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

1. D'Amico, D. J.; McDougal, M. A.; Amenta, D. S.; Gilje, J. W.; Wang, S.; Hrib, C. G.; Edelmann, F. T. Synthesis and supramolecular structures of manganese complexes with n-pyrazolylpropanamide-derived ligands. *Polyhedron* **2015**, *88*, 19-28. **REU CHE-1062629**

2. Heerschap, S.; Marafino, J. N.; McKenna, K.; Caran, K. L.; Feitosa, K. Foams stabilized by tricationic amphiphilic surfactants. *Colloids Surf. A* **2015**, *487*, 190-197. **RCSA SICCSA 21041, RCSA MICCSA 10709, REU CHE-1062629, REU CHE-1461175, MRI DMR-1229383**

3. Marafino, J. N.; Gallagher, T. M.; Barragan, J.; Volkers, B. L.; LaDow, J. E.; Bonifer, K.; Fitzgerald, G.; Floyd, J. L.; McKenna, K.; Minahan, N. T.; Walsh, B.; Seifert, K.; Caran, K. L. Colloidal and antibacterial properties of novel triple-headed, double-tailed amphiphiles: Exploring structure-activity relationships and synergistic mixtures. *Bioorg. Med. Chem.* **2015**, *23*, 3566-3573. **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521, MRI CHE-0922935, MRI CHE-1046630**

4. Reeves, B. J.; Shircliff, D. M.; Shott, J. L.; Boardman, B. M. Synthesis and investigation of cobalt chalcogenide clusters with thienyl phosphine ligands as new acceptor materials for P3HT. *Dalton Transactions* **2015**, *44*, 718-724. **Cottrell College Science Award 22628**, **REU CHE-1062629**

5. Reisner, B. A.; Smith, S. R.; Stewart, J. S.; Raker, J. R.; Crane, J. L.; Sobel, S. B.; Pesterfield, L. Great Expectations: Using an analysis of current practices to propose a framework for the undergraduate inorganic curriculum. *Inorg. Chem.* **2015,** *54,* 8859-8868. **DOI**: 10.1021/ acs.inorgchem.5b01320. **TUES DUE-1225792**

6. Rudloff M. W.; Woosley A. N.; Wright N. T.; Biophysical characterization of naturally occurring titin M10 mutations. *Prot. Sci*. **2015**, *24(6*): 946-55. **REU CHE-1062629**

7. Bagley, A. C.; AbuNada, I.; Jun Y.; DeVore, T. C. Investigations of NMR chemical shifts using DFT-B_3LYP- GIAO calculations. *NMR Spectroscopy in the Undergraduate Curriculum* **2016,** *2***,** 67-77, **DOI:** 10.1021/bk-2016-1225.ch005. **REU CHE-1461175**

8. Cruz, S. S.; Amenta, D. S.; Gilje, J. W.; Yap, G. P. A. A re-examination of the reaction of dicloro-tris-(triphenylphosphino)ruthenium (II): Crystal structures of triphenylphosphine chloro ruthenium complexes. *Polyhedron* **2016**, 179-183. **REU CHE-1062629**

9. DuPont, K. E.; McKenzie, A. M.; Kokhan, O.; Sumner, I.; Berndsen, C. E. The disulfide bonds within BST-2 enhance tensile strength during viral tethering. *Biochemistry* **2016**, *55*, 940-947. **REU CHE-1461175**

10. Hughey, C. A.; McMinn, C. M.; Phung, J. Beeromics: from quality control to identification of differentially expressed compounds in beer. *Metabolomics* **2016**, 12:11. **MRI CHE-0958973**

11. Minbiole, K. P. C.; Jennings, M. C.; Ator, L. E.; Black, J. W.; Grenier, M. C.; LaDow, J. E.; Caran, K. L.; Seifert, K.; Wuest, W. M. From antimicrobial activity to mechanism of resistance: the multifaceted role of simple quaternary ammonium compounds in bacterial

eradication. *Tetrahedron* **2016**, *72(25)*, 3559-3566. **University City Science Center S1403, RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521, DGE-1144462**

12. Rogers, B. A.; Thompson, T. S.; Zhang, Y. J. Specific anion effects on thermodynamics of caffeine partitioning between aqueous and cyclohexane phases. *J. Phys. Chem. B*, **2016**, *120*, 12596–12603. **REU CHE-1461175**

13. Shircliff, D. M.; Pastore,V. J.; Poltash, M. L.; Boardman, B. M. Synthesis and characterization of pendant phenyl ester-substituted thiophene based copolymers. *Materials Today Communications* **2016**, *8*, 15-22. **REU CHE-1461175**

14. Amenta, D. S.; Liebing, P.; Biero, J. E.; Sherman, R. J.; Gilje, J. W.; Edelmann, F. T. Synthesis and crystal structures of three new benzotriazolylpropanamides. *Acta Cryst*. **2017**, E73. **REU CHE-1461175**

15. Brock, L. R.; Keister, J. W.; France, M.; Fierro, N.; DeVore, T. C. The thermal decomposition of ammonium meta-vanadate under restricted flow conditions. *American Journal of Analytical Chemistry* **2017**, *8,* No.1, DOI: 10.4236/ajac.2017.81003. **REU CHE-0754521**, MRI CHE-0320245, and IMR DMR-0315345

16. Corbin, D. A.; Shircliff, D. M.; Reeves, B. J.; Boardman, B. M. Metallopolymers from direct polymerization of functionalized cobalt chalcogenide clusters and thiophene comonomers. *Polym. Chem.* **2017**, *8*, 3801-3809. **Cottrell College Science Award 22628**, **REU CHE-1461175**

17. Gallagher, T. M.; Marafino, J. N.; Wimbish, B. K.; Volkers, B.; Fitzgerald, G.; McKenna, K.; Floyd, J.; Minahan, J. T.; Walsh, B.; Thompson, K.; Bruno, D.; Paneru, M.; Djikeng, S.; Masters, S.; Haji, S.; Seifert, K.; Caran. K. L. Hydra amphiphiles: Using three heads and one tail to influence aggregate formation and to kill pathogenic bacteria. *Colloids Surf. B.* **2017**, *157*, 440-448. **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521, REU CHE-1461175, MRI CHE-0922935, MRI CHE-1046630**

18. Hu L. R.; Ackermann M. A.; Hecker P. A.; Prosser B. L.; King B.; O'Connell K. A.; Asico L. D.; Jose P. A.; Meyer L. C.; Berndsen C. E.; Wright N. T.; Lederer W. J.; Kontrogianni-Konstantopoulos A. Arrhythmia and deregulated Ca^{2+} cycling underlie the development of hypertrophic cardiomyopathy due to mutant obscurins. *Science Advances* **2017** Jun 7; 3(6). **REU CHE-1461175**

