

Ernest A-Williams Education

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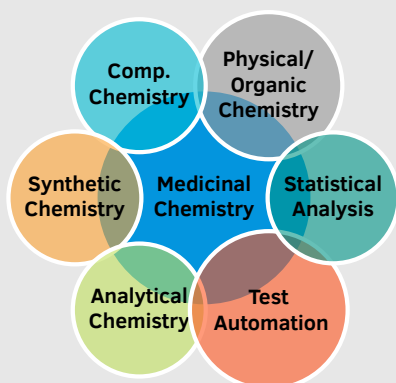


<https://awoonor.github.io/>



esaw83@mun.ca

Skills



Interests

Drug Design & Discovery



Medicinal Chemistry



Computational Biophysics



Molecular Dynamics



Pharmacology



2014 – 2020

Completed

PhD., Chemistry

St. John's, NL, Canada

Supervisor: **Prof. Chris Rowley**

Specialization: Theoretical & Computational Chemistry

Memorial University

2010 – 2014

BSc. (Hons), Chemistry

Sackville, NB, Canada

Supervisor: **Prof. Khashayar Ghandi**

Specialization: Physical Chemistry

Mount Allison University

Research Experience

Sep. 2014 –

Apr. 2020

Graduate Research Assistant

Dept. of Chemistry, Memorial University

- Developing and exploring new computational methods to predict the reactivity of druggable targets in protein kinase enzymes.

Jan. – May

2019

Visiting Researcher

Centre for Chemical and Synthetic Biology, Uottawa

- Design, synthesis, and evaluation of targeted covalent inhibitors for human tissue transglutaminase enzyme.

May 2013 –

Aug. 2014

Research Associate

ChemGreen Innovation Inc.

- Explored the chemistry of free radical reactions in green solvents, particularly supercritical CO₂, and its applications.

Jan. 2014 –

May. 2014

Independent Student Researcher

Metal Heads Research Group, MtA

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

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 CO₂. This research was part of BSc. (Hons) thesis work.

Sept. 2011 –

Aug. 2012

Research Assistant

The Wild Toads Research Group, MtA

- Conducted experimental research work 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. Novel compounds were characterized using a suite of spectroscopic techniques and were tested for their potential as anti-fungal and antibacterial agents.

Select Publications

1. **Awoonor-Williams, E.** ; Rowley, C. N. *How Reactive are Druggable Cysteines in Protein Kinases?* J. Chem. Inf. Model. (2018).
DOI: <https://doi.org/10.1021/acs.jcim.8b00454>
2. **Awoonor-Williams, E.** ; Rowley, C. N. *The Hydration Structure of Methylthiolate from QM/MM MD* J. Chem. Phys. (2018).
DOI: <https://doi.org/10.1063/1.5038010>
3. **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>
4. **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>
5. 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>
6. **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>
7. **Awoonor-Williams, E.** ; Rowley, C. N. *Molecular Simulation of Nonfacilitated Membrane Premeation* BBA – Biomembranes (2016), 1858(7).
DOI: <https://doi.org/10.1016/j.bbamem.2015.12.014>
8. 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>
9. 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>
10. 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

- 2015–present
Chemical Institute of Canada (CIC), *Member*
- 2014–present
Biophysical Society of Canada, *Member*
- 2017–2020
Memorial University Students' Biophysical Society, *President*

Skills & Abilities

- Programming Languages: Python, Bash Scripting.
- LaTeX, Linux, Schödingler/Maestro, MOE, NAMD, CHARMM, AMBER, etc.