Christian Ieritano BSc, PhD

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Education

Sept 2017 – Aug 2023 **PhD – Chemistry** (University of Waterloo)
Supervisor: Prof. W. Scott Hopkins.

Dissertation title: *Towards Understanding Differential Ion Mobility and its Applications for Analytical and Medicinal Chemistry*

Sept 2012 – Apr 2017 **BSc – Medicinal Chemistry** (University of Waterloo)

Experience

Sept 2023 – Present **WaterFEL Project Coordinator**
University of Waterloo, Waterloo ON, Canada.

- Coordinated operations and managed instrumentation for the new infrared free electron laser (FEL) facility coming to UW, and analogous facilities at the University of British Columbia and TRIUMF.
- Modified commercial mass spectrometers to enable Infrared Multiple Photon Dissociation (IRMPD) experiments using IR light generated from the FEL.
- Developed software for data acquisition and processing for IRMPD experiments, in preparation for the FEL's activation.
- Prepared infrastructure and servers for data storage, screening user proposals, and provided safety training to users for upcoming public-access to FEL operations.

Sept 2017 – Aug 2023 **Graduate Research Assistant (Vanier Canada Scholar)**
University of Waterloo, Waterloo ON, Canada. **Supervisor**: Prof. W. Scott Hopkins

- 20+ publications (15 first author, 3 cover articles) on research concerning applications of ion mobility and mass spectrometry for separations of complex metabolite mixtures, prediction of molecular properties relevant to the drug-design process, trapped ion spectroscopy using UVPD, and modelling of ion mobility *in silico* using self written codes.
- Senior graduate student responsible for maintenance and upkeep of two SelexION Differential Mobility Spectrometers (DMSs) coupled to QTRAP 5500 triple quadrupole mass spectrometers, with modifications that enable action spectroscopy.
- Additional responsibilities included maintenance and upkeep of the Nd:YAG pump laser and OPO used for UVPD action spectroscopy on the DMS platform, organization of group meetings, and training of undergraduate/graduate students on all instruments listed.

May 2022 – Sept 2022 **Sessional Lecturer**
Organic Chemistry Lab (CHEM 265L at the University of Waterloo)

- As a laboratory instructor for CHEM 265L (Organic Chemistry Lab 1), I managed setup and supervised lab sessions for a class of 65 students. Additionally, I independently rewrote the entire course manual to link experiments with real world examples and introduced two new experiments to the curriculum.

May 2015 – Aug 2023 **Teaching Assistant (TA), Curriculum Development, and NSERC-USRA**
University of Waterloo. **Supervisors**: Prof. Eric Fillion (NSERC-USRA) Julie M. Goll, M.Sc. (TA)

- Held graduate and undergraduate TA positions for the senior organic chemistry labs (CHEM 265L and 360L) and advanced senior synthesis lab (CHEM 382L).

- Developed an experiment (CHEM 360L) to determine activation energy differences between kinetic and thermodynamic Diels-Alder reaction pathways (*J. Chem. Ed.* ***2021****. 98, 577 – 586.*)
- As a USRA, I performed synthesis (Schlenk techniques, dry-box) and characterization (NMR, HRMS, XRD, FT-IR) of organometallic complexes for hydrogenolysis, resulting in 1 publication in *Chem. Comm.*

Jan 2016 – Aug 2016 **Radiochemistry Research Assistant**
TRIUMF, Vancouver BC, Canada. **Supervisor**: Prof. Yann Seimbille

- 3 publications in *Organic and Biomolecular Chem.*, *Chem. Open* (cover article), and *Molecules*.
- Developed and synthesized multifunctional cancer treatment agents exhibiting therapeutic and diagnostic properties using bioorthogonal click-chemistry.
- Optimized synthesis of novel peptides to target biomarkers characteristic to neoplastic tissue.

Publications in Refereed Journals

(28) Abaeva, M., Ieritano, C., Hopkins, W. S., Unsymmetrical Imidazopyrimidine-Based Ligand and Bimetallic Complexes. *Inorg. Chem.* **2024**, 63 (2), 1010 - 1019.

(27) Ashworth, E. K., Dezalay, J., Ryan, C. R. M., Ieritano, C., Hopkins, W. S., Chambrier, I., Cammidge, A. N., Stockett, M. H., Noble, J. A., & Bull, J. N. Protomers of the green and cyan fluorescent protein chromophores investigated using action spectroscopy. *Phys. Chem. Chem. Phys.* **2023**, 25, 20405 – 20413.

