



# Caitlin Simopoulos, PhD

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## SUMMARY

- Computational biologist with 10 years of interdisciplinary and collaborative research experience focused on Next Generation Sequencing and proteomic technologies.
- Passionate about deciphering complex drug-human gut microbiome interactions using multi-omics.
- Develops and applies machine learning and statistical tools as solutions to molecular biology data analysis problems.
- Experienced in developing both user-friendly GUI software tools (R/Shiny) and Unix-based command line interface bioinformatic tools for specialized data analysis.
- Lead author of numerous peer-reviewed publications, and highly skilled in verbal communication to the public, students, and scientist peers at local, national and international levels.

## EDUCATION

**Doctor of Philosophy** in Computational Biology 2019  
*McMaster University Hamilton, ON, Canada*

- *Supervisors:* Elizabeth Weretilnyk and Brian Golding
- *Thesis:* [Using machine learning to predict long non-coding RNAs and exploring their evolutionary patterns and prevalence in plant transcriptomes.](#)
- *Awarded:* (2016-2018) Catherine Jane Stevenson Memorial Award, by competition, for research supporting Northern Canada, specifically research supporting the plant *Eutrema salsgunieum* native to Yukon.

**Master of Bioinformatics** (MBinf) 2014  
*University of Guelph Guelph, ON, Canada*

- *Supervisors:* Paul McNicholas and Steven Rothstein
- *Major Research Project:* Weighted gene correlation network analysis of maize and rice undergoing nitrogen stress.
- *Awarded:* (2014) Queen Elizabeth II Award in Science and Technology, by nomination, for academic merit, research strength, leadership, and communication skills.

**Bachelor of Science** in Molecular Biology and Genetics 2012  
*University of Guelph, Guelph, ON, Canada*

## RESEARCH EXPERIENCE

**University of Ottawa, Ottawa, ON** Faculty of Medicine 2019-present  
*Postdoctoral Associate, Funded by Technomise NSERC-CREATE*

*Supervisors:* Daniel Figeys and Mathieu Lavallée-Adam  
Computational biology and the microbiome

- Computational lead of group's high-throughput machine learning-based metaproteomic drug-microbiome interaction study in collaboration with microbiologists and other bioinformaticians.

- Develops and applies machine learning bioinformatic software tools to “omics” data for acceleration of inflammatory bowel disease and drug-microbiome interaction studies.
- Writes software tools using both R and Python ([MetaProClust-MS1](#) as command line tool, [pepFunk](#) as an R/Shiny app).
- Collaborates with both internal wet lab scientists and external academic and industry groups to push the boundaries of microbiome science.
- Publishes peer-reviewed manuscripts in highly respected scientific journals (*e.g.* [Bioinformatics](#)).

#### Leadership

- Trains wet lab scientists in highly sought-after computational skills in R (*e.g.* [Intro to R](#), [Intro to stats in R](#), [Intro to metaproteomic analysis in R](#)).
- Organizes and hosts microbiome-focused monthly seminar series.
- Mentors students in bioinformatic pipeline development and software creation specific to translational molecular medicine.

#### **IMPACTT - Integrated Microbiome Platforms for Advancing Causation Testing and Translation** 2022-present

##### *IMPACTT Mentee*

- Receiving mentorship support to develop an independent research program and to build a strong scientific network.
- Support to attend and present at the “Having IMPACTT: Advancing Microbiome Research” symposium.

#### **Genetics Society of America** 2019-present

##### *Early Career Researcher Committee: Communication and Outreach, Member*

- Communicates relevant science associated topics in online blogs or articles accessible to both scientists and the general public (*e.g.* [Navigating fake news as a scientist](#)).
- Works collaboratively with early career scientists across North America.

#### **McMaster University, Hamilton, ON** Department of Biology 2014-2019

##### *Graduate Researcher*

- Developed a machine learning tool for predicting plant lncRNAs from transcriptomic data ([CREMA](#)) that has been incorporated into the [PLncDB v2.0](#).
- Acted as bioinformatics lead in plant molecular biology and biochemistry lab.
- Presented interdisciplinary research at local, national, and international conferences.

#### **McMaster University, Hamilton, ON** Department of Biology 2014-2019

##### *Teaching Assistant*

- Developed and delivered lectures for a bioinformatics-focused plant biotechnology course.
- Led ecology, evolution and plant molecular biology labs.
- Awarded “Outstanding Achievement as Teaching Assistant” during the 2014/2015 school year.