19. Johnson, N. O.; Light, T. P.; MacDonald, G.; Zhang, Y. J. Anion-caffeine interactions studied by ^{13}C and ^{1}H NMR and ATR-FTIR spectroscopy. *J. Phys. Chem. B*, **2017**, *121*, 1649–1659. **REU CHE-1461175**

20. Wilson, R. H.; Zamfir, S.; Sumner, I. Molecular dynamics simulations reveal a new role for a conserved active site asparagine in a ubiquitin-conjugating enzyme. J. Mol. Graph. Model. **2017,** in press. **REU CHE-1062629, REU CHE-1461175**

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

1. Blackard, R. T.; Mattila, J. M.; Odenkirk, M. T.; Lucas, S. K.; Hughey, C. A. Effect of functional groups on the decarboxylation of benzoic and phenylpropanoic acids during in-source collision induced dissociation. *Rapid Communications in Mass Spectrometry*, submitted. **RUI CHE-1307226, MRI CHE-0922935, MRI CHE-1046630, REU CHE-1461175**

2. Morales, A. C.; Cooper, N. D.; Reisner, B. A.; DeVore, T. C. Variable temperature PXRD investigation of the phase changes during the dehydration of potassium Tutton Salts. *J. Thermal Analysis and* Calorimetry, submitted. **REU CHE-1461175**

3. Morales, A.; Cooper, N. C.; Reisner, B. A.; DeVore, T. C. Decomposition pathways for the Tutton Salts $K_2M(SO_4)_2 \cdot 6\ H_2O$ (M = Mg, Co, Ni, Cu, Zn). *J. Therm Anal. Calor.*, submitted. **REU CHE-1461175**, MRI CHE-0320245, and IMR DMR-0315345

4. Morales, A. C.; Cooper, N. C.; Reisner, B. A.; DeVore, T. C. Enthalpy of formation of $K_2M(SO_4)_2 \cdot 6\ H_2O$ (M = Mg, Co, Ni, Cu, Zn). *J. Therm Ana., Calor*, submitted. **REU CHE-1461175**, MRI CHE-0320245, and IMR DMR-0315345

5. Rossi D.; Palmio J.; Galli L.; Barone V.; Caldwell T. A.; Policke R. A.; Berndsen C. E.; Wright N. T.; Romero N.; Malfatti E.; Brochier G.; Stojkovic; Jordanova A.; Guergueltcheva A.; Hackman P.; Romero N. B.; Eymard B.; Udd B.; Sorrentino V. Digenic inheretence of a FLNC frameshift and an OBSCN variant in a family with distal muscular dystrophy. *PlosOne*, submitted. **REU CHE-1461175**

6. Snell-Feikema, R.; DeVore, T. C. Can DSC be used to determine the enthalpy of formation for metal oxalates? *J. Therm Anal. 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 $RuCl_3(NO)(PPh_3)_2$ and $RuCl_3(NO) \cdot H_2O$ with $Ph_2P(CH_2)_nP(O)Ph_2$, n = 1, 2, or 3: Crystal structures of ruthenium nitrosyl complexes containing monodentate and chelating $Ph_2P(CH_2)_nP(O)Ph_2$ ligands. *Polyhedron*, submitted. **REU CHE-1062629** and **REU CHE-1461175**

8. Giersch, G. E. W.; Boyett, J. C.; Hargens, T. A.; Luden, N. D.; Saunders, M. J.; Daley, H.; Hughey, C. A.; El-Sohemy, A.; Womack, C. J. The effect of the CYP1A2 -163 C>A polymorphism on the metabolism of caffeine and effect on performance. *J. Caffeine Research*, submitted. **REU CHE-1461175**

NSF-supported non-JMU presentations:

Amenta/Gilje

1. Mitchell, J.; McDougal, M.; Amenta, D. S.; Gilje, J. W. Some chemistry of hemilabile ligands. Presented at 17th Annual Undergraduate Research Symposium, Baltimore, MD, October 25, 2014. **REU CHE-1062629**

2. Cruz, S. S.*; Gilje, J. W.; Amenta, D. S.; Yap, G. P. A. An Evaluation of the chemistry of $RuCl_2(PPh_3)_3$ with nitriles. Presented at 17th Annual Undergraduate Research Symposium, Baltimore, MD, October 25, 2014. **REU CHE-1062629**

3. Beiro, J. E.; Amenta, D. S.; Gilje, J. W. Preparation and characterization of metal/ligand complexes using substituted n-triazolylpropanamide ligands**.** Presented at 18th Annual Undergraduate Research Symposium, Baltimore, MD, October 3, 2015. **REU CHE-1461175**

4. Sherman, R. J.; Amenta, D. S.; Gilje, J. W. Preparation of ruthenium complexes of N-triazolylpropanamide derivatives. Presented at 18th Annual Undergraduate Research Symposium, Baltimore, MD, October 3, 2015. **REU CHE-1461175**

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

6. Shircliff, D. M.; Reeves, B. J.; Boardman, B. M. The investigation of charge transfer between cobalt chalcogenide clusters and thiophene based polymers, Presented at 17th Annual Undergraduate Research Symposium, Baltimore, MD, October 25, 2014. Won 1st place poster in chemical sciences. **Cottrell College Science Award**, **22628, REU CHE-1062629**

7. Shott, J. L.; Reeves, B. J.; Boardman, B. M. Synthesis, characterization, and polymerization of thienyl phosphine palladium (II) complexes. Presented at 17th Annual Undergraduate Research Symposium, Baltimore, MD, October 25, 2014. Won 1st place poster in chemical sciences. **Cottrell College Science Award**, **22628, REU CHE-1062629**

8. Boardman, B. M.; Reeves, B. J.; Shircliff, D. M.; Shott, J. L. Synthesis, characterization, and investigation of cobalt chalcogenide clusters with thienyl phosphine 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**

9. Shircliff, D. M.; Boardman, B. M. Synthesis and characterization of new low band gap polymers containing ethyl and phenyl ester functionalized polythiophene derivatives. Presented at 249th American Chemical Society National Meeting & Exposition, Denver, CO, March 22-26, 2015; POLY-291 **REU CHE-1062629**

10. Shott, J. L.; Reeves, B. J.; Boardman, B. M. Synthesis, characterization, and polymerization of thienyl phosphine palladium (II) complexes. Presented at 249th American Chemical Society National Meeting & Exposition, Denver, CO, March 22-26, 2015; INORG-645. **Also selected for Sci-Mix **REU CHE-1062629**

