Ernest A-Williams

LinkedIn /in/eawoonorwilliams

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https://awoonor.github.io/

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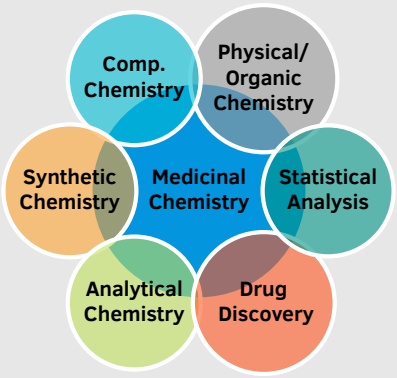
Skills



Interests

- Drug Design & Discovery
- Medicinal Chemistry
- Computational Biophysics
- Molecular Dynamics / QM/MM
- Data Science

Education

2014 – 2020 **PhD., Chemistry** — Memorial University
St. John's, NL, Canada
Supervisor: **Prof. Chris Rowley**
Specialization: Theoretical & Computational Chemistry

2010 – 2014 **BSc. (Hons), Chemistry** — Mount Allison University
Sackville, NB, Canada
Supervisor: **Prof. Khashayar Ghandi**
Specialization: Physical Chemistry

Research Experience

May 2021 – Present **Innovation Postdoc** — Novartis Institutes for BioMedical Research

- Exploring *in silico* approaches towards drug discovery

Sep. 2014 – May 2021 **Graduate Research Associate** — 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 CO_2, and its applications.

Jan. – 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 CO_2. 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 Nonfacilated 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

- 2019–present
  American Chemical Society (ACS), *Member*
- 2015–present
  Chemical Institute of Canada (CIC), *Member*
- 2014–present
  Biophysical Society of Canada, *Member*

Skills & Abilities

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