## TEACHING EXPERIENCE

#### **Undergraduate Student Mentoring** 2020 - present

##### *University of Ottawa, Ottawa, ON*

Isaac Kuk, Translational and Molecular Medicine

*Project title: "Expanding pepFunk to support eggNOG and GO annotations"*

- Meets weekly to discuss project progress and future plans
- Teaches introductory R and statistics through project based learning

**TMM3107: Introduction to high-throughput and systems biology methods relevant to diseases** March 14, 2022

*University of Ottawa, Ottawa, ON*

“Using metaproteomics to explore the effects of drugs on the human microbiome”

- Guest lecture on metaproteomics and bioinformatics.
- Discussed challenges in metaproteomic data analysis.
- Explored how different bioinformatic tools can solve these challenges.
- Introduced applications of computational tools on real world data.

**TMM3009: Translational Molecular Medicine Virtual Lab Rotation** March-April 2021

*University of Ottawa, Ottawa, ON*

- Developed own material for 5 weeks of virtual lab rotations
- Created interactive tutorials for [introductory data analysis in R](#)
  - [Introduction to R](#)
  - [Introduction to Statistics in R](#)
  - [Introduction to Metaproteomics in R](#)

**Teaching Assistant**

2014-2018

*McMaster University, Hamilton, ON*

Awarded “Outstanding Achievement as a Teaching Assistant” during the 2014/2015 school year.

Biology 1M03: Biodiversity, Evolution & Humanity

*Tutorial TA (2014, 2017-2018)*

- Led an engaging, hands-on and discussion friendly tutorial
- Marked weekly assignment and final group project
- Answered online discussion board questions

*Lead lecture TA (2015-2017)*

- Acted as first contact for all first year undergraduate life sciences students
- Held office hours to discuss lecture material
- Answered online discussion board questions

Biology 1A03: Cellular & Molecular Biology

*Lead lecture TA (2015-2017)*

- Acted as first contact for all first year undergraduate life sciences students
- Held office hours to discuss lecture material
- Answered online discussion board questions

Biology 4BB3: Plant Metabolism and Molecular Biology

*Lecture TA (2017)*

- Developed and presented lectures throughout the semester on appropriate material
- Curated data for bioinformatics-focused final project
- Graded final project

Biology 3B03: Plant Physiology

*Lab TA (2018)*

- Led plant physiology based wet labs
- Marked weekly lab reports

**SCIENCE  
OUTREACH**

**TECHNOMISE Special Seminar Organizing Committee** 2020-present  
*Member*

- Invite respected researchers in the field of microbiomes to speak to TECHNOMISE-CREATE trainees
- Co-host monthly seminar series

**Early Career Leadership Program** 2019-present  
*Communication and Outreach, Member, Genetics Society of America*

- Work within a diverse team of early career scientists who are dedicated to science communication
- Communicate novel scientific discoveries by writing pieces published in online blogs or articles accessible to both scientists and the general public

**Pint of Science** 2019-present  
*Local organizer*

- In charge of three day event that brings scientists into cafes and pubs
- Organize event logistics
- Invite speakers to the events
- Host the three day speaker series
- Lead other local volunteers

**Pulsar Collective** 2019-present  
*Mentor*

- Visit highschools virtually
- Highlight underrepresented genders in STEM
- Communicate that STEM is accessible to all genders

**Skype a Scientist** 2020-present  
*Scientist volunteer*

- Visit classrooms virtually
- Answer student questions about science and research

**Plant Molecular Workshop** 2013-2019  
*McMaster University, Hamilton, ON*

- Lead high school students through typical plant molecular biology experiments
- Develop young people's interest in biology

**Researcher's Night Hamilton** 2018  
*Presenter*

- Combined art and science for fun and approachable science outreach
- Presented computational work in a visual manner to the public

**Software Carpentry** 2017  
*Workshop Assistant*

- Offer hands-on assistance to workshop attendees
- Promote inclusivity in computer and data science

**TECHNICAL  
SKILLS**

**Programming languages:** Python, R, R Shiny, Unix, sysadmin responsibilities.

**Statistical Analysis and ML:** Supervised learning: SVM, random forest, regression, multi-model ensemble methods; Unsupervised learning: hierarchical clustering, k-medoids, k-means; Predictive modeling and feature selection: Elastic Net, Lasso, logistic regression.

