# Caitlin Simopoulos, PhD

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caitsimop

#### DISCIPLINES

Bioinformatics, Computational Biology, Molecular Biology, -omics Technologies, Machine Learning

#### **EDUCATION**

#### Doctor of Philosophy - Computational Biology

2019

McMaster University, Hamilton, ON

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

#### Master of Bioinformatics (MBinf)

2014

University of Guelph, Guelph, ON

Supervisors: Paul McNicholas and Steven Rothstein

Major Research Project: Weighted gene correlation network analysis of maize and rice undergoing nitrogen stress

# Bachelor of Science, Molecular Biology and Genetics

2012

University of Guelph, Guelph, ON

#### **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

#### RELEVANT **EXPERIENCE**

#### TECHNOMISE-CREATE Postdoctoral Associate

2019-present

University of Ottawa, Ottawa, ON

Supervisor: Daniel Figeys

Co-supervisor: Mathieu Lavallée-Adam

Research topic:

- Identify effects of drugs on human gut microbiomes based on a machine learning framework
- Reclassify drugs according to their effects on the gut microbiota
- Contribute to computational methodology for metaproteomic data analysis including the creation of web applications written in R shiny
- Working on an interdisciplinary and collaborative research team

#### Research Assistant

January 2014-August 2014

University of Guelph, Guelph, ON

Responsibilities:

- Identified transcriptional responses to nitrogen stress in rice.
- Created an efficient R package for genetic network analysis.
- Collaborated with a multi-disciplinary team.

#### MBinf Research Project

May 2013-December 2013

University of Guelph, Guelph, ON

Responsibilities:

- Analyzed microarray data of important crops undergoing nitrogen stress.
- Used and further developed programming skills in R.

### Undergraduate Research Project

September 2011-April 2012

University of Guelph, Guelph, ON

Research topic:

Member

• The effects of stress on S. mediterrinea after RNAi knock-down of age-1.

USEL Position Summer 2011

University of Guelph and OMAFRA, Guelph, ON Responsibilities:

- Created a viral infection identification protocol for Ontario strawberries.
  - Established relationships to maintain communication between OMAFRA and Ontario farmers.

### SCIENTIFIC OUTREACH

# TECHNOMISE Special Seminar Organizing Committee

2020-present

- 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

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

Local organizer

- In charge of three day event that brings scientists into cases 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

 $Scientist\ volunteer$ 

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

#### Plant Molecular Workshop

2013-2019

2020-present

McMaster University, Hamilton, ON

- Lead high school students though 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

#### TEACHING EXPERIENCE

#### Student Mentoring

2020 - present

University of Ottawa

Isaac Kuk, Translational and Molecular Medicine

Expanding pepFunk to support eggNOG and GO annotations

#### Teaching Assistant

2014-2018

McMaster University, Hamilton, ON

Biology 1M03: Biodiversity, Evolution & Humanity

Tutorial TA (2014, 2017-2018)

- Lead an engaging, hands-on and discussion friendly tutorial
- Mark weekly assignment and final group project
- Answer online discussion board questions

Lead lecture TA (2015-2017)

- Act as first contact for all first year undergraduate life sciences students
- Hold office hours to discuss lecture material
- Answer online discussion board questions

Biology 1A03: Cellular & Molecular Biology

Lead lecture TA (2015-2017)

- Act as first contact for all first year undergraduate life sciences students
- Hold office hours to discuss lecture material
- Answer online discussion board questions

Biology 4BB3: Plant Metabolism and Molecular Biology Lecture TA (2017)

- Develop and present lectures throughout the semester on appropriate material
  - Curate data for bioinformatics-focused final project

#### • Grade final project

Biology 3B03: Plant Physiology Lab TA (2018)

- Lead plant physiology based wet labs
- Mark weekly lab reports

#### **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

Awarded for travel to attend CSPB-CSBV, 2016

# 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

Simopoulos, CMA, Ning, Z, Li, L, Khamis, MM, Zhang, X, Lavallée-Adam, M, PUBLICATIONS 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 salsuqineum 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 phyloge

netic 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

mittee.

# **OUTREACH**

Carla Bautista, Elisabeth Adkins Marnik, Caitlin MA Simopoulos\*, Anna Drangowska-**PUBLICATIONS** Way, Thomas James Smyth Merritt (2020) What is the new way scientists edit DNA? Frontiers for Young Minds. (In press).

> 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 Subcom-

CONFERENCE Simopoulos, C, Ning, Z, Zhang, X, Li, L, Walker, K, Lavallée-Adam, M, Figeys, D. PRESENTATION 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: peptid-ceentric functional enrichment for metraproteomic gut microbiome data. Virtual oral presentation at ISMB2020.

> 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 lncR-

> 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.

<sup>\*</sup> Shared first authorship

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 proba-

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 salsuqineum 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.

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.

# **AFFILIATIONS**

PROFESSIONAL International Society for Computational Biology Genetics Society of America The Canadian Society for Plant Biologists Canadian Association for Plant Biotechnology

2020-present 2019-present 2014-2019 2018

# **JOURNAL** REVIEW ACTIVITIES

- Molecular Omics
- Journal of Proteomics
- Nature Protocols
- Scientific Reports
- Interface Focus
- F1000 Research

<sup>\*</sup> Shared first authorship