11. Boardman, B. M. Cobalt chalcogenide clusters with thienyl phosphine ligands as new acceptor materials for hybrid photovoltaic devices. Presented at 12th International Symposium on Functional π-Electron Systems, Seattle, WA, July 19-24 2015. **Only PUI faculty invited to present. **Cottrell College Science Award 22628, REU CHE-1062629**

12. Moore, A. M.; Shott, J. L.; Boardman, B. M. Polymerization and characterization of functionalized palladium complexes with benzothiadiazole co-monomers. Presented at 18th Annual Undergraduate Research Symposium, Baltimore, MD, October 3, 2015. **REU CHE-1461175**

13. Shircliff, D. M.; Pastore,V. J.; Boardman, B. M. Synthesis and characterization of pendant phenyl ester-substituted thiophene based copolymers. Presented at 18th Annual Undergraduate Research Symposium, Baltimore, MD, October 3, 2015. **REU CHE-1461175**

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**

15. Boardman, B. M. Direct polymerization of cobalt chalcogenide clusters for hybrid photovoltaic materials. Presented at Virginia Commonwealth University, Physics Colloquia, Richmond, VA, February 12, 2016. **Cottrell College Science Award 22628**, **REU CHE-1461175**

16. Corbin, D. A.; Boardman, B. M. The synthesis and characterization of polymerized cobalt selenide clusters with photovoltaic applications. Presented at The Colonial Academic Alliance 2016 Undergraduate Research Conference, Williamsburg, VA, April 15-17, 2016. **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**

18. Boardman, B. M. Hybrid systems vs. hybrid materials for photovoltaic applications. Presented at University of North Carolina, Charlotte, Chemistry Colloquia, Charlotte, NC, January 30, 2017. **Cottrell College Science Award 22628**, **REU CHE-1461175**

19. Shott, J. L.; Boardman, B. M. Thienyl phosphine palladium(II) complexes: An introduction to hybrid materials in undergraduate laboratories. Presented at ACS 253rd National Meeting, San Francisco, CA, April 2, 2017; CHED 135, **REU CHE-1461175**

20. Boardman, B. M. Direct polymerization of cobalt chalcogenide clusters for hybrid photovoltaic materials. Presented at ACS 253rd National Meeting, San Francisco, CA, April 4, 2017; INOR 707, **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

22. Caran, K. L. Amphiphiles and Gelators. 4-VA Soft Matter Workshop, James Madison University, February 11, 2014. Sound bite (oral) presentation. **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521**

23. Caran, K. L. Amphiphiles and Gelators: Designing Molecules to Self-Assemble. Chemistry Department, Villanova University, March 25, 2014. *Invited seminar.* **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521**

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**

25. Gallagher, T.; Marafino, J. N.; Volkers, B.; Walsh, B.; Thompson, K.; Minahan, N.; Floyd, J.; Irby, J.; Bonnifer, K.; Damiano, L.; McKenna, K.; Caran, K.; Seifert, K. Antibacterial activity of triscationic amphiphiles. Presented at the Virginia Branch of the American Society for Microbiology, Department of Biology, James Madison University, November 7-8, 2014. **Tara won first prize for her poster presentation at this meeting.* **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521**

26. Heerschap, S.; Marafino, J.; McKenna, K.; Caran, K.; Feitosa, K. Aqueous Foam Stabilized by Tricationic Amphiphilic Surfactants. Presented at the March Meeting of the American Physical Society (APS), San Antonio, TX, March 2-6, 2015; poster presentation. **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521**

27. Walsh, B.; Thompson, K.; Marafino, J. N.; Damiano, L.; McKenna, K.; Gallagher, T. M.; Schmachtenberg, M.; Kou, K.; Wenzel, M.; Seifert, K.; Caran, K. L. Synthesis and study of polycationic amphiphiles as potent antiseptics and novel colloids: Exploring structure activity relationships. Presented at the Regional Meeting of the American Chemical Society, Department of Chemistry, University of Virginia, April 17, 2015; poster presentation. **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521**

28. Walsh, B. J. C.; Kou, K.; Marafino, J. N.; McKenna, K.; Thompson, K.; Gallagher, T. M.; Seifert, K.; Caran, K. L. Synthesis and Study of Polcationic Amphiphiles as Potent

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**

31. Walsh, B. J. C.; Kou, K.; Seifert, K.; Caran, K. L. Synthesis and Study of Polycationic Amphiphiles as Potent Antiseptics and Novel Colloids: Exploring Structure Activity Relationships. 30th Annual National Conference on Undergraduate Research (NCUR), University of North Carolina Asheville, Asheville, NC, April 7-9, 2016. Oral presentation. **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521**

32. Thompson, K. A.; Caran, K. L. The Effect of Hofmeister Series Counterions on the Colloidal and Antimicrobial Properties of a Triple-headed Single-tailed Amphiphile. 30th Annual National Conference on Undergraduate Research (NCUR), University of North Carolina Asheville, Asheville, NC, April 7-9, 2016. Oral presentation. **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**

35. Caran, K. L. Colloidal and antibacterial activity of non-conventional amphiphiles. Virginia Soft Matter Workshop, Virginia Commonwealth University, Richmond, VA, October 29, 2016. *Invited plenary presentation*. **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521**

36. Caran, K. L.; Seifert, K.; Feitosa, K.; Marafino, J.; Rogers, E.; Thompson, K.; Walsh, B.; Kendrick, S.; McKenna, K.; Ashamole, B.; Lauer, M.; Rauer, S.; Rister, A. Colloidal and antibacterial studies of non-conventional polycationic amphiphiles. 253rd National Meeting of the American Chemical Society, San Francisco, CA, April 2-6, 2017. oral presentation (ORGN 651). **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521**

37. Ashamole, B.; Rogers, E.; Ogunjirin, E.; Seifert, K.; Caran, K. L. Antimicrobial and colloidal properties of novel polycationic amphiphiles. 253rd National Meeting of the American Chemical Society, San Francisco, CA, April 2-6, 2017. oral presentation (CHED 42). **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521**

38. Lauer, M.; Rogers, E.; Kubow, C.; Seifert, K.; Caran, K. L. Study of fluorescent quaternary ammonium amphiphiles to gain insight into the mechanism of antibacterial activity. 253rd National Meeting of the American Chemical Society, San Francisco, CA, April 2-6, 2017. oral presentation (CHED 43). **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521**

39. Kendrick, S.; Rogers, S.; Seifert, K.; Caran, K. L. Synthesis and study of triple-headed, double-tailed amphiphiles as potent antiseptics. 253rd National Meeting of the American Chemical Society, San Francisco, CA, April 2-6, 2017. poster presentation (CHED 1232). **RCSA MICCSA 10709, REU CHE-1062629, REU CHE-0754521**