**Communication:** Fluent in English and French, excellent written and verbal communication skills.

**Data visualisation:** ggplot2, Adobe Illustrator.

**Biology:** Human gut microbiome, genomics, transcriptomics, metaproteomics, metagenomics, evolution, lncRNA

## SOFTWARE

### MetaProClust-MS1

- Tool for clustering metaproteomes using Rapid MS1 profiles
- Written using R and Python
- Approach to intentional and resource conscious metaproteomic research

### pepFunk

- R Shiny app built for metaproteomic functional analysis
- Written in R
- Part of iMetaLab suite

### CREMA

- Prediction of lncRNAs from transcript sequences
- Unix command line interface
- Written using Python and R

## CONTINUING EDUCATION

<b>From Lab 2 Fulfillment</b>	Entrepreneur workshop	2020
<b>WinSETT</b>	Becoming Leaders, professional development	2019
<b>TECHNOMISE-CREATE</b>	Professional development bootcamp	2019
<b>Canadian Bioinformatics Training</b>	Metabolomics workshop	2013

## HONOURS AND AWARDS

<b>IAPB Travel Grant</b>	Awarded to present a seminar at IAPB Dublin, August 2018	2018
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<b>Catherine Jane Stevenson Memorial Bursary</b>	Awarded for research supporting Northern Canada	2016-2018
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<b>McMaster University Department of Biology Travel Scholarship</b>	Awarded for travel to attend CSPB-CSBV, 2016	2016
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<b>George H. Duff Student Travel Bursary</b>	Awarded for travel to attend CSPB-CSBV, 2016	2016
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<b>Outstanding Achievement as a Teaching Assistant</b>	Awarded to a graduate student in the Department of Biology for their outstanding achievement as a teaching assistant during the 2014/2015 school year.	2015
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<b>Graduate Scholarship</b>	McMaster University, Hamilton, Canada Total funding: \$1070/year	2014
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<b>Queen Elizabeth II Award in Science and Technology</b>	Awarded by nomination for academic merit, research strength, leadership, and communication skills. Total funding: \$5,000/semester	2013
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<b>University of Guelph Entrance Scholarship</b>	Awarded to students with a minimum 85% admission average.	2008
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Total funding: \$1000

**SELECT  
PUBLICATIONS**

Li, L, Ning, Z, Cheng, K, Zhang, X, **Simopoulos, C**, Figeys, D. (2022) iMetaLab Suite: A One-stop Toolset for Metaproteomics. iMeta. <https://doi.org/10.1002/imt2.25>

**Simopoulos, C**, Figeys, D, Lavalley-Adam, M. (2022) Novel Bioinformatics Strategies Driving Dynamic Metaproteomic Studies. In Jennifer Geddes-McAlister (Eds). Proteomics in Systems Biology. Methods in Molecular Biology, vol. 2456. Humana, New York, NY. [https://doi.org/10.1007/978-1-0716-2124-0\\_22](https://doi.org/10.1007/978-1-0716-2124-0_22)

Li, L, Ning, Z, Zhang, X, Butcher, J, **Simopoulos CMA**, Mayne, J, Stintzi, A, Mack DR, Liu, Y-Y, Figeys, D. (2021) Revealing Protein-Level Functional Redundancy in the Human Gut Microbiome using Ultra-deep Metaproteomics. bioRxiv. <https://doi.org/10.1101/2021.07.15.452564>

**Simopoulos, CMA**, Ning, Z, Li, L, Khamis, MM, Zhang, X, Lavallée-Adam, M, Figeys, D. (2021). MetaProClust-MS1: A tool for clustering metaproteomes using rapid MS1 profiling. bioRxiv. <https://doi.org/10.1101/2021.03.31.43786>

**Simopoulos, CMA\***, MacLeod, MJR\*, Irani, S, Sung, WWL, Champigny, MJ, Summers, PS, Golding, GB, Weretilnyk, EA. (2020) Coding and long non-coding RNAs provide evidence of distinct transcriptional reprogramming for two ecotypes of the extremophile plant *Eutrema salsugineum* undergoing water deficit stress. BMC Genomics 21, 396 <https://doi.org/10.1186/s12864-020-06793-7>

**Simopoulos, CMA**, Ning, Z, Zhang, X, Li, L, Walker, K, Lavallée-Adam, M, Figeys, D. (2020). pepFunk, a tool for peptide-centric functional analysis in metaproteomic human gut microbiome studies. Bioinformatics, btaa289 <https://doi.org/10.1093/bioinformatics/btaa289>

**Simopoulos, CMA**, Weretilnyk, EA, Golding, GB. (2019) Molecular traits of long non-protein coding RNAs from diverse plant species show little evidence of phylogenetic relationships. (2019) G3. 9(8), 2511-2520 <https://doi.org/10.1534/g3.119.400201>

**Simopoulos CMA**, Weretilnyk, EA, Golding, GB. (2018). Prediction of plant lncRNA by ensemble machine learning classifiers. BMC Genomics. 19, 316 <https://doi.org/10.1186/s12864-018-4665-2>

Coneva, V\*, **Simopoulos, C\***, Casaretto, JA, El-kereamy, A, Guevara, D R, *et al.* (2014). Metabolic and co-expression network-based analyses associated with nitrate response in rice. BMC Genomics, 15, 1056 <http://www.biomedcentral.com/1471-2164/15/1056>

\* Shared first authorship

**OUTREACH  
PUBLICATIONS**

Carla Bautista, Elisabeth Adkins Marnik, **Caitlin MA Simopoulos\***, Anna Drangowska-Way, Thomas James Smyth Merritt (2020) What is the new way scientists edit DNA? Frontiers for Young Minds. 9:600133. doi:10.3389/frym.2021.600133

**GSA Communications & Outreach Subcommittee\*** (November 26, 2020) Hurdles and advances to making science gender-neutral. ecrLife.

