

2021:

1. Cresti, J.R., Manfredonia, A.J., Bragança, C.E., Boscia, J.A., Hurley, C.M., Cundiff, M.D., and Kraut, D.A., 2021. Proteasomal conformation controls unfolding ability. *Proceedings of the National Academy of Sciences*, 118(25).
2. Pinca, J.R., Duborg, W.G. and Jorn, R., 2021. Ion Association and Electrolyte Structure at Surface Films in Lithium-Ion Batteries. *The Journal of Physical Chemistry C*, 125(13), pp.7054-7066.
3. Repash, E.M., Pensabene, K.M., Palenchar, P.M. and Eggler, A.L., 2021. Solving the Problem of Assessing Synergy and Antagonism for Non-Traditional Dosing Curve Compounds Using the DE/ZI Method: Application to Nrf2 Activators. *Frontiers in pharmacology*, 12, p.1384.
4. Zhai, T., Zhang, F., Haider, S., Kraut, D. and Huang, Z., 2021. An Integrated Computational and Experimental Approach to Identifying Inhibitors for SARS-CoV-2 3CL Protease. *Frontiers in molecular biosciences*, 8, p.267.
5. Benson, K.R., Stash, J., Moffa, K.L., Schmehl, R.H., Dudley, T.J. and Paul, J., 2021. Ruthenium complexes with asymmetric hydroxy-and methoxy-substituted bipyridine ligands. *Polyhedron*, p.115300.
6. Martinez, K., Benson, K., Paul, J. and Schmehl, R.H., 2021. Photophysics of Ru (II) complexes with hydroxylated diimine ligands: Photoinduced electron/proton transfer to anthraquinone. *Polyhedron*, 207, p.115376.
7. Saghatforoush, L., Hosseinpour, S., Moeini, K., Mardani, Z., Bezpalko, M.W. and Kassel, W.S., 2021. Investigation Of The Binding Ability Of A New Thiosemicarbazone-Based Ligand And Its Zn (II) Complex Toward Proteins And DNA: Spectral, Structural, Theoretical, And Docking Studies. *Journal of Structural Chemistry*, 62(5), pp.748-761.
8. Sauerland, M., Mertes, R., Morozzi, C., Eggler, A.L., Gamon, L.F. and Davies, M.J., 2021. Kinetic assessment of Michael addition reactions of alpha, beta-unsaturated carbonyl compounds to amino acid and protein thiols. *Free Radical Biology and Medicine*, 169, pp.1-11.
9. Domingo, L.R., Seif, A., Mazarei, E., Zahedi, E. and Ahmadi, T.S., 2021. Quasi-RRHO approximation and DFT study for understanding the mechanism and kinetics of nitration reaction of benzonitrile with nitronium ion. *Computational and Theoretical Chemistry*, 1199, p.113209.
10. Domingo, L.R., Mazarei, E., Seif, A., Ríos-Gutiérrez, M., Zahedi, E. and Ahmadi, T.S., 2021. Closer Investigation of the Kinetics and Mechanism of Spirovinylcyclopropyl Oxindole Reaction with $3\Sigma-g$ -O₂ by Topological Approaches and Unraveling the Role of the I₂ Catalyst. *The Journal of Physical Chemistry A*.

11. Boschi, V. and Willenbring, J.K., Chemical and physical drivers of beryllium retention in two soil endmembers. *Science of The Total Environment*, **2021**, 754, p.141591. <https://doi.org/10.1016/j.scitotenv.2020.141591>
12. Sundberg, B.N. and Lagalante, A.F., Characterization of non-ionic surfactants in Winsor & Newton's water-mixable oil paints. *Journal of Cultural Heritage*, **2021**, 48, pp.54-64. <https://doi.org/10.1016/j.culher.2020.12.008>
13. Michal P. Glogowski, Jay M. Matthews, Brian G. Lawhorn, Kevin P. C. Minbolie. Diastereoselective Copper-Mediated Conjugate Addition of Functionalized Magnesiates for the Preparation of Bisaryl NRF2 Activators. *Journal of Organic Chemistry* **2021**, 86, 4, 3120–3137. DOI: [10.1021/acs.joc.0c02639](https://doi.org/10.1021/acs.joc.0c02639)
14. Lea Barny, Julia Tasca, Hugo Sanchez, Chelsea Smith, Suzanne Koptur, Tatyana Livshultz, Kevin P.C. Minbolie. Chemotaxonomic Investigation of Apocynaceae for Retronecine-Type Pyrrolizidine Alkaloids Using HPLC-MS/MS. *Phytochemistry* **2021**, Volume 185, May 2021, 112662. DOI: <https://doi.org/10.1016/j.phytochem.2021.112662>
15. Javier A Feliciano; Austin J. Leitgeb; Cassandra L. Schrank; Ryan A. Allen; Kevin PC Minbolie; William M. Wuest, Robert Carden. Trivalent Sulfonium Compounds (TSCs): Tetrahydrothiophene-based amphiphiles exhibit similar antimicrobial activity to analogous ammonium-based amphiphiles. *Bioorganic and Medicinal Chemistry Letters* **2021**, 37, p.127809. DOI: [10.1016/j.bmcl.2021.127809](https://doi.org/10.1016/j.bmcl.2021.127809)
16. Jenifer Walke, Matthew Becker, Arianna Krinos, Elizabeth (Burzynski) Chang, Celina Santiago, Thomas Umile, Kevin Minbolie, Lisa Belden. Seasonal changes and the unexpected impact of environmental disturbance on skin bacteria of individual amphibians in a natural habitat. *FEMS Microbiology Ecology* **2021**, Volume 97, Issue 3, March 2021, fiaa248. DOI: [10.1093/femsec/fiaa248](https://doi.org/10.1093/femsec/fiaa248)
17. Kyle J. Sommers, Brian S. Bentley, Robert G. Carden, Savannah J. Post, Ryan A. Allen, Renee C. Kontos, Jacob W. Black, William M. Wuest, Kevin P. C. Minbolie. Metallocene QACs: The Incorporation of Ferrocene Moieties into monoQAC and bisQAC Structures. *ChemMedChem* **2021**, 16, 3, 467-471. DOI: [10.1002/cmdc.202000605](https://doi.org/10.1002/cmdc.202000605)
18. Silverberg, L.J., Mal, T.K., Pacheco, C.N., Povelones, M.L., Malfara, M.F., Lagalante, A.F., Olsen, M.A., Yennawar, H.P., Sobhi, H.F., Baney, K.R. and Bozeman, R.L., **2021**. T3P-Promoted Synthesis of a Series of 2-Aryl-3-phenyl-2, 3-dihydro-4H-pyrido [3, 2-e][1, 3] thiazin-4-ones and Their Activity against the Kinetoplastid Parasite Trypanosoma brucei. *Molecules*, 26(20), p.6099.
19. O'Reilly, M.C., Stoffregen, S.A., Peterson, K.P., Maddox III, M.P. and Schrank, C., **2021**. Discovery-Based Bromination of Alcohols: An Organic Chemistry Experiment Supporting Spectroscopic Analysis and Mechanistic Reasoning. *Journal of Chemical Education*, 98(10), pp.3326-3332.