(26) Haack, A.,* Ieritano, C.,* Hopkins, W. S. MobCal-MPI 2.0: An Accurate and Parallelized Package for Calculating Field-Dependent Collision Cross Sections and Ion Mobilities. *Analyst.* **2023**, 148, 3257 – 3273. *Equal contribution.

(25) Steinstra, C. M. K., Ieritano, C., Haack, A., Hopkins, W. S. Bridging the Gap between Differential Mobility, Log S, and Log P Using Machine Learning and SHAP Analysis. *Anal. Chem.* **2023**, 95 (27), 10309 – 10321.

(24) Ieritano, C., Haack, A., Hopkins, W. S. Chemical Transformations can Occur during DMS Separations: Lessons Learned from Beer's Bittering Compounds. *J. Am. Soc. Mass Spectrom.* **2023**, 34 (7), 1315 – 1329.

(23) Ieritano, C., Thomas, P., Hopkins, W. S. Argentination: A Silver Bullet for Cannabinoid Analysis by Differential Mobiltiy Spectrometry. *Anal. Chem.* **2023**, 95 (22), 8668 – 8678.

(22) Bissonnette, J. R., Ryan, C. R., Haack, A., Ieritano, C., Hopkins, W. S. First-Principles Modeling of Preferential Solvation in Mixed-Modifier Differential Mobility Spectrometry. *J. Am. Soc. Mass Spectrom.* **2023**, 34 (7), 1417 – 1427.

(21) Ieritano, C., Hopkins, W. S. The hitchhiker's guide to dynamic ion–solvent clustering: applications in differential ion mobility spectrometry. *Phys. Chem. Chem. Phys.* **2022**, 24, 20594 – 20615.

(20) Haack, A., Bissonnette, J. R., Ieritano, C., Hopkins, W. S. Improved First-Principles Model of Differential Mobility Using Higher Order Two-Temperature Theory. *J. Am. Soc. Mass Spectrom.* **2022**, 33 (3), 535 – 547.

(19) Ieritano, C., Le Blanc, J. C. Y., Schneider, B. B., Bissonnette, J. R., Haack, A., Hopkins, W. S. Protonation-Induced Chirality Drives Separation by Differential Ion Mobility Spectrometry. *Angew. Chemie Int. Ed.* **2022**, 61 (9), e202116794. *Frontispiece*.

(18) Ieritano, C., Campbell, J. L., Hopkins, W. S. Predicting Differential Ion Mobility Behaviour *in silico* using Machine Learning. *Analyst.* **2021**, 146 (*15*), 4737 – 4743.

(17) Ieritano, C., Lee, A., Crouse, J., Bowman, Z., Mashmoushi, N., Crossley, P. M., Friebe, B. P., Campbell, J. L., Hopkins, W. S. Determining Collision Cross Sections from Differential Ion Mobility. *Anal. Chem.* **2021,** 93 (*25*), 8937 – 8944.

(16) Ieritano, C., Hopkins, W. S. "Thermometer" Ions Can Fragment Through an Unexpected Intramolecular Elimination: These Are Not the Fragents You Are Looking For. *J. Phys. Chem. Lett.* **2021,** 12 (*25*), 5994 – 5999.

(15) Ieritano, C., Rickert, D., Featherstone, J., Honek, J. F., Campbell, J. L., Le Blanc, J. C. Y., Schneider, B. B., Hopkins, W. S. The Charge-State and Structural Stability of Peptides Conferred by Microsolvating Environments in Differential Mobility Spectrometry. *J. Am. Soc. Mass Spectrom.* **2021**, 32 (*4*), 956 – 968. ***Cover Article.***

(14) Ieritano, C., Hopkins, W. S. Assessing collision cross section calculations using MobCal-MPI with a variety of commonly used computational methods. *Mat. Today Comm.* **2021**, 27, 102226.

(13) Ieritano, C., Montgomery, C. A., Goll, J. M., Chan, H. Y. Some Like It Hot: Experimentally determining $\Delta\Delta H^{\ddagger}$, $\Delta\Delta S^{\ddagger}$, and $\Delta\Delta G^{\ddagger}$ between Kinetic and Thermodynamic Diels-Alder Pathways using Microwave-Assisted Synthesis. *J. Chem. Ed.* **2021**, 98 (*2*), 577 – 586.