40. Caran, K. L.; MacDonald, G. Summer REU program integrating deaf and hearing participants in chemistry research. 253rd National Meeting of the American Chemical Society, San Francisco, CA, April 2-6, 2017. oral presentation (CHED 2144). **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

44. DeVore, T. C.; Cooper, N. Why doesn't thermal analysis give consistent Arrhenius parameters for simple systems? 2015 SERMACS- SWRM, Memphis TN, November 5 - 7, 2015. Presentation 1117. **REU CHE-1461175**, MRI CHE-0320245, and IMR DMR-0315345

45. DeVore, T. C.; Snell-Feikema, R., Method for determining the enthalpy of reaction for metal oxalates using DSC, 2015 SERMACS- SWRM, Memphis TN, November 5 -7, 2015. Presentation 1118. **REU CHE-1461175**, MRI CHE-0320245, and IMR DMR-0315345

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

47. DeVore, T. C. Effect of sample mass on the thermal decomposition of "simple" systems, SERMACS – 861, Oct 23, 2016. **REU CHE-1461175**, MRI CHE-0320245, and IMR DMR-0315345

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

52. Hughey, C. A. Electrospray ionization liquid chromatography mass spectrometry (ESI LC/MS): Foodomics and Fundamentals. Suter Science Seminar, Eastern Mennonite University, Harrisonburg, VA, September 19, 2014. *Invited talk.* **MRI CHE-0958973, REU CHE-1062629**

53. Hughey, C. A.; McMinn, C. M.; Phung, J. Beeromics: From QC to IDs of differentially expressed compounds in craft beers. Presented at 63rd ASMS Conference on Mass Spectrometry & Allied Topics, St. Louis, MO, May 31-June 4, 2015; Oral WOE, 2:30 (Food Chemistry & Safety). **MRI CHE-0958973, REU CHE-1062629**

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**

59. Foss, K. M.; Fortmann, K. T.; Hughey, C. A. LC/MS metabolomic profiling of an amber ale fermented with four different yeast strains. World Brewing Congress, August 13-17, 2016, Denver, CO, Poster 82. **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**

61. Carter, L. C.; Fortmann, K. T.; Hughey, C. A. Effect of yeast strain on the volatile profile of beer as determined by solid phase microextraction (SPME) GC/MS. 65th Annual Conference on Mass Spectrometry and Allied Topics, Indianapolis, June 4-9, 2017, Wednesday Poster (WP) 182. **REU CHE-1461175**

62. Foss, K. M.; Fortmann, K. T.; Hughey, C. A. Targeted and untargeted metabolomic profiling of a pale ale brewed with genetically different yeast strains. 65th Annual Conference on Mass Spectrometry and Allied Topics, Indianapolis, June 4-9, 2017, Wednesday Poster (WP) 170. **MRI CHE-0958973, REU CHE-1461175**

63. Odenkirk, M. T.; Mattilla, J. M.; Blackard, R. T.; Poltash, M. L.; Lucas, S. K. Jones, J.; Hughey, C. A. Predictive Models of Negative Ion Electrospray Response Explored Through Machine Learning Applications. 65th Annual Conference on Mass Spectrometry and Allied Topics, Indianapolis, June 4-9, 2017, Wednesday Poster (WP) 028. **MRI CHE-0922935, MRI CHE-1046630, RUI CHE-1307226**

MacDonald

64. Zhang, Y. J.; Rogers, B. A.; Johnson, N. O.; Light, T. P.; Thompson, T. S. l 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

68. Bentley, A.; Eppley, H.; Jamieson, E.; Johnson, A.; Nataro, C.; Reisner, B.; Stewart, J.; Smith, S.; Williams, N.; Watson, L. Mg deficient IONiC/VIPEr: An online community for inorganic chemists. Presented at the 249th National Meeting of the American Chemical Society, Denver, CO, March 22, 2015; CHED 11. **TUES DUE-1225792**

69. Eppley, H.; Johnson, A.; Williams, N.; Bentley, A.; Jamieson, E.; Nataro, C.; Raker, J.; Reisner, B.; Smith, S.; Stewart, J.; Watson, L. VIPEr faculty development workshops; Cutting edge content development and sharing pedagogical best practices. Presented at the 249th National Meeting of the American Chemical Society, Denver, CO, March 22, 2015; CHED 45. **TUES DUE-1225792**

70. Reisner, B. A.; Price, W. T.; Muetterties, A. M. Solvent loss and reuptake in $Na[BH(C_2H_3N_3)_3]$ frameworks. Presented at the 249th National Meeting of the American Chemical Society, Denver, CO, March 23, 2015; INOR 366. **REU CHE-1062629**

71. Price, W. T.; Reisner, B. A. Mechanisms and kinetics of solvent loss in $Na[BH(C_2H_3N_3)_3]$.solvent. Presented at the National Conference on Undergraduate Research, Eastern Washington University, Cheney, WA, April 18, 2015; Poster 9 – 48B. **REU CHE-1062629**

72. Price, W. T.; Reisner, B. A. Synthesis of metal organic frameworks and their activation kinetics. Presented at the Virginia Academy of Sciences, James Madison University, Harrisonburg, VA, May 22, 2015. **REU CHE-1062629**

73. Reisner, B. A. Building Community in Inorganic Chemistry Education. Chemical Education Research and Practice Gordon Conference, Bates College, Lewiston, ME, June 21-26, 2015. **TUES DUE-1225792**

74. Eppley, H. J.; Nataro, C.; Bentley, A. K.; Jamieson, E. R.; Johnson, A. R.; Reisner, B. A.; Stewart, J. L.; Smith, S. R.; Watson, L. A.; Williams, N. S. B. Expanding the frontiers of

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**

76. Reisner, B. A.; Cresawn, K. O.; Paulson, S. A.; Pyle, E. J.; Higdon, R. L.; Almarode, J. T. EPIC science education at James Madison University: Expanding pathways, identity and capacity (EPIC) in science education. Presented at the Biennial Conference of Chemical Education, University of Northern Colorado, Greeley, CO, August 1, 2016. **Noyce DUE-1439849**

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-1,2,54-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**

79. Higdon, R.; Reisner, B.; Cresawn, K.; Pyle, E. Being Unicorns: Preservice teachers and professional identity. Presented at the Virginia Association of Science Teachers Professional Development Institute, Williamsburg, VA, November 18, 2016. **Noyce DUE-1439849**

80. Reisner, B. A. One eye on the past, one eye on the future: A reflection on the undergraduate inorganic chemistry curriculum. Presented at the 251st ACS Meeting of the American Chemical Society, San Diego, CA, March 13, 2016: INOR 1. **TUES DUE-1225792**

