Ernest A-Williams

Ph.D. Candidate,
Aspiring Medicinal Chemist

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https://awoonor.github.io/

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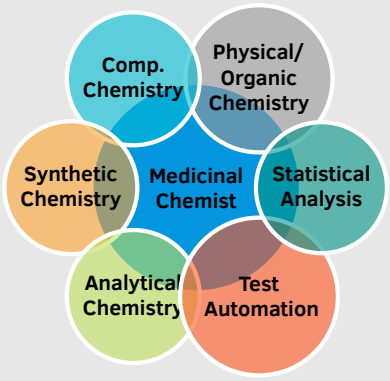
Skills



Interests

- Drug Design & Discovery
- Medicinal Chemistry
- Computational Biophysics
- Molecular Dynamics
- Pharmacology

Education

2014 - Pres. (Expected) **PhD., Chemistry** — Memorial University
St. John's, NL, Canada
Supervisor: **Prof. Chris Rowley**
Specialization: Physical, Theoretical & Computational Chemistry

2010 - 2014 **BSc. (Hons), Chemistry** — Mount Allison University
Sackville, NB, Canada
First Class Honours with Distinction

Research

2014 - Pres. **Graduate Research Assistant** — Memorial University

- Developing computational methods to better predict the pK_a's of cysteine residues in proteins and kinase enzymes

2013 - 2014 **Research Associate** — ChemGreen Innovation Inc.

- Worked as a research associate for ChemGreen Inc. exploring physical chemistry and chemistry physics, and its applications to green chemistry and energy.

Jan.2014 - May.2014 **Independent Student Researcher** — Metal Heads Research Group

- Special topics research project in inorganic chemistry under the supervision of Dr. Glen Briand of Mount Allison University. The project involved synthetizing bismuth amine-thiol complexes and testing them for their catalytic properties.

May 2013 - May 2014 **Honours Research Student** — Mount Allison University

- Explored the kinetics and thermodynamics of hexafluoropropene radical polymerization in supercritical carbon dioxide. The research was conducted under the supervision of Prof. Khashayar Ghandi (Mount Allison University), and combined both experimental and computational methods.

May 2013 - Jul. 2013 **Research Scientist** — TRIUMF National Laboratory

- Worked with a team of research scientists at TRIUMF National Laboratory exploring muonium free radical chemistry in supercritical fluids such as carbon dioxide

Sept.2011 - Aug. 2012 **Research Assistant** — The Wild Toads Research Group

- Conducted experimental research in Prof. Stephen Westcott's lab (Mount Allison University) investigating the synthesis and biological activity of novel Schiff-base compounds derived from long chain amines. New compounds were characterized using a number of experimental techniques and were tested for their potential as anti-fungal and antibacterial agents.

Select Publications

1. **Awoonor-Williams, E.** ; Walsh, A. G.; Rowley, C. N. ***Modeling Covalent Modifier-Drugs*** BBA – Proteins and Proteomics (2017).
   DOI: https://doi.org/10.1016/j.bbapap.2017.05.009
2. **Awoonor-Williams, E.** ; Rowley, C. N. ***The Hydration Structure of Carbon Monoxide by Ab Initio Methods*** J. Chem. Phys. 146 (2017).
   DOI: http://dx.doi.org/10.1063/1.4974164
3. Gaalswyk, K.;**Awoonor-Williams, E.** ; Rowley, C. N. ***Generalized Langevin Methods for Calculating Transmembrane Diffusivity*** J. Chem. Theory Comput. (2016), 12(11).
   DOI: http://dx.doi.org/10.1021/acs.jctc.6b00747
4. **Awoonor-Williams, E.** ; Rowley, C. N. ***Evaluation of Methods for the Calculation of the pK_a's of Cysteine Residues in Proteins*** J. Chem. Theory Comput. (2016), 12(9).
   DOI: http://dx.doi.org/10.1021/acs.jctc.6b00631
5. **Awoonor-Williams, E.** ; Rowley, C. N. ***Molecular Simulation of Nonfacilated Membrane Premeation*** BBA – Biomembranes (2016), 1858(7).
   DOI: https://doi.org/10.1016/j.bbamem.2015.12.014
6. Erika N. Daley; Keshia A. Moffat; Maria N. Wilson; Matthew M. Brown; **Awoonor-Williams, E.**; Marco I. Farren-Dai; Christopher M. Vogels; Allan A. Letourneau; Taylor M. Brooks; Andreas Decken; Felix J. Baerlocher; Stephen A. Westcott ***Synthesis and Antimicrobial Properties of Lipophilic Schiff Base Copper and Palladium Complexes*** Transition Metal Chem. (2015), 12(9).
   DOI: http://dx.doi.org/10.1007/s11243-015-9953-y
7. Khashayar Ghandi; Alexander D. Findlater; Zahid Mahimwalla; Connor S. MacNeil; **Awoonor-Williams, E.**; Federico Zahariev; Mark S. Gordon ***Ultra-fast Electron Capture by Electrosterically-Stabilized Gold Nanoparticles*** Nanoscale (2015), 7.
   DOI: http://dx.doi.org/10.1039/C5NR02291F
8. Farren-Dai, M.; **Awoonor-Williams, E.**; MacNeil, C. S.; Mahimwalla, Z.; Ghandi, K. ***A Novel Gold Nanoparticle Stabilization and its Muon Chemistry*** Chemical Physics Letters, ***Editors Choice*** (2015), 610–611.
   DOI: https://doi.org/10.1016/j.cplett.2014.06.051

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Affiliations

- 2014–present
  Teaching Assistants' Union of Memorial University of Newfoundland (TAUMUN)
- 2014–present
  Biophysical Society of Canada, *Member*
- 2015–present
  Chemical Institute of Canada (CIC), *Member*
- 2015–present
  Memorial University Chemistry Graduate Society (MUNCGS), *Secretary*
- 2015–present
  Memorial University Graduate Student Safety Committee

Skills & Abilities

- Programming Languages: Python, LabVIEW, MATLAB
- LaTeX, Linux, Adobe Illustrator, Schödinger/Maestro, MOE.