(12) Ieritano, C. Featherstone, J., Haack, A., Guna, M., Campbell, J. L., Hopkins, W. S. How Hot are your Ions in Differential Mobility Sepctrometry? *J. Am. Soc. Mass Spectrom.* **2020**, *31 (3)*, 582–593.

(11) Ieritano, C., Crouse, J., Campbell, J. L., Hopkins, W. S. A Parallelized Molecular Collision Cross Section Package with Optimized Accuracy and Efficiency. *Analyst* **2019**, *144* (5), 1660–1670.

(10) Zhou, C., Ieritano, C., Hopkins, W. S. Augmenting Basin-Hopping With Techniques From Unsupervised Machine Learning : Applications in Spectroscopy and Ion Mobility. *Front. Chem.* **2019**, *7*, 519.

(9) Ieritano, C., Campbell, J. L., Hopkins, W. S. Unravelling the Factors That Drive Separation in Differential Mobility Spectrometry: A Case Study of Regioisomeric Phosphatidylcholine Adducts. *Int. J. Mass Spectrom.* **2019**, *444*, 116182.

(8) Ieritano, C., Featherstone, J., Carr, P. J. J., Marta, R. A., Loire, E., McMahon, T. B., Hopkins, W. S. The Structures and Properties of Anionic Tryptophan Complexes. *Phys. Chem. Chem. Phys.* **2018**, *20* (41), 26532–26541.

(7) Gao, F., Ieritano, C., Chen, K. T., Dias, G. M., Rousseau, J., Bénard, F., Seimbille, Y. Two Bifunctional Desferrioxamine Chelators for Bioorthogonal Labeling of Biovectors with Zirconium-89. *Org. Biomol. Chem.* **2018**, *16* (28), 5102–5106.

(6) Chen, K. T., Ieritano, C., Seimbille, Y. Early-Stage Incorporation Strategy for Regioselective Labeling of Peptides Using the 2-Cyanobenzothiazole/ 1,2-Aminothiol Bioorthogonal Click Reaction. *ChemistryOpen* **2018**, *7* (3), 256–261. ***Cover Article.***

(5) Chen, K. T., Nguyen, K., Ieritano, C., Gao, F., Seimbille, Y. A Flexible Synthesis of 68Ga-Labeled Carbonic Anhydrase IX (CAIX)-Targeted Molecules via CBT/1,2-Aminothiol Click Reaction. *Molecules.* **2018**, *24* (1), 23.

(4) Liu, C., Le Blanc, J. C. Y., Schneider, B. B., Shields, J., Federico, J. J., Zhang, H., Stroh, J. G., Kauffman, G. W., Kung, D. W., Ieritano, C., et al. Assessing Physicochemical Properties of Drug Molecules via Microsolvation Measurements with Differential Mobility Spectrometry. *ACS Cent. Sci.* **2017**, *3* (2), 101–109. ***Cover Article.***

(3) Fillion, E., Kavoosi, A., Nguyen, K., Ieritano, C. $B(C_6F_5)_3$-Catalyzed Transfer 1,4-Hydrostannylation of α,β-Unsaturated Carbonyls Using *i*Pr-Tricarbastannatrane. *Chem. Comm.* **2016**, *52*, 12813–12816.

(2) Ieritano, C., Carr, P. J. J., Hasan, M., Burt, M., Marta, R. A., Steinmetz, V., Fillion, E., Mcmahon, T. B., Hopkins, W. S. The Structures and Properties of Proton- and Alkali-Bound Cysteine Dimers. *Phys. Chem. Chem. Phys.* **2016**, *18*, 4704–4710.

(1) Liu, C., Le Blanc, J. C. Y., Shields, J., Janiszewski, J. S., Ieritano, C., Ye, G. F., Hawes, G. F., Hopkins, W. S., Campbell, J. L. Using Differential Mobility Spectrometry to Measure Ion Solvation: An Examination of the Roles of Solvents and Ionic Structures in Separating Quinoline-Based Drugs. *Analyst* **2015**, *140*, 6897–6903. ***Cover Article.***