81. Salvatore, K. L.; Reisner, B. A. Synthesis of metal coordination compounds derived from 3,5-dimethyl-1,2,4-trizaole. 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 incorporationg the hydrotris(3,5-dimethyl-1,2,4-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**

83. Johnson, A.; Stewart, J.; Bentley, A.; Eppley, H.; Jamieson, E.; Nataro, C.; Reisner, B.; Smith, S.; Watson, L.; Williams, N. IONiC bonding: Building a lattice using attractive forces. To be presented at the 253rd National Meeting of the American Chemical Society, San Francisco, CA, April 2, 2017: INOR 221. **TUES DUE-1225792**

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

presented at the 253rd National Meeting of the American Chemical Society, San Francisco, CA, April 3, 2017: INOR 519. **REU CHE-1461175**

85. Reisner, B. A.; Nataro, C.; Smith, S.; Bentley, A.; Eppley, H.; Jamieson, E.; Johnson, A.; Stewart, J.; Watson, L.; Williams, N. Building community in (inorganic) chemistry: Ideas from IONiC. To be presented at the 253rd National Meeting of the American Chemical Society, San Francisco, CA, April 3, 2017: CHED 245. **TUES DUE-1225792**

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**

87. Reisner, B. A.; Raker, J. R.; Stewart, J. L.; Smith, S. R. Changing practice at the frontiers of inorganic chemistry. Presented at the Gordon Research Conference on Chemistry Education: Research and Practice, Lewiston, ME, June 21, 2017 **TUES DUE-1225792**

88. Reisner, B. A.; Cresawn, K.; Pyle, E.; Paulson, S.; Higdon, R. EPIC science education at James Madison University: Expanding Pathways, Identity and Capacity (EPIC) in secondary education. Presented at the 254th National Meeting of the American Chemical Society, Washington, DC, August 20, 2017: CHED 58. **Noyce DUE-1439849**

89. Reisner, B. A.; Stewart, J. L.; Bentley, A. K.; Eppley, H. J.; Jamieson, E. R.; Johnson, A. R.; Lin, S.; Nataro, C.; Plass, K.; Smith, S. R.; Watson, L. A.; Williams, N. IONiC connection: Increasing interactions in the inorganic community. Presented at the 254th National Meeting of the American Chemical Society, Washington, DC, August 22, 2017: INOR 547. **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 hydortris(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

91. Iuga, A.; McKaig, D. E.; Sumner, I. Understanding force field bias in Pin1WW. Presented at the 59th Annual Meeting of the Biophysical Society, Baltimore, MD, February 7–11, 2015. **REU CHE-1062629**

92. Zamfir, S.; Sumner, I. Molecular dynamics studies of the ubiquitin conjugation mechanism. Presented at the 59th Annual Meeting of the Biophysical Society, Baltimore, MD, February 7–11, 2015. **REU CHE-1062629**

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**

95. Jones, W. M.; Davis, A. G.; Sumner, I. QM/MM analysis of the mechanism of the ubiquitin conjugating enzyme Ubc13. Presented at the 251st American Chemical Society National Meeting & Exposition. San Diego, CA, March 11-16, 2016; COMP-318. **REU CHE-1062629, REU CHE-1461175**

96. Davis, A. G.; Jones, W. M.; Sumner, I. Determining the mechanism of the ubiquitin-conjugating enzyme Ubc13 with QM/MM and metadynamics. Presented at the 251st American Chemical Society National Meeting & Exposition. San Diego, CA, March 11-16, 2016; COMP-361. **REU CHE-1062629, REU CHE-1461175**

97. Sumner, I. Electron trajectories in molecular orbitals. Presented at the 251st American Chemical Society National Meeting & Exposition. San Diego, CA, March 11-16, 2016; COMP-223. **REU CHE-1062629**

98. Sumner, I. Mechanistic insights into Ubc13-catalyzed ubiquitination. Presented at the 94th Annual Meeting of the Virginia Academy of Science, U. of Mary Washington, Fredericksburg, VA, May 19, 2016. **REU CHE-1062629, REU CHE-1461175**

99. Davis, A. G.; Jones, W. M.; Zamfir, S.; Sumner, I. Determining the mechanism of the ubiquitin conjugating enzyme, Ubc13, with QM/MM and metadynamics. Presented at the 15th MERCURY Conference on Undergraduate Computational Chemistry, Bucknell U., Lewisburg, PA, July 21 - 23, 2016. **REU CHE-1062629, REU CHE-1461175**

100. Jones, W. M.; Davis, A. G.; Zamfir, S.; Sumner, I. Computational analysis of the mechanism of the ubiquitin conjugating enzyme, Ubc13. Presented at the 15th MERCURY Conference on Undergraduate Computational Chemistry, Bucknell U., Lewisburg, PA, July 21 - 23, 2016. **REU CHE-1062629, REU CHE-1461175**

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 Biologial Sciences, University of Maryland, Baltimore County, Baltimore, MD, Oct. 22, 2016. **REU CHE-1062629**

104. Sumner, I.; Wilson, R. H.; Jones, W. M.; Davis, A. G.; Zamfir, S. Mechanistic insights into Ubc13-catalyzed ubiquitination. Presented at the Biophysical Society 61st Annual Meeting, New Orleans, LA, Feb. 11-15, 2017; 328-Pos. **REU CHE-1062629, REU CHE-1461175**

105. Jones, W. M.; Davis, A. G.; Sumner, I.; Zamfir, S. Computational analysis of the mechanism of the ubiquitin conjugating enzyme, Ubc13. Presented at the Biophysical Society 61st Annual Meeting, New Orleans, LA, Feb. 11-15, 2017; 1431-Pos. **REU CHE-1062629, REU CHE-1461175**

106. Wilson, R. H.; Sumner, I. A computational investigation into the mechanism of the histone acetyltransferase, Gcn5. Presented at the Biophysical Society 61st Annual Meeting, New Orleans, LA, Feb. 11-15, 2017; 330-Pos. **REU CHE-1461175**

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**

109. Miller, A.; Sumner, I. Comparing force fields with density functional theory in small, solvated peptides. Presented at the 95th Annual Meeting of the Virginia Academy of Science, Virginia Commonwealth University, Richmond, VA May 17-19, 2017. **REU CHE-1062629**

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. Letournaeu 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**

119. Caldwell T. A.; Policke R. A.; Wright N. T. Structural analysis of the Ig5958 Domain of Obscurin, Biophysical Society (poster), Baltimore ,MD, Feb 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. Rudloff M. W.; Woosley A. N.; Wright N. T. Biophysical characterization of naturally occurring titin M10 mutations (poster), Biophysical Society, Baltimore, MD, Feb 2015. **REU CHE-1062629**

