

Student Publications: 2015 – 2019

(Chemistry undergraduate authors are underlined)

2015

Bruce, C.D.; Ferrara, M.M.; Manka, J.L.; Davis, Z.S.; Register, J. Dynamic hydrogen bonding and DNA flexibility in minor groove binders: molecular dynamics simulation of the polyamide f-ImPyIm bound to the Miu1 (MCB) sequence 5'-ACGCGT-3' in 2:1 motif. *J. Mol. Recog.* **2015**, 28, 325-337.

Satam, V.; Babu, B.; Patil, P.; Brien, K. A.; Olson, K.; Savagain, M.; Lee, M.; Mephram, A.; Jobe, L. B.; Bingham, J. P.; Pett, L.; Wang, S.; Ferrara, M.; Bruce, C. D.; Wilson, W. D.; Lee, M.; Hartley, J. A.; Kiakos, K. AzaHx, a Novel Fluorescent, DNA Minor Groove and G-C Recognition Element: Synthesis and DNA Binding Properties of a p-Anisyl-4-Aza-Benzimidazole-Pyrrole-Imidazole (AzaHx-PI) Polyamide. *Bioorg. Med. Chem. Lett.*, **2015**, 25, 3681–3685.

2016

2017

Hunter, N.H.; Bakula, B.C.; Bruce, C.D. Molecular dynamics simulations of apo and holo forms of fatty acid binding protein 5 and cellular retinoic acid binding protein II reveal highly mobile protein, retinoic acid ligand, and water molecules. *Journal of Biomolecular Structure and Dynamics*, **2017**, online.

Student Presentations: 2015 – 2019

(Chemistry undergraduate presenters are underlined; awards received are **bold underlined**)

2015

Bou-Anak, S.; Burgett, M.; Nowacki, A.; Ahluwalia, M.; Gladson, C. Correlation of Higher Levels of Soluble TNF-R1 in Plasma with Increasing Age and Obesity in Patients with Glioblastoma Tumors. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Bou-Anak, S.; Kaltenbach, J. Examination of Tinnitus: Study of Synapses on Fusiform Cells in the Dorsal Cochlear Nucleus. Senior Honors Program Project (Advisors: Dr. Helen Murphy and Dr. Cyrilla Wideman, Neuroscience Program). Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Brown, B.; Hunter, N.; Bruce, C.D. Docking studies of a series of long-chain carboxylic acids in the Fatty Acid Binding Protein FABP5 as a potential cancer therapy. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Bukszar, Z.; Challen, P.; Solomon, V.; Dyck, J.S. Nanopowder Synthesis and Characterization of Bismuth Telluride Nanoparticles for Prospective Thermoelectric Materials. Presented at Annual Spring Meeting of the American Physical Society, Ohio-Region Section, Kent State University, Kent, OH, March 2015.

Bukszar, Z.; Dyck, J.; Challen, P.; Solomon, V. Bottom-Up Wet Chemical Synthesis of Bismuth Telluride Nanoparticles. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Buzalka, N.; Peshel, E.; Longworth, M. Identifying New Interactors of Condensin II Subunit dCAP-03. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Clark, K.; Dukes, D.; Rohde, D.E. Analysis of Synthetic Cannabinoids, Cathinones and Phenethylamines in Northeast Ohio. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Huber, A.; Harrington, R.; Otolowski, C.; Rice, D.; Barnett, Dr. Computational modeling of ionic liquids for use in dye-sensitized solar cells. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Hunter, N.; Bruce, C.D. Molecular Dynamics Studies of Retinoid Ligands in the Fatty Acid Binding Protein FABP5 as a Potential Cancer Therapy. Presented at 14th MERCURY Conference on Undergraduate Computational Chemistry, Bucknell University, Lewisburg, PA, July 2015.