Awards, Honours, and Distinctions

Award	Awarding source	Year awarded	Months held	Total value
CSC Award for Best Oral Presentation, Symposium of Chemical Physics (SCP)	Canadian Society for Chemistry (CSC)	2023	1	100 CAD
ISIMS Graduate Student Travel Award	International Society of Ion Mobility Spectrometry (ISIMS)	2022	1	250 USD
Graduate Student Excellence Award	University of Waterloo (GWC²)	2022	1	1,000 CAD
CSMS Student Travel Award to the Lake Louise Tandem MS Workshop	SCIEX	2021	1	2,000 CAD
Bill Davidson Graduate Student Award	ETP Symposium	2021	1	2,000 CAD
Bruker Biospin Graduate Scholarship	University of Waterloo (GWC²)	2021	1	1,000 CAD
W. S. Rickert Graduate Student Fellowship in Science	University of Waterloo	2021	12	25,000 CAD
Waterloo AI Graduate Scholarship	Waterloo Artificial Intelligence Institute	2021	1	5,000 CAD
Vanier Canada Graduate Scholarship	NSERC	2020-2023	36	150,000 CAD
Paul Bridger Graduate Award	University of Waterloo	2020	1	2,000 CAD

ASMS Graduate Student Travel Award	American Society for Mass Spectrometry (ASMS)	2020	1	1,000 USD
WIN Nanofellowship	Waterloo Institute for Nanotechnology (WIN)	2019 and 2020	24	20,000 CAD
Robert J. LeRoy poster award	Symposium on Chemical Physics (SCP)	2019	1	500 CAD
Don E. Irish Graduate Award	University of Waterloo	2019	1	1,000 CAD
Ontario Graduate Scholarship	Province of Ontario	2018 and 2019	24	30,000 CAD
Graduate Teaching Excellence award	University of Waterloo Dept. of Chemistry	2018 and 2019	4	200 CAD
NSERC CGS M	NSERC	2017	12	17,500 CAD
NSERC USRA	NSERC	2015	4	4,500 CAD
Award for academic excellence	VCNA/ St. Mary's CBM	2013-2017	56	10,000 USD
President's Entrance Scholarship	University of Waterloo	2012	4	2,000 CAD

Conference Presentations

(14) Ieritano, C., Thomas, P., Hopkins, W. S. (2023) Argentination: A Silver Bullet for Cannabinoid Analysis by Differential Mobility Spectroemtry. Lake Louise Tandem Mass Spectrometry Workshop. Lake Louise, Alberta. (Poster)

(13) Ieritano, C., Bissonnette, J. R., Haack, A., Le Blanc, J. C. Y., Schneider, B. B., Hopkins, W. S. (2023) Protonation-Induced Chirality Drives Separation by Differential Ion Mobility Spectrometry. Symposium on Chemical Physics. Waterloo, Ontario. (Oral)

(12) Ieritano, C., Thomas, P., Hopkins, W. S. (2023) Argentination: A Silver Bullet for Cannabinoid Analysis by Differential Mobility Spectroemtry. ASMS Conference Proceedings. Houston, Texas. (Poster)

(11) Ieritano, C., Haack, A., Hopkins, W. S. (2023) Chemical Transformations can Occur during DMS Separations: Lessons Learned from Beer's Bittering Compounds. ASMS Conference Proceedings. Houston, Texas. (Poster)

(10) Ieritano, C., Haack, A., Hopkins, W. S. (2022) Analysis of Beer by Differential Mobility Spectrometry (DMS) Unexpectedly Revealed that Dynamic Ion Microsolvation can Promote Chemical Transformations. Lake Louise Tandem Mass Spectrometry Workshop. Lake Louise, Alberta. (Poster)

(9) Ieritano, C., Haack, A., Hopkins, W. S. (2022) Kinetic vs Thermodynamic Control within Differential Mobility Spectrometry: An Unexpected Observation from Alpha-Acids found in Brewing Hops. ISIMS Conference Proceedings. Memphis, Tenessee. (Oral)

(8) Ieritano, C., Le Blanc, J. C. Y., Schneider, B. B., Bissonnette, J. R., Haack, A., Hopkins, W. S. (2022) Protonation-Induced Chirality Drives Separation by Differential Ion Mobility Spectrometry. ASMS Conference Proceedings. Minneapolis, Minnesota. (Oral)

(7) Ieritano, C., Le Blanc, J. C. Y., Schneider, B. B., Bissonnette, J. R., Haack, A., Hopkins, W. S. (2021) Protonation-Induced Chirality Drives Separation by Differential Ion Mobility Spectrometry: The Curious Case of Verapamil. Lake Louise Tandem Mass Spectrometry Workshop. Lake Louise, Alberta. (Oral)

