properties of Novel Polycationic Amphiphiles. Presented at the 19th Annual Undergraduate Research Symposium in the Chemical and Biological Sciences at the University of Maryland, Baltimore County (UMBC), Baltimore, MD, October 22, 2016; poster presentation. RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521

34. Lauer, M. K.; Caran, K. L.; Rogers, E.; Seifert, K. A Study of Fluorescent Quaternary Ammonium Amphiphiles to Gain Insight Into The Mechanism of Antibacterial Activity. Presented at the 19th Annual Undergraduate Research Symposium in the Chemical and Biological Sciences at the University of Maryland, Baltimore County (UMBC), Baltimore, MD, October 22, 2016; poster presentation. RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521


Devore

Oral

41. DeVore, T. C.; Snell-Feikema, R. Can DSC be used to Determine the Enthalpy of Formation for Metal Oxalates? VA Acad of Sciences, James Madison University, Harrisonburg, VA, May 21-23, 2015, Presentation CHEM 11. REU CHE-1461175, MRI CHE-0320245, and IMR DMR-0315345

42. DeVore, T. C. Coupling experiment with DFT calculations: On the road to discovery, VA Acad of Sciences, James Madison University, Harrisonburg, VA, May 21-23, 2015, Presentation EDU 3. REU CHE-1461175, MRI CHE-0320245, and IMR DMR-0315345

43. DeVore, T. C.; Bagley, A.; Yin, J. Coupling DFT calculations with experiment in the physical chemistry laboratory. 2015 SERMACS- SWRM, Memphis, TN, Presentation 52. REU CHE-1461175, MRI CHE-0320245, and IMR DMR-0315345


46. DeVore, T. C. Chemistry and spectroscopy in KBr matrices, VAS, May 19, 2016.


48. DeVore, T. C.; Morales, A.; Reisner, B. A., Decomposition pathways for the Tutton Salts $K_2M(SO_4)_2 \cdot 6 H_2O$ (M = Mg, Co, Ni, Cu, Zn), SERMACS – 1087, Oct 26, 2016. REU CHE-1461175, MRI CHE-0320245, and IMR DMR-0315345

49. DeVore, T. C.; Morales, A. C.; Cooper, N. C.; Reisner, B. A., Enthalpy of formation of $K_2M(SO_4)_2 \cdot 6 H_2O$ (M = Mg, Co, Ni, Cu, Zn), SERMACS – 1169, Oct 26, 2016. REU CHE-1461175, MRI CHE-0320245, and IMR DMR-0315345

Poster

50. Morales, A. C.; Cooper, N. C.; Reisner, B. A.; DeVore, T. C. Thermal decomposition of $K_2M(SO_4)_2 \cdot 6 H_2O$ (M = Mg, Co, Ni, Cu, Zn) SERC, Oct 20 – 21, 2016. REU CHE-1461175, MRI CHE-0320245, and IMR DMR-0315345

51. Morales, A. C.; Cooper, N. C.; Reisner, B. A.; DeVore, T. C. Thermal decomposition of $K_2M(SO_4)_2 \cdot 6 H_2O$ (M = Mg, Co, Ni, Cu, Zn) UMBC Undergrad Research Conference, Oct 22, 2016. REU CHE-1461175, MRI CHE-0320245, and IMR DMR-0315345

Hughey


54. Mattilla, J. M.; Hurdle, S. A; Lucas, S. K. Comparison of negative ion ESI ionization efficiencies for a diversity of small acidic molecules with widely varying pKas. Presented at 63rd ASMS Conference on Mass Spectrometry & Allied Topics, St. Louis, MO, May
31-June 4, 2015; Poster ThP01-006 (Ambient Ionization: Fundamentals). MRI CHE-0922935, MRI CHE-1046630, RUI CHE-1307226

55. Hughey, C. A.; McMinn, C. M.; Phung, J. Beeromics: From QC to IDs of differentially expressed compounds. 2015 American Society of Brewing Chemists Annual Meeting, La Quinta, CA, June 14-17, 2015; Oral (Methods of Analysis). MRI CHE-1046630,

56. MRI CHE-0958973, REU CHE-1062629

57. Hughey, C. A.; Foss, K. M.; Fortmann, K. LC/MS metabolomic profiling of an amber ale fermented with four different yeast strains. 251st American Chemical Society National Meeting & Exposition, March 13-17, 2016, AGFC 179. MRI CHE-0922935, MRI CHE-1046630

