

Caitlin Simopoulos, PhD

4501C, Roger Guindon Hall, University of Ottawa
451 Smyth Road, Ottawa, Ontario, K1H 8L1
+1.647.280.6247 — csimopou@uottawa.ca

  caitsimop
caitlinsimopoulos.com

SUMMARY

- Computational biologist with nine years of interdisciplinary and collaborative research experience focused on “omics” technologies.
- Current focus is the development and application of machine learning tools as solutions to molecular biology data analysis problems.
- Experience in developing both user-friendly GUI software tools and command line interface bioinformatic tools for specialized data analysis.
- Passionate about deciphering complex drug-human gut microbiome interactions using multi-omics.
- 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

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

- *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 salsgunicum* native to Yukon.

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

- *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.

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

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](#), [pepFunk](#)).

- 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.

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

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 Scientist Committee

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	From Lab 2 Fulfillment Entrepreneur workshop	2020
	WinSETT Becoming Leaders, professional development	2019
	TECHNOMISE-CREATE Professional development bootcamp	2019
	Canadian Bioinformatics Training Metabolomics workshop	2013
HONOURS AND AWARDS	IAPB Travel Grant	2018
	Awarded to present a seminar at IAPB Dublin, August 2018	
	Catherine Jane Stevenson Memorial Bursary	2016-2018
	Awarded for research supporting Northern Canada	
	McMaster University Department of Biology Travel Scholarship	2016
	Awarded for travel to attend CSPB-CSBV, 2016	
	George H. Duff Student Travel Bursary	2016
	Awarded for travel to attend CSPB-CSBV, 2016	
	Outstanding Achievement as a Teaching Assistant	2015
	Awarded to a graduate student in the Department of Biology for their outstanding achievement as a teaching assistant during the 2014/2015 school year.	
	Graduate Scholarship	2014
	McMaster University, Hamilton, Canada	
	Total funding: \$1070/year	
	Queen Elizabeth II Award in Science and Technology	2013
	Awarded by nomination for academic merit, research strength, leadership, and communication skills.	
	Total funding: \$5,000/semester	
	University of Guelph Entrance Scholarship	2008
	Awarded to students with a minimum 85% admission average.	
	Total funding: \$1000	
SELECT PUBLICATIONS	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 <i>Eutrema salsugineum</i> 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](https://doi.org/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.

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/ze2bA0QsRKI>

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 adapta-*

tion 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.

PROFESSIONAL AFFILIATIONS	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