(6) Ieritano, C., Haack, A., Hopkins, W.S. (2021) "Thermometer" Ions Can Fragment Through an Unexpected Intramolecular Elimination: These are not the Fragments you are Looking For. Trent Conference for Mass Spectrometry. Virtual Symposium. (Oral)

(5) Ieritano, C., Rickert, D., Featherstone, J., Honek, J. F., Campbell, J. L., Le Blanc, J. C. Y., Schneider, B. B., Hopkins, W. S. (2021) The Charge-State and Structural Stability of Peptides Conferred by Microsolvating Environments in DMS. ISIMS 2021 Conference Proceedings. Virtual Symposium. (Oral)

(4) Ieritano, C., Featherstone, J., Haack, A., Guna, M., Cambell, J.L., Hopkins, W.S. (2020) How hot are your ions in differential mobiltiy spectrometry? ASMS Conference Proceedings. Houston, Texas. (Oral recording)

(3) Campbell, J.L., Ieritano, C., Le Blanc, J.C.Y., Seale, B., Bowman, Z., Crouse, J., Zhou, C., Hopkins, W.S. (2019) Exploring the physicochemical properties of pesticides using differential mobility spectrometry and machine learning-based modelling. ASMS Conference Proceedings. Atlanta, Georgia. (Poster)

(2) Liu C, Le Blanc J. C. Y, Shields J, Janiszewski J. S, Ieritano C, Ye G. F, Hawes G. F, Hopkins W. S, Campbell J. L. (2016) Combining Rapid Isomer Separations and Physicochemical Property Predictions for Drug Molecules with Differential Mobility Spectrometry. ASMS Conference Proceedings. San Antonio, Texas. (Oral)

(1) Lock C. J, Campbell J. L, Liu C, Le Blanc J. C. Y, Shields J, Janiszewski J, Ieritano C, Ye G. F, Hawes G. F, Hasan M, Hopkins W. S. (2015) Understanding the Roles of Steric and Effects in Separating Isomers using Differential Mobility Spectrometry. American Society for Mass Spectrometry Conference Proceedings, St. Louis, Missouri. (Poster)

Git Repositories

(3) PodPals: A Graphical User Interface (GUI) designed to streamline the creation and analysis of files generated by the ORCA computational chemistry package. (2024)

(2) Lights, Spectra, Action!: A user-friendly GUI for analyzing data generated from action spectroscopy experiments on SCIEX mass spectrometers. (2023)

(1) MobCal-MPI: A globally recognized, paralellized code for accurately calculating ion mobility and collision cross sections. (2020)

Community Service and Public Outreach

May 2017 – Aug 2023 **Ride Leader**
University of Waterloo Cycling Club
- Organized and led weekly road rides for the A, B, and C groups of the UW cycling club (3 – 10 riders).
- Provided instruction to new group members of the techniques/etiquette involved in group riding.

May 2014 – Aug 2022 **Team Leader for Medicinal Chemistry**
University of Waterloo Science Ambassadors
- Served as Team Lead and mentor for the Medicinal Chemistry ambassador team (5 members), providing training on how to effectively communicate with prospective students by sharing my own perspectives on undergraduate life and post-secondary education.
- Represented the Faculty of Science at recruitment events, such as the Ontario University Fair (100,000+ attendees). Provided guidance and answered questions for prospective students.

Jan 2014 – Dec 2015 **President**
University of Waterloo Chemistry Club
- Organized and led social events such as movie nights and Student-Prof outings at local breweries.
- Introduced student vs. professor sporting contests, including an annual baseball game and video-game tournaments, which have become recurring traditions within the club.

Mentoring Activities

Since joining the Hopkins group in 2017 for my graduate studies, I have had the privilege of mentoring and supervising 13 undergraduate chemistry students, guiding them through their projects. As part of my role, I trained these students in the utilization of the Differential Mobility Spectrometer (DMS) and various computational packages, including basin hopping, Gaussian, ORCA, and MobCal-MPI, which are regularly employed in our work. I also familiarized them with the essential safety protocols and standard operating procedures (SOPs) necessary for laboratory work.

These students come from a variety of backgrounds ranging from co-op students to 4th-year honours project students and summer volunteers. In addition to introducing them to the lab environment, I served as their indirect supervisor during their time in the group. Within this role, I provided my students with guidance on their projects and assisted them in choosing future experiments to perform based on their results. To ensure consistent communication between myself and my students, we maintained a weekly meeting schedule to discuss their results and plan the next steps, which was also complemented by informal discussions that occurred throughout the week.