58. Foss, K. M.; Fortmann, K. T.; Hughey, C. A. LC/MS metabolomic profiling of an amber ale fermented with four different yeast strains. 64th Annual Conference on Mass Spectrometry and Allied Topics, San Antonio, June 5-9, 2016, Tuesday Poster (TP) 248. MRI CHE-0922935, MRI CHE-1046630


60. Odenkirk, M. T.; Lucas, S. K.; Hughey, C. A. A functional group approach to determining the effects of mobile phase modifiers on the negative ion ESI ionization efficiency. 64th Annual Conference on Mass Spectrometry and Allied Topics, San Antonio, June 5-9, 2016, Tuesday Poster (TP) 484. RUI CHE-1307226, REU CHE-1461175


MacDonald

64. Zhang, Y. J.; Rogers, B. A.; Johnson, N. O.; Light, T. P.; Thompson, T. S. I MacDonald, G. Specific anion effects on caffeine partitioning between aqueous and cyclohexane phases", 253rd ACS National Meeting, San Francisco, CA, April 2-6, COLL 129 (oral). REU CHE-1461175 Year
Ogunjirin

65. Davenport, Z.; Mekonnen, A.; Ogunjirin, A. E. Synthesis and characterization of Boc protected N-n-Pentyl-3-pyridyl pyrrolidine ether. Presented at the Annual Biomedical Research Conference for Minority Students in Tampa, Florida, November 9-12, 2016. Zachary won a partial travel award to present at this meeting. **REU CHE-1461175**

66. Davenport, Z.; Mekonnen, A.; Ogunjirin, A. E. Synthesis and characterization of Boc protected N-n-Pentyl-3-pyridyl pyrrolidine ether. Presented at the 20th Undergraduate Research Symposium in the Chemical and Biological Sciences, Saturday, October 14, 2017. **REU CHE-1461175**

67. Mekonnen, A.; Davenport, Z.; Ogunjirin, A. E. An approach to synthesize and determine the Partition Coefficient of Two Analogs of Pyridyl Ether Compound. Presented at the Annual Biomedical Research Conference for Minority Students in Tampa, Florida, November 9-12, 2016. Zachary won a partial travel award to present at this meeting. Afomeya won a travel award to present at this meeting. **REU CHE-1461175**

Reisner


inorganic chemistry. Presented at the 251st ACS Meeting of the American Chemical Society, San Diego, CA, March 13, 2016: INOR 418. TUES DUE-1225792

75. Johnson, A. R.; Lin, S.; Nataro, C.; Raker, J. R.; Reisner, B. A.; Stewart, J. L. Organometallic chemistry at the frontiers of inorganic chemistry, A six-day workshop presented at the University of Michigan, June 26-July 1, 2016. TUES DUE-1225792


77. Salvatore, K. L.; Reisner, B. A. Synthesis of metal coordination compounds derived from 3,5-dimethyl-1,2,4-triazole. Presented at the 19th Annual UMBC Undergraduate Research Symposium in the Chemical and Biological Sciences, Baltimore, MD, October 22, 2016. REU CHE-1461175

78. Roberts, E. T.; Reisner, B. A. Synthesis and characterization of new metal-organic materials incorporating the hydrotris(3,5-dimethyl-1,2,5-triazolyl)borate ligand. Presented at the 19th Annual UMBC Undergraduate Research Symposium in the Chemical and Biological Sciences, Baltimore, MD, October 22, 2016. REU CHE-1461175


81. Salvatore, K. L.; Reisner, B. A. Synthesis of metal coordination compounds derived from 3,5-dimethyl-1,2,4-triazole. Presented at the 2017 Colonial Academic Alliance Undergraduate Research Conference, Elon University, Elon, NC, March 31-April 1, 2017. REU CHE-1461175

82. Roberts, E. T.; Reisner, B. A. Synthesis and characterization of new metal-organic materials incorporating the hydrotris(3,5-dimethyl-1,2,5-triazolyl)borate ligand. Presented at the 2017 Colonial Academic Alliance Undergraduate Research Conference, Elon University, Elon, NC, March 31-April 1, 2017. REU CHE-1461175


84. Roberts, E.; Salvatore, K.; Chan, B.; Reisner, B. A. Coordination compounds and hybrid materials containing the hydrotris(3,5-dimethyl-1,2,4-triazolyl)borate ligand. To be