Hurd, A.; Myers, A.; Mandato, D.; Fadoul, M.; Challen, P.; Kwan, D. Synthesis of a Pincer Complex with Sulfur Donor Atoms. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Indiano, B.; Rohde, D. Addition of Amphetamine Assay to an ELISA Drug Menu. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Kwit, A. Diverse Leadership: A Contemporary Recipe for Success. Leadership Scholars Program. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Kwit, A. Structural changes in DNA upon binding in a 2:1 motif to a polyamide minor groove binder: f-IPP in 5'-TAGCTA-3'. Senior Honors Program Project (Advisor: Dr. Chrystal Bruce, Chemistry). Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Lee, M.; Chandrasekharan, U.; Braley, C.; Dicorleto, P. Regulatory role of novel post-translational modifications of Signal Transducer and Activator of Transcription 3 (STAT3) in Human Endothelial Cells. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

McCabe, M.; Shinaver, R.; Meyer, M. The Heroin Trend. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Myers, A. Custom-synthesized Nutrient Derivatives as Inhibitors for Onset of Atherosclerosis. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Rocco, S. The Therapeutic Effects of Ataluren on BMPR2 Nonsense Mutations Leading to Pulmonary Arterial Hypertension. Senior Honors Program Project (Advisor: Dr. Jim Lissemore, Biology). Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Sammon, R. Everyday Leaders. Leadership Scholars Program. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015.

Stahon, K.; Bastian, C.; Kidd, G.; Brunet, S.; Baltan, S. Age dependent modifications of axons, mitochondrial dynamics, and Ca²⁺ homeostasis underlie the vulnerability of aging white matter to ischemia. Senior Honors Program Project (Advisor: Dr. Erin Johnson, Biology). Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2015. **The Provost's Award**

2016

Bakula, B. Interaction Simulations of Fatty Acid Binding Protein 5 with Fatty Acid Substituted Ligands. Presented at 15th MERCURY Conference on Undergraduate Computational Chemistry, Bucknell University, Lewisberg, PA, July 2016.

Beer, A.; Chai, Y. Peroxide Induced Specific Protein Modification in HeLa Cells. Presented at Cleveland Section ACS Meeting-in-Miniature, Cleveland State University, Cleveland, OH, March 2016.

Beer, A.; Chai, Y. Peroxide Induced Specific Protein Modification in HeLa Cells. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Blask, S. Characterization of the Bandwidth Gap of Graphene Quantum Dots. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Brown, B. Molecular Dynamics of Ligand Binding into FABP5. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Brown, B. Molecular dynamics simulations of a series of experimentally active ligands bound to Fatty Acid Binding Protein 5. Presented at the 252nd ACS National Meeting, Philadelphia, PA, August 2016.

Hadib Nissan, R. Hydrazone synthesis: E/Z conformational selectivity. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Hunter, N. Molecular Dynamics Studies of CRABP-II. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Hunter, N. Molecular dynamics studies of the binding of retinoic acid to the transport proteins CRABP-II and FABP5. Presented at the 252nd ACS National Meeting, Philadelphia, PA, August 2016.

Lee, M. Tumor Necrosis Factor Receptors in Psoriasis. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016. **Poster of Special Merit**

Mihas, A.; Murphy, H.; Wideman, C. Effects of a High-Fat/High-Sucrose Diet on Metabolism, Spatial Working Memory, and Anxiety-Like Behavior in Rats. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Monahan, A. Oxidative Stress and Alzheimer's Disease. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Mualem, J. The Economics Perspective of Gene Patents: Myriad Genetics Case Study. Presented at Celebration of Scholarship Panel Presentation, John Carroll University, University Heights, OH, April 2016.

Mualem, J.; Smith, J.; O'Dell, K. Transformational Leadership: From Theory to Board Room. Leadership Scholars Program. Presented at Celebration of Scholarship, John Carroll University, University Heights, OH, April 2016.

Nyaanga, J.; Nichols, M. Lipid Peroxidation of Linoleic Acid. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.
Poster of Special Merit

Osiecki, N.; Nichols, M. Proton NMR Studies of the Equilibrium of Ethyl Acetylacetate. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Parr, B.; Bastian, C.; Stahon, K.; Brunet, S.; Baltan, S. NOS Inhibition Promotes Axon Function Recovery by Preserving Axonal Mitochondrial after Ischemia. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Parr, B.; Piccillo, E.; Mascotti, D. Celis, E. Binding Properties of Peptide (RRWRRRRRRAAATAPDNLGYM) with Poly-IC. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Parr, B.; Smith, J.; O'Dell, K. An Analysis of Transformational Leadership and Its Application amongst Different Leaders. Leadership Scholars Program. Presented at Celebration of Scholarship, John Carroll University, University Heights, OH, April 2016.