Zhang

124. 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**

125. Zhang, Y. J.; Rogers, B. A.; Thompson, T. S.; Wu, T. Y. Specific ion effects on the thermodynamics of caffeine partition between organic and aqueous phases, The 248th ACS National Meeting, San Francisco, California, August 10-14, 2014 (oral). **REU CHE-1062629**

126. Al Husseini, D.; Zhang, Y. J. Effects of anions and amino acids on surface tension of water, UMBC Undergraduate Research Symposium, Baltimore, MD, October 25, 2014 (Poster). **REU CHE-1062629**

127. Johnson, N. O.; 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**

130. Thompson, T. S.; Allsbrook, A. P.; Zhang, Y. J. Effects of osmolytes on caffeine partitioning thermodynamics, 253rd ACS National Meeting, San Francisco, CA, April 2-6, COLL 361 (poster). **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:

1. Reisner, B. A.; Vaughn, K. T. L.; Shorish, Y. L. Making data management accessible in the undergraduate chemistry curriculum. *J. Chem. Educ.* **2014**, *91*, 1943-1946. **DOI**: 10.1021/ed500099h

2. Mandernach, M. A.; Shorish, Y. L.; Reisner, B. A. The evolution of instruction delivery in the chemistry curriculum informed by mixed assessment methods. *Issues Sci. Tech. Lib. (ISTL)* **2014**, *77*. **DOI:** 10.5062/F46H4FDD

3. Caldwell, T. A.; Sumner, I.; Wright, N. T. Mechanical dissociation of the M-band titin/obscurin complex is directionally dependent FEBS *Lett*., **2015**, 589, 1735-1739. **Research Corporation Award 22450** and **Jeffress Memorial Trust**

4. Metrick, M. A.; MacDonald, G. Hofmeister ion effects on the solvation and thermal Stability of model proteins lysozyme and myoglobin*. Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2015**, *469*, 242-251.

5. Ogunjirin, A. E.; Fortunak, J. M.; Brown, L. L.; Xiao, Y.; Davilla-Garcia, M. I. Competition, selectivity and efficacy of analogs of A-84543 for nicotinic acetylcholine receptors with repositioning of pyridine nitrogen. *Nuerochem. Res.* **2015**, *40*, 2131-2142. *This work was partially supported by the National Institutes of Health grants 5R24MH067627 and NIGMSNIH S06 GM08016-34.*

6. Raker, J. R.; Reisner, B. A.; Smith, S. R.; Stewart, J. L.; Crane, J. L.; Pesterfield, L.; Sobel, S. B. In-depth coursework in undergraduate inorganic chemistry: Results from a national survey of inorganic chemistry faculty. *J. Chem. Educ.* **2015**, 92, 980-985. **DOI**: 10.1021/ed500625f. Selected as an ACS Editors Choice article.

7. Raker, J. R.; Reisner, B. A.; Smith, S. R.; Stewart, J. L.; Crane, J. L.; Pesterfield, L.; Sobel, S. B. Foundation coursework in undergraduate inorganic chemistry: Results from a national survey of inorganic chemistry faculty. *J. Chem. Educ.* **2015**, 92, 973-979. **DOI**: 10.1021/ed500624t. Selected as an ACS Editors Choice article.

8. Ann, J.; Ki, Y.; Yoon, S.; Kim, M. S.; Lee, J. U.; Kim, C.; Lee, S; AJung, A.; Baek, J.; Hong, S.; Choi, S.; Pearce, L. V.; Esch, T. E.; Turcios, N. A.; Lewin, N. E.; Ogunjirin, A. E.; Herold, B. K.; McCall, A. K.; Blumberg, P. M.; Lee, J. 2-Sulfonamidopyridine C-region analogs of 2-(3-fluoro-4-methylsulfonamidophenyl)propanamides as potent TRPV1 antagonists. *Bioorg. Med. Chem.* **2016**, *24*(6), 1231-1240. *This research was supported by research grants from the Korea Science and Engineering Foundation (KOSEF) (NRF-2007-0056817) and the National Leading Research Lab (NLRL) program (2011-0028885) in South Korea, and in part by the Intramural Research Program of the NIH, Center for Cancer Research, NCI (Project Z1A BC 005270) in the USA*

9. Baiady, N.; Padala, P.; Mashahreh, B.; Cohen-Kfir, E.; Todd, E. A.; Du Pont, K. E.; Berndsen, C. E.; Wiener, R. The Vps27/Hrs/STAM (VHS) domain of the signal-transducing adaptor molecule (STAM) directs associated molecule with the SH3 Domain of STAM (AMSH) specificity to longer Ubiquitin chains and dictates the position of cleavage. *J Biol Chem*. **2016** Jan 22;291(4):2033-42. doi: 10.1074/jbc.M115.689869. PubMed PMID:26601948

10. Boyett, J. C.; Giersch, G. E.; Womack, C. J.; Saunders, M. J.; Hughey, C. A.; Daley, H. M.; Lunden, N. D. "Time of day and training status both impact the efficacy of caffeine for short duration cycling performance," *Nutrients*, **2016**, 8(10).

11. Light, T. P.; Corbett, K. M.; Metrick, M. A.; MacDonald, G. Hofmeister ion-induced changes in water structure correlate with changes in solvation of an aggregated protein complex *Langmuir*, **2016**, *32*, 1360-1369.

12. Oweis W.; Padala P.; Hassouna F.; Cohen-Kfir E.; Gibbs D. R.; Todd E. A.; Berndsen C. E.; Wiener R. Trans-Binding mechanism of ubiquitin-like protein activation revealed by a UBA5-UFM1 Complex Cell Rep. **2016** Sep 20;16(12):3113-20. doi: 10.1016/j.celrep.2016.08.067.

13. Nguyen-Phan, T. D.; Baber, A. E.; Rodriguez, J. A.; Senanayake, S. D. Au and Pt nanoparticle supported catalysts tailored for H_2 production: From models to powder catalysts, *Appl. Cat. A.*, **2016**, 518, 18-47. (Review article written while at JMU, with Brookhaven National Lab postdocs and scientists who are funded by U.S. Department of Energy DE-SC0012704)

14. Shorish, Y.; Reisner, B. A. Building Data and Information Literacy in the Undergraduate Chemistry Curriculum. In *Integrating Information Literacy into the Chemistry Curriculum*; Lovitt, C. F.; Shuyler, K.; Li, Y., Eds.; ACS Symposium Series 1232; American Chemical Society: Washington, DC, **2016**; pp. 31-56. **DOI:** 10.1021/bk-2016-1232.ch002

15. Boyle, D. T.; Wilke, J. A.; Palomino, R. M.; Lam, V. H.; Schlosser, D. A.; Andahazy, W. J.; Stopak, C. Z.; Stacchiola, D. J.; Rodriguez, J. A.; Baber, A. E. Elucidation of active sites for the reaction of ethanol on TiO_2/Au(111), *J. Phys. Chem. C*, **2017**, *121*, 7794-7802. Grant: **4-VA**, **U.S. Department of Energy DE-SC0012704 (for work done at Brookhaven National Laboratory, IR experiments)**.