86. Eppley, H. J.; Lin, S.; Nataro, C.; Plass, K.; Reisner, B. A. VIPEr - Teaching at the Frontiers of Inorganic Chemistry, Several talks presented at a three day work hosted at Franklin and Marshall College, June 1-3, 2017. TUES DUE-1225792


90. Krist, E. C.; Roberts, E. T.; Chan, B. C.; Reisner, B. A. Synthesis and characterization of new alkali metal and divalent transition metal materials derived from the hydrotris(3,5-dimethyl-1,2,4-triazolyl)borate ligand. Presented at the 254th National Meeting of the American Chemical Society, Washington, DC, August 22, 2017: INOR 548. REU CHE-1461175

Sumner


93. Zamfir, S.; Sumner, I. Molecular dynamics studies of the ubiquitin conjugation mechanism. Presented at the 93rd Annual Virginia Academy of Science Meeting, JMU, Harrisonburg, VA, May 22, 2015. REU CHE-1062629

94. Jones, W.; Davis, A.; Sumner, I. Computational analysis of the mechanism of the ubiquitin conjugating enzyme Ubc13. Presented at the 18th Annual Undergraduate Research Symposium in the Chemical and Biological Sciences. University of Maryland -
Baltimore County, Baltimore, MD, October 3, 2015. (2nd place) REU CHE-1062629


101. Wilson, R. H.; Sumner, I. A computational investigation into the mechanism of the histone acetyltransferase, Gcn5. Presented at the 15th MERCURY Conference on Undergraduate Computational Chemistry, Bucknell University, Lewisburg, PA, July 21 - 23, 2016. REU CHE-1461175

102. Wilson, R. H.; Sumner, I. A computational investigation into the mechanism of the histone acetyltransferase, Gcn5. Presented at the 19th Undergraduate Research Symposium in the Chemical and Biological Sciences, University of Maryland, Baltimore County, Baltimore, MD, Oct. 22, 2016. (1st place) REU CHE-1461175

103. Miller, A.; Sumner, I. Comparing force fields with density functional theory in small, solvated peptides. Presented at the 19th Undergraduate Research Symposium in the Chemical and Biological Sciences, University of Maryland, Baltimore County, Baltimore, MD, Oct. 22, 2016. REU CHE-1062629


107. Noll, C.; Sumner, I. A computational study of the interactions between the histone acetyltransferase, Gcn5, and a histone tail. Presented at the 95th Annual Meeting of the Virginia Academy of Science, Virginia Commonwealth University, Richmond, VA May 17-19, 2017; SBBB-8. REU CHE-1461175

108. Wilson, R. H.; Sumner, I. A computational investigation into the mechanism of the histone acetyltransferase, Gcn5. Presented at the 95th Annual Meeting of the Virginia Academy of Science, Virginia Commonwealth University, Richmond, VA May 17-19, 2017. REU CHE-1461175


Wright

110. Willey, A. M.; Sumner, I. C.; Caldwell, T. A.; Wright, N. T. Obscurin acts as a variable force resistor (15 min talk), Virginia Academy of Science, May 2017. REU CHE-1461175

111. Willey, A. M.; Sumner, I. C.; Caldwell, T. A.; Wright, N. T. Obscurin acts as a variable force resistor (poster), Biophysical Society Annual Meeting, New Orleans LA, February 2017. REU CHE-1461175

112. Willey, A. M.; Sumner, I. C.; Caldwell, T. A.; Wright, N. T. Analysis of the structure and force resistance of Obscurin Ig domains 35/36 and 58/59 (poster), University of Maryland Baltimore County, Baltimore, VA, October 2016. REU CHE-1461175

113. Letournaeu A. L.; Wright N. T. Analysis of muscle proteins Titin and Obscurin, University of Maryland Baltimore County, Baltimore, VA, October 2016. REU CHE-1461175

114. Policke R. A.; Berndsen C. E.; Wright N. T. Structural analysis of the Ig59 domain of Obscurin (poster), CAA undergraduate meeting, Williamsburg, VA, Apr. 2016. REU CHE-1461175

115. Policke R. A.; Berndsen C. E.; Wright N. T. Re-examination of the titin I6 structure (15 min. talk), Virginia Academy of Science, Fredericksburg, VA, May 2016. REU CHE-1461175

116. Letournaeu A. L.; Wright N. T. Analysis of muscle proteins Titin and Obscurin (15 min. talk), Virginia Academy of Science, Fredericksburg, VA, May 2016. REU CHE-1461175
117. Letourneau A. L.; Wright N. T. Towards the structural determination of the titin ZIg9 structure (poster), UMBC undergraduate research symposium, University of Maryland Baltimore-County, Oct 2015. REU CHE-1461175