Salemme, R.; Lee, M.; Braley, C.; Chandrasekharan, U.; DiCorleto, P. Small Interfering RNAs (siRNAs) Targeting 3'-UTR Region of Protein Arginine Methyl Transferase 5 (PRMT5) Inhibited TNF Induction of Proinflammatory Genes in Endothelial Cells. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Seiter, E.M.; Bolton, S.K.; Saporito, R.A. A New Method for Extracting Alkaloid Defenses from Poison Frog Skins. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Sternbach, S.; Nichols, M. The Study of Intermediates of a Deprotonation Reaction of a Ketone with a Lithium Amide Base using ^6Li , ^{15}N NMR Spectroscopy and Molecular Modeling. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Sternbach, S.; Murphy, H.; Wideman, C. Effects of a High Fat Diet on Metabolism and Working Memory in Rats. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Taleff, N. Proton NMR Studies of the Equilibrium of Acetylacetone. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Volpe, D.; Dyck, J.; Challen, P. Bottom-Up Wet Chemical Synthesis of the Infinitely Adaptable Bismuth Telluride Series. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2016.

Volpe, D.J.; Challen, P.R.; Solomon, V.C.; Dyck, J.S. Bottom-Up Wet Chemical Synthesis of Nanostructured Materials from the Infinitely Adaptable Bismuth Telluride Series. Presented at Annual Spring Meeting of the American Physical Society, Ohio-Region Section, Dayton, OH, April 2016.

2017

Altabbaa, R.; Dweik, R.; Aulak, K.; Tian, L.; Mellor. A Role for Transforming Growth Factor- β in Pulmonary Arterial Hypertension. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Bakula, B.; Perugini, A. Molecular Dynamics Simulations of Fatty Acid Binding Protein 5 with Fatty Acid Substituted Ligands. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Beer, A. Comparing the Middle and C-terminal Domains of the SOXE Proteins. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Brown, B. Bottom-up wet chemical synthesis and characterization of the infinitely adaptable $(\text{Bi}_2)_m(\text{Bi}_2\text{Te}_3)_n$ (PC). Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Brown, B. Molecular Dynamics study of the protein-ligand interactions of a Fatty Acid Binding Protein. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Ekstrand, E.; Murphy, H.; Wideman, C. The Effects of Vyvanse on Spatial Working Memory, Body Weight, and Adiposity in Rats. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Ellis, E. Analysis of Thiophene- and Pyrrole- Substituted Fatty Acids in FABP5 by Molecular Dynamics Simulations. Presented at 16th MERCURY Conference on Undergraduate Computational Chemistry, Furman University, Greenville, SC, July 2017.

Exler, R.J.; O'Dell, K. Leadership in Financial Service Professionals. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Koetting, P. Initial Coordinates Impact on Trajectory of Protein-Ligand Binding Interactions with FABP5. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Mahoney, M.; Rishavy, M.A.; Hallgren, K.W.; Berkner, K.L. Generating Vitamin K Oxidoreductase Complex 1 Mutants. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

May, N. Principle Component Analysis of Lavender Essential Oils. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Nyaanga, J. Characterization of Missense Mutations in Factor VIII That Lead to Abnormal N-Linked Glycosylation. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Piccillo, E.; Perkins, B.; Lessieur, E.; Nivar, G.; Murphy, H.; Wideman, C. Visual Performance Evaluation of Zebrafish with Mutations in Cilia Transition Zone Proteins CEP290, AHI1, and ARL13B. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Ponsart, K. Leadership in the Medical Field. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Posney, E. Alterations in the Hind Limb Vasculature of STS-135 Mice. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Posney, E. Leadership Essentials for Pharmacists. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.

Rey, G.; Hoffman, G.; Skerl, E.; Altabbaa, R.; Kwan, M.L. Preparation of ¹⁹F NMR-Reporter Pincer Ligand: Trying to be greener. Presented at Celebration of Scholarship Poster Session, John Carroll University, University Heights, OH, April 2017.