<https://ecrlife.org/hurdles-and-advances-to-making-science-gender-neutral/>

**GSA Communications & Outreach Subcommittee\*** (October 8, 2020) Navigating fake news as a scientist. ecrLife.

<https://ecrlife.org/navigating-fake-news-as-a-scientist/>

\* Written as a collaboration with the GSA Communications & Outreach Subcommittee.

**INVITED  
TALKS**

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

**CONFERENCE  
PRESENTATION** **Simopoulos, C.** Ning, Z, Li, L, Zhang, X, Hamada, M, Lavallée-Adam, M, Figeys, D. MetaProClust-MS1 can cluster metaproteomes using MS1 profiling only. Virtual oral presentation at GLBIO2021. <https://youtu.be/tET-YVuyB7Y>

**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. Video presentation at user!2020. <https://youtu.be/UZtpi-Bg9i0>

**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 at ISMB2020. <https://youtu.be/ze2bAQsRKI>

**Simopoulos, C. 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. Poster at the 2020 meeting for the European Conference on Computational Biology. (*Poster presentations cancelled due to the COVID-19 pandemic.*)

**Simopoulos, C.,** Weretilnyk, E. A., Golding, G. B. (August 21, 2018) *Local adaptation in the extremophile Eutrema salsugineum: Exploring the roles of putative lncRNAs*

Oral presentation at the 2018 meeting of the International Association for Plant Biotechnology, Dublin, Ireland.

**Simopoulos, C.,** Weretilnyk, E. A., Golding, G. B. (July 15, 2018) *Using machine learning to predict long non-protein coding RNAs from plant transcriptome*  
Poster presented at the joint meeting of ASPB and CSPB, Montreal, Quebec.

**Simopoulos, C.,** Golding, G. B., Weretilnyk, E. A. (Nov 19, 2016) *An improved method for long non-coding RNA prediction that includes small ORF coding probabilities*

Presented at the annual Biology Graduate Research Day at McMaster University in Hamilton, Ontario.

**Simopoulos, C.,** Golding, G. B., Weretilnyk, E. A. (Nov 19, 2016) *An improved method for long non-coding RNA prediction that includes small ORF coding probabilities*

Presented at the annual Eastern meeting of the Canadian Society of Plant Biologists at McMaster University, Hamilton, Ontario

**Simopoulos, C.** Golding, G. B., Weretilnyk, E. A. (June 16, 2016) *Insights into the*

*abiotic stress response of Eutrema salsugineum by co-expression network analysis*  
Poster presented at the annual national meeting of the Canadian Society of Plant Biologists at Queen's University, Kingston, Ontario.

Garvin, A.\*, **Simopoulos, C.\***, Sung, W., Golding, B., Weretilnyk, E. (Nov. 21, 2015) *A long non-coding RNA associated with nutrition in Eutrema salsugineum: An example of local adaptation?*

Poster presented at the annual Eastern meeting of the Canadian Society of Plant Biologists at the University of Toronto, Toronto, Ontario.

\* Shared first authorship

**Simopoulos, C.** Garvin, A., Sung, W., Golding, B., Weretilnyk, E. (Oct. 15, 2015) *How do outlier samples affect the results of a co-expression network?*

Poster presented annual Biology Graduate Research Day at McMaster University in Hamilton, Ontario.

**Simopoulos, C.**, Garvin, A., Sung, W., Golding, B., Weretilnyk, E. (Dec 4, 2014) *Does Yukon Eutrema salsugineum require elevated sulfur and, if so, why?*

Poster presented at annual Biology Graduate Research Day at McMaster University in Hamilton, Ontario.

<b>PROFESSIONAL AFFILIATIONS</b>	Canadian National Proteomics Network	2021-present
	Human Proteome Organization	2021-present
	International Society for Computational Biology	2020-present
	Genetics Society of America	2019-present
	The Canadian Society for Plant Biologists	2014-2019
	Canadian Association for Plant Biotechnology	2018

**JOURNAL REVIEW ACTIVITIES**

- Molecular Omics
- Journal of Proteomics
- Nature Protocols
- Scientific Reports
- Interface Focus
- F1000 Research
- Molecular Ecology Resources
- Mass Spectrometry Reviews
- Bioinformatics