118. Caldwell T. A.; Sumner I. C.; Wright N. T; SMD studies on M10/Ig1 titin/obscurincomplex (15 min. talk), Virginia Academy of Sciences, Harrisonburg, VA, May 2015. REU CHE-1062629


120. Rudloff M. W.; Woosley A. N.; Wright N. T. Biophysical characterization of naturally occurring titin M10 mutations (15 min. talk), CAA meeting, Philadelphia, PA, April 2015. REU CHE-1062629

121. Rudloff M. W.; Woosley A. N.; Wright N. T. Biophysical characterization of naturally occurring titin M10 mutations (15 min. talk), Virginia Academy of Sciences, Harrisonburg, VA, May 2015. REU CHE-1062629

122. Todd E. A.; Wright N. T.; Berndsen C. E. Solution dynamics of Ubc13 (15 min. talk), Biophysical Society, Baltimore, MD, Feb 2015. REU CHE-1062629

123. Zhang, Y. J. Ions effects on caffeine partitioning and polymer aggregation, Telluride Science Research Center Workshop, Interfacial Molecular and Electronic Structure and Dynamics, July 7-11, 2014 (Invited Talk). REU CHE-1062629


127. Johnson, N. Q.; Zhang, Y. J. An NMR study on interactions of Hofmeister ions with caffeine, UMBC Undergraduate Research Symposium, Baltimore, MD, October 3, 2015, #253 (Poster, won the second place poster award in chemical sciences). REU CHE-1461175

128. Price, W. T.; Thompson, T. S.; Allsbrook, A. P.; Zhang, Y. J. Cation effects on thermodynamics of caffeine partitioning between aqueous and cyclohexane phases, UMBC Undergraduate Research Symposium, Baltimore, MD, October 3, 2015, #252 (Poster, won the second place poster award in chemical sciences). REU CHE-1461175
129. Thompson, T. S.; Allsbrook, A. P.; Zhang, Y. J. The effects of osmolytes on caffeine partitioning thermodynamics and aqueous interactions, UMBC Undergraduate Research Symposium, Baltimore, MD, October 22, 2016, Poster #128 (won the first place poster award in chemical sciences). REU CHE-1461175


131. Zhang, Y. J.; Rogers, B. A.; Johnson, N. O.; Light, T. P.; Thompson, T. S.; MacDonald, G. Specific anion effects on caffeine partitioning between aqueous and cyclohexane phases, 253rd ACS National Meeting, San Francisco, CA, April 2-6, COLL 129 (oral). REU CHE-1461175
Non-NSF Peer Reviewed Publications:


22. Caldwell C.; Sumner I.; Wright N. T.; Mechanical dissociation of the M-band titin/obscurin complex is directionally dependent, FEBS Letters, 2015 Jul 8; 589(15), 1735-9. (Research Corporation)
Non-NSF supported non-JMU presentations

Baber


Berndsen


17. Hilliard, M. T.; Wright, N. T.; Wiener, R.; Berndsen, C. E.; Characterization of the UFM1 interacting motif in UBA5. 2015 NIH Undergraduate Research Symposium at UMBC.


22. Young, B. H.; Berndsen, C. E. Investigating the GCN5 histone acetyltransferase chemical mechanism ASBMB, San Diego, Apr 2 to 6, 2016; 1083.18.


Foust/Hughey


Kokhan


34. Swaim, C.; Kokhan, O. Biological semiconductors: structural control of heme redox potentials in PpcA, a 3-heme cytochrome, poster presented at Biophysical Society Meeting, February 13, 2017, 1504-pos


MacDonald

38. Temple, J. E.; MacDonald, G. Probing buffer-specific effects on nucleotide binding to RecA using difference FTIR. Biophysical Society Meeting, 2015, Baltimore, MD.


Raston


Reisner

44. Reisner, B. A. Seven courses, two exams: Designing the ACS Inorganic Chemistry Exams for a diverse undergraduate curriculum. Presented at the 249th National Meeting of the American Chemical Society, Denver, CO, March 22, 2015; CHED 11.

45. Marek, K.; Murphy, K.; Raker, J.; Reisner, B. A. Bringing the other elements to shore: Development of the anchoring concept content map for inorganic chemistry. To be presented at the 253rd National Meeting of the American Chemical Society, San Francisco, CA, April 5, 2017: CHED 2013. ACS Exams Institute