20. **Hurley C.M.**, Kraut D.A. (2021) Determination of Proteasomal Unfolding Ability. In: Cacace A.M., Hickey C.M., Békés M. (eds) Targeted Protein Degradation. Methods in Molecular Biology, vol 2365. Humana, New York, NY. https://doi.org/10.1007/978-1-0716-1665-9_12

2022:

1. **Fumo, VM**; Roberts, RC; Zhang, JY ; and O'Reilly, MC. "Diastereoselective synthesis of cyclic tetrapeptide pseudoxyllemycin A illuminates the impact of base during macrolactamization" Organic and Biomolecular Chemistry, February 1, 2023. DOI: 10.1039/d2ob02126a

2. Atom Economical QPCs: Phenyl-Free Biscationic Quaternary Phosphonium Compounds as Potent Disinfectants Author(s): Thierer, LM; Petersen, AA; Michaud, ME; Sanchez, CA; **Brayton, SR**; Wuest, WM; Minbile, KPC, ACS INFECTIOUS DISEASES, FEB 2023. DOI: 10.1021/acsinfecdis.2c00575

3. An integrated physiological perspective on anthropogenic stressors in the Gulf coast toad (*Incilius nebulifer*), Monroe, DJ; Barny, Lea A.; Wu, Alice; Minbile, Kevin P. C.; Gabor, Caitlin R. FRONTIERS IN ECOLOGY AND EVOLUTION Volume: 11; FEB 2 2023DOI: 10.3389/fevo.2023.1112982

4. Bimolecular Excited-State Proton-Coupled Electron Transfer within Encounter Complexes. Martinez, Kristina; Koehne, Sydney M.; **Benson, Kaitlyn**; Paul, Jared J.; Schmehl, I.; Russell H. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY FEB 2023. 10.1021/jacs.2c10165

5. Crystal structures of the sulfones of 2,3-diphenyl2,3-dihydro-4H-1,3-benzothiazin-4-one and 2,3diphenyl-2,3-dihydro-4H-pyrido[3,2-e][1,3]thiazin- 4-one. Yennawar, Hemant P.; Mal, Tapas K.; Pacheco, Carlos N.; Lagalante, Anthony F.; Olsen, Mark A.; Russell, Michael W.; Muench, Grace C.; Moyer, Quentin J.; Silverberg, Lee J. ACTA CRYSTALLOGRAPHICA SECTION E-CRYSTALLOGRAPHIC COMMUNICATIONS Volume: 79, MAR 2023. DOI: 10.1107/S2056989023001524

6. Metabolite compositions on skins of eastern hellbenders *Cryptobranchus alleganiensis alleganiensis* differ with location and captivity. Loudon, Andrew H.; Terrell, Kimberly A.; **Davis, Robert W.**; Umile, Thomas P.; Lipps, Gregory J.; Greathouse, Joe; Chapman, Eric; Roblee, Kenneth; Kleopfer, John D.; Bales, Emma K.; Hyman, Oliver J.; Harris, Reid N.; Minbile, Kevin P. C. DISEASES OF AQUATIC ORGANISMS Volume: 153 Pages: 9-16, FEB 2 2023. DOI: 10.3354/dao03715

7. Soft QPCs: Biscationic Quaternary Phosphonium Compounds as Soft Antimicrobial Agents. **Brayton, SR**; Toles, ZEA; Sanchez, CA; Michaud, ME; Thierer, LM; Keller, TM; Risener, CJ; Quave, CL; Wuest, WM; Minbile, KPC. ACS INFECTIOUS DISEASES Volume: 9, APR 14 2023 DOI: 10.1021/acsinfecdis.2c00624

8. Scalable and Chromatography-Free Synthesis of Efflux Pump Inhibitor Phenylalanine Arginine beta-Naphthylamide for Its Validation in Wild-Type Bacterial Strains. Russo, CM; Howey, KG; O'Reilly, MC; CHEMMEDCHEM, May 2023, 1860-7187. <http://dx.doi.org/10.1002/cmdc.202300128>