16. Padala P.; Oweis W.; Mashahreh B.; Soudah N.; Cohen-Kfir E.; Todd E. A.; Berndsen C. E.; Wiener R. Novel insights into the interaction of UBA5 with UFM1 via a UFM1-interacting sequence. *Sci Rep*. **2017** Mar 30;7(1):508. doi: 10.1038/s41598-017-00610-0.

17. Wang, S.; Liebing, P.; Oehler, F.; Gilje, J. W.; Hrib, C. G.; Edelmann, F. T. Supramolecular layer structures of Mn(II), Co(II) and Cu(II) complexes with the 3-(1*H*-benzotriazol-1-yl)-propanamide ligand – Metal coordination vs. hydrogen bonding, *Cryst. Growth Des*. **2017**, *17*, 3402-3410.

18. Ackermann M. A.; King B.; Perry N. A.; Bobbili P. J.; Rudloff M.; Berndsen C. E.; Wright N. T.; Hecker P. A.; Kontrogianni-Konstantopoulos A. Small obscurins at the intercalted disc Mediate Cardiomyocyte Adhesion and size via the PI3K/AKT/mTOR pathway (submitted to Cardiovascular Research July 2017). (**Research Corporation**)

19. Santiago A. E.; Yan M. B.; Tran M. B.; Wright N. T.; Luzader D. H.; Kendall M. M.; Ruiz-Perez F.; Nataro J. P. A large family of anti-activator accompanying XylS/AraC family regulatory proteins, *Molecular Microbiology* **2016,** Jul; 101(2), 314-32. (**Research Corporation**)

20. Temple J. E.; Oehler M. C.; Wright N. T.; Chemical shift assignments of the 2nd domain of human obscurin A, *J. Biomolecular NMR Assignments*, **2016** Apr; 10(1), 63-5.

21. Wright N. T. Heteronuclear multidimensional NMR in a teaching laboratory, *J. Chem. Educ.*, **2016**; 93(2), 287-91.

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

1. Baber, A. E. Surface chemistry over inverse model catalysts from ultrahigh vacuum to near-ambient pressures, Appalachian State Seminar Series, Boone, NC, November 6, 2015. Invited oral presentation.

2. Baber, A. E. Unraveling the Relationship between Structure and Activity using Model Catalysts under Near-Ambient Pressures, 250th American Chemical Society National Meeting, Boston, MA, August 17, 2015. Invited Oral Presentation.

3. Baber, A. E.; Boyle, D. T.; Stopak, C. Z. Fundamental Catalytic Studies of Bimetallic and Oxide Nanomaterials for CO oxidation and the Reverse Water Gas Shift Reaction, poster presentation, 250th American Chemical Society National Meeting, Boston, MA, August 16, 2015. Poster.

4. Baber, A. E., Boyle, D. T.; Andahazy, W. J.; Lam, V. H.; Schlosser, D. A.; Tosti, N.; Wilke, J. A. Titania/gold inverse model catalysts for acetaldehyde formation from ethanol, 63rd International American Vacuum Society Symposium & Exhibition, Nashville, TN, November 9, 2016. Oral presentation number 1384.

5. Baber, A. E. Direct visualization of atomic–scale model catalyst features from ultrahigh vacuum to near-ambient pressures, Southeastern Regional Meeting of the American Chemical Society, Columbia, SC, October 25, 2016. Invited oral presentation number 603.

6. Boyle, D. T.; Wilke, J. A.; Lam, V. H.; Baber, A. E. Low temperature adsorption of ethanol on TiO_2/Au(111) inverse model catalysts, oral, Southeastern Regional Meeting of the American Chemical Society, Columbia, SC, October 25, 2016. Oral presentation number 862.

7. Wilke, J. A.; Baber, A. E. Stabilization and reaction of small molecules on TiO_2/Au(111) inverse model catalysts, Southeastern Regional Meeting of the American Chemical Society, Columbia, SC, October 24, 2016. Poster 445.

8. Andahazy, W. J.; Boyle, D. T.; Stopak, C. Z.; Baber, A. E. Using inverse model catalysts to investigate CO_2 chemistry, poster, 251st American Chemical Society National Meeting, San Diego, March 14, 2016. Poster 2421106

9. Boyle, D. T.; Andahazy, W. J.; Stopak, C. Z.; Lam, V. H.; Schlosser, D. A.; Boeckmann, D. M.; Baber, A. E. Adsorption and reactivity of ethanol on Au(111)-based inverse model catalysts, 251st American Chemical Society National Meeting, San Diego, March 14, 2016. Poster 2418246.

10. Baber, A. E. Unraveling the relationship between structure and activity using model catalysts under near-ambient pressures, Loyola University Chicago, April 27, 2017. Guest video conference lecture given in a joint undergraduate/graduate course “Structure and Reactivity of Solid Surfaces” Chem 395/435.

11. Andahazy, W. J.; Baber, A. E.; Constantin, C. Correlation between optical and electrical properties of acid treated PEDOT-PSS films, Material Research Society Spring Meeting and Exhibit, Phoenix, AZ, April 18, 2017. Poster ED8.4.13.

12. Boyle, D. T.; Wilke, J. A.; Lam, V. H.; Baber, A. E., poster. Elucidating distinct Au(111) and TiO2 /Au(111) surface sites for the selective oxidation of ethanol to acetaldehyde, 253rd American Chemical Society National Meeting, San Francisco, April 2, 2017. COLL poster 362.

13. Wilke, J. A.; Baber, A. E., poster. Stabilization and reaction of small molecules on TiO2/ Au(111) inverse model catalysts, 253rd American Chemical Society National Meeting, San Francisco, April 2, 2017. COLL poster 263.

14. Baber, A. E.; Boyle, D. T.; Andahazy, W. J.; Lam, V. H.; Schlosser, D. A.; Tosti, N.; Wilke, J. A. Determining optimum surface preparations to control the selectivity of ethanol chemistry over TiO_2/Au(111), 253rd American Chemical Society National Meeting, San Francisco, April 6, 2017. COLL oral presentation 798.

