Caitlin Simopoulos, PhD

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Summary

A computational biologist with a decade of interdisciplinary and collaborative research experience leveraging R and Python in High-Performance Computing environments. Demonstrated expertise in developing and deploying machine learning and statistical tools to analyze complex biological data. Lead author on multiple peer-reviewed publications with exceptional communication skills, delivering impactful presentations to diverse audiences including the public, students, and scientific peers at local, national, and international levels.

Experience

Senior Computational Biologist 2   2024–Present

Recursion, Toronto, ON

- Leads computational biology strategy for two pre-clinical drug programs, driving target validation, patient selection, and translational research efforts.
- Serves as primary computational point-of-contact, orchestrating cross-functional collaboration with biologists, chemists, and project leads to advance critical program milestones.
- Founded and launched the 2025 Computational Biology Internship Program, directly mentoring early-career scientists and cultivating organizational talent.

Senior Computational Biologist   2023–2024

Roche Canada, Mississauga, ON

- Partnered with Principal Scientists at Genentech (gRED) to architect and deploy novel analytical pipelines using R, Python, and Unix scripting.
- Spearheaded independent, cutting-edge single-cell transcriptomic research advancing the understanding of lung disease mechanisms.
- Translated complex research findings to bench scientists, driving experimental design and strategic decision-making.
- Championed workplace culture initiatives and assumed leadership roles across multiple teams.

Computational Biologist   2022–2023

Roche Canada (Contract), Mississauga, ON

- Collaborated directly with gRED computational scientists to investigate lung disease pathology within a single-cell framework.
- Delivered actionable insights through rigorous data analysis, enabling bench scientists to draw meaningful biological conclusions.
- Communicated research findings with clarity to internal stakeholders and collaborators.

Postdoctoral Researcher   2019–2022

University of Ottawa, Ottawa, ON

- Led computational strategy for high-throughput, machine learning-based metaproteomic drug-microbiome interaction studies in collaboration with microbiologists and bioinformaticians.
- Developed and deployed bioinformatic software tools (MetaProClust-MS1, pepFunk) to accelerate IBD and drug-microbiome interaction research.
- Empowered wet-lab scientists through comprehensive training in computational skills using R.

EDUCATION

PhD in Computational Biology   2019

McMaster University, Hamilton, ON

Master of Bioinformatics (MBinf)   2014

University of Guelph, Guelph, ON

BSc in Molecular Biology & Genetics   2012

University of Guelph, Guelph, ON

SELECTED PRESENTATIONS

Simopoulos, C. A novel mass spectrometry profiling approach for large-scale drug-microbiome screening. Flash talk, Having IMPACTT Conference, Canmore, AB, June 2, 2022. ***Selected as Best Flash Talk.***

Simopoulos, C. A novel mass spectrometry profiling approach for large-scale drug-microbiome screening. Oral presentation, CNPN 2022, Montreal, QC, May 17, 2022.

Simopoulos, C. MetaProClust-MS1: An MS1-only profiling approach to metaproteome screening. Invited talk, CNPN Seminar Series, July 27, 2021.

Simopoulos, C., Ning, Z, Zhang, X, Li, L, Walker, K, Lavallée-Adam, M, Figeys, D. pepFunk: peptide-centric functional enrichment for metaproteomic gut microbiome data. Virtual oral presentation, ISMB2020. [Video]

Simopoulos, C., Weretilnyk, E.A., Golding, G.B. Local adaptation in the extremophile *Eutrema salsugineum*: Exploring the roles of putative lncRNAs. Oral presentation, International Association for Plant Biotechnology, Dublin, Ireland, 2018.

SELECTED PUBLICATIONS

1. Li, L, **Simopoulos, CMA**, Mayne, J, et al. Systematic Metaproteomics Mapping Reveals Functional and Ecological Landscapes of Human Gut Microbiota Responses to Therapeutic Drugs. (2025) *Nature Communications.* doi:10.1038/s41467-025-64433-8

2. Wang, L, Simopoulos, CMA, Serrana, J, et al. PhyloFunc: phylogeny-informed functional distance as a new ecological metric for metaproteomic data analysis. (2025) *Microbiome.* doi:10.1186/s40168-024-02015-4

3. Li, L, Wang, T, Ning, Z, et al., incl. **Simopoulos, CMA**. Revealing proteome-level functional redundancy in the human gut microbiome using ultra-deep metaproteomics. (2023) *Nature Communications.* doi:10.1038/s41467-023-39149-2

4. **Simopoulos, CMA**, Ning, Z, Li, L, et al. MetaProClust-MS1: A tool for clustering metaproteomes using rapid MS1 profiling. (2022) *mSystems.* doi:10.1128/msystems.00381-22

5. **Simopoulos, CMA**, Ning, Z, Zhang, X, et al. pepFunk, a tool for peptide-centric functional analysis in metaproteomic human gut microbiome studies. (2020) *Bioinformatics.* doi:10.1093/bioinformatics/btaa289

6. **Simopoulos CMA**, Weretilnyk, EA, Golding, GB. Prediction of plant lncRNA by ensemble machine learning classifiers. (2018) *BMC Genomics.* doi:10.1186/s12864-018-4665-2

A complete list of publications is available on my Google Scholar profile.