Berndsen

15. Young, B. H.; Caldwell, T. A.; McKenzie, A. M.; Kokhan, O.; Berndsen, C. E. Characterization of the structure and catalytic activity of Legionella pneumophila VipF Midwest Enzyme Chemistry Conference, Chicago, Sept 12, 2015.

16. Berndsen, C. E.; Hilliard, M. T.; Gibbs, D. R.; Bijani, S.; Wright, N. T.; Wiener, R.; Identification of novel substrate binding sites in the Ufm1 activating enzyme, Midwest Enzyme Chemistry Conference, Chicago, Sept 12, 2015.

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.

18. Berndsen, C. E. Viral tethering by Tetherin. Presented to the Department of Chemistry at Wake Forest University, September 9th, 2015.

19. Ozcan, K. A.; Berndsen, C. E. Simulation of viral tethering by membrane anchored anti-viral protein BST-2. Presented at 19th CNMS Undergraduate Research Symposium, UMBC, Baltimore, MD October 22, 2016.

20. Henderson, M.; Berndsen, C. E. Structural and functional studies of aquifex aeolicus proteins AQ_328, AQ_1359, AND AQ_1482; Presented at Presented at 19th CNMS Undergraduate Research Symposium, UMBC, Baltimore, MD October 22, 2016.

21. Kelly, R. T.; South, E. J.; Berndsen, C. E. Investigation into allosteric effects of UFM1; Presented at Presented at 19th CNMS Undergraduate Research Symposium, UMBC, Baltimore, MD 10-22-2016.

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

23. Jackson, C. E.; Berndsen, C. E. Fluorescent assay of Ubiquitin conjugation. ASBMB, San Diego, Apr 2 to 6, 2016; 834.14.

24. Ozcan, K. A.; Berndsen, C. E. Structural mechanism of viral tethering by the anti-viral protein BST-2. Presented at ASBMB 2017, Chicago, IL, 4-23-2017.

25. Kelly, R. T.; Berndsen, C. E. Conformation locking and unlocking in the Ubiquitin family of proteins; Presented at ASBMB 2017, Chicago, IL, 4-25-2017.

Foust/Hughey

26. Foust, R. D.; Hughey, C. A.; Ralston, D. Detection limit and limit of quantitation: An instrumental anlaysis exercise with statistics. 251st American Society National Meeting & Exposition, March 13-17, 2016, ANYL 259.

Kokhan

27. McKenzie, A. M.; Marzolf, D. R.; O'Malley, M. C.; Kokhan, O. Ultrafast limits of photo-induced electron transfer rates in PpcA, a multi-heme c-type cytochrome. Presented at Biophysical Society Meeting, Los Angeles, CA, February 28, 2016, 102-platform

28. Marzolf, D. R.; McKenzie, A. M.; Hudson, C. A.; Kokhan, O. Multimerization of solution-state proteins by water-soluble porphyrins. Presented at Biophysical Society Meeting, Los Angeles, CA, February 28, 2016, 254-poster

29. Kokhan, O.; Marzolf, D. R.; Hudson, C. A.; McKenzie, A. M. Photo-induced charged and energy transfer in complexes of c-type cytochromes with water-soluble porphyrins. Presented at Biophysical Society Meeting, Los Angeles, CA, February 29, 2016, 1540-poster

30. McKenzie, A. M.; Marzolf, D. R.; O'Malley, M. C.; Kokhan, O. Ultrafast limits of photo-induced electron transfer rates in PpcA, a multi-heme c-type cytochrome. Presented at UMBC Undergraduate Symposium, Baltimore, MD, October 3, 2015, 130-poster

31. Marzolf, D. R.; McKenzie, A. M.; Hudson, C. A.; Kokhan, O. Multimerization of solution-state proteins by water-soluble porphyrins. Presented at UMBC Undergraduate Symposium, Baltimore, MD, October 3, 2015, 118-poster

32. Hudson, C. A.; Kokhan, O. Interactions between water-soluble porphyrins and c-type cytochromes. Presented at UMBC Undergraduate Symposium, Baltimore, MD, October 3, 2015, 165-poster

33. Kokhan, O. Molecular mechanisms of short-range electron transfer in metalloproteins, seminar presented at Department of Chemistry, University of Michigan at Ann Arbor, November 4, 2016.

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

35. Kokhan, O.; Marzolf, D. R.; Hudson, C. A.; McKenzie, A. M. Photoinduced charge and energy transfer in complexes of c-type cytochromes with water-soluble porphyrins, poster presented at Biophysical Society Meeting February 13, 2017, 2172-pos

36. O'Malley, M. C.; McKenzie, A. M.; Marzolf, D. R.; Swaim, C.; Kokhan, O. Mimicking natural photosynthesis: ultrafast charge transfer in PpcA-Ru(bpy)3 complexes, poster presented at Biophysical Society Meeting, February 14, 2017, 2171-pos.

37. Marzolf, D. R.; Swaim C. M.; McKenzie A. M.; Hudson C. A.; Wright N. T.; Kokhan, O. Porphyrin-induced multimerization of solution-state proteins, poster presented at Biophysical Society Meeting, February 15, 2017, 2427-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.

39. Light, T. P.; Metrick, M. A.; MacDonald, G. Cation–specific influences on the solvation and solvent accessibility of alanine-rich peptides. Biophysical Society Meeting, 2016, Los Angeles, CA.

Raston

40. Raston, P. L.; Bunn, H. Far-Infrared spectroscopy of syn-vinyl alcohol. Presented at the 71st International Symposium on Molecular Spectroscopy, Champaign-Urbana, Il, USA, June 20-24, 2016.

41. Raston, P. L.; Bunn, H. Infrared spectroscopy of the O_2-H_2/HD/D_2 van der Waals complexes. Presented at the 71st International Symposium on Molecular Spectroscopy, Champaign-Urbana, Il, USA, June 20-24, 2016.

42. Raston, P. L.; Bunn, H. Far-Infrared spectroscopy of anti-vinyl alcohol. Presented at the 71st International Symposium on Molecular Spectroscopy, Champaign-Urbana, Il, USA, June 20-24, 2016.

43. Bunn, H.; Raston, P. L.; Douberly, G. E. Laser spectroscopy of vinyl alcohol embedded in helium nanodroplets. Presented at the 72nd International Symposium on Molecular Spectroscopy, Champaign-Urbana, Il, USA, June 19-23, 2017.

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

46. Reisner, B. A.; Pazicni. S. Engaging in Feedback Part II: Research on illusory competence and self-assessment. Presented at the 254th National Meeting of the American Chemical Society, Washington, DC, August 21, 2017: CHED 95.