

# Rana A. Barghout

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 <https://ranaabarghout.github.io/>



## Education

Sept 2021–Aug 2026 **PhD, Chemical Engineering & Applied Chemistry, University of Toronto & Vector Institute, Toronto, ON**  
Thesis: “Deep learning for improving metabolic modeling and strain engineering”  
Supervisors: R. Mahadevan & B. Sanchez-Lengeling  
Abstract: Exploration of SOTA deep learning & optimization to enhance computational metabolic modeling across scales.  
Skills: Python (PyTorch, Pyomo, RDKit, Scikit-learn), Linux, MATLAB, SQL.

Sept 2016–May 2021 **BASc, Chemical and Biological Engineering, University of British Columbia, Vancouver, BC**  
Dean’s Honor List (3 years)

## Research Experience

Sept 2021–Present **PhD Candidate, Machine Learning for Genome-Scale Strain Fitness Prediction, University of Toronto, Toronto, ON**

- Designed and implemented CPI-Pred: deep learning model integrating protein language models & molecular embeddings to predict enzyme kinetics ( $k_{cat}$ ,  $K_M$ ,  $K_I$ ,  $k_{cat}/K_M$ ).
- Integrated ML-predicted parameters into genome-scale models via kinGEMs pipeline; improved gene lethality prediction by 3%.
- Conducted large-scale benchmarking on sequence-compound datasets; demonstrated out-of-distribution generalization improvements.

Sept 2020–Aug 2021 **Undergraduate Thesis, Integrating Machine Learning with Kinetic Models, University of British Columbia, Vancouver, BC**

- Developed decision tree and LSTM models to interpret xylose yield predictions from experimental data.
- Formulated and solved large-scale Pyomo and SciPy optimization problems to estimate kinetic parameters.
- Preprocessed and analyzed data with Scikit-learn, Pandas, TensorFlow, improving predictive accuracy by 10%.

Sept 2018–Apr 2019 **Chemical Engineering Support (Co-op), BC Research Inc., Vancouver, BC**

- Optimized meso-scale experimental workflows; reduced data collection time by 50%.
- Conducted PIV fluid dynamics analysis for open-channel flumes; enhanced measurement accuracy.
- Delivered operational training on advanced PIV and sonic wave gauge systems; ensured compliance with WHMIS and laser safety.

## Other Work Experience

Jan 2021–Present **Teaching Assistant, Chemical Engineering & Applied Chemistry Depts., UofT & UBC, Courses: CHE204, CHE205, CHE305, CHE222, CHE322, CHE499, CHBE221.**

- Led weekly tutorials for 70 students on dynamic modeling, process control, MATLAB & Python.
- Graded assignments/quizzes; improved learning outcomes for 140+ students.

Oct 2020–Apr 2021 **Laboratory Assistant, Dr. Louise Creagh Labs, UBC,**

- Prepared cell culture media and autoclaved bioreactors; maintained fed-batch systems for *Pichia pastoris*.
- Revised instructional materials for improved clarity and engagement.

## Publications and Presentations

- [1] R. Ahmed Barghout, L. Chinas, Z. Xu, B. Sanchez-Lengeling, and R. Mahadevan. *Bridging sequence and kinetics: utilizing multi-scale representations for genome-scale metabolic models*. Spotlight Talk. Singapore, Apr. 2025.
- [2] R. Ahmed Barghout, M. Kirby, A. Zheng, L. Chinas Serrano, Z. Xu, and M. Mohammadi. "Machine Learning for Sequence to Function Approaches". In: *Machine Learning and Big-Data Enabled Biotechnology*. Ed. by H. Alper. Advanced Biotechnology Series. Forthcoming. Springer, 2025.
- [3] J. Barraza, R. Ahmed Barghout, R. Almada, A. Jinich, and B. Sanchez-Lengeling. "Graph Data Modeling: Molecules, Proteins, Chemical Processes". In: *ACS In Focus (accepted)* (2025).
- [4] Z. Xu, R. Ahmed Barghout, J. Wu, and D. Garg. *CPI-Pred: A General-Purpose Compound-Protein Interaction Prediction Model*. Submitted for review; preprint at <https://www.biorxiv.org/content/10.1101/2025.01.16.633372v1.full.pdf>. 2025.
- [5] R. Ahmed Barghout, L. Chinas, and R. Mahadevan. "kinGEMs: Advancing enzyme-constrained genome-scale modeling with deep learning-predicted kinetic parameters". In: *COBRA Conference*. San Diego, CA, Oct. 2024.
- [6] R. Ahmed Barghout, Z. Xu, and R. Mahadevan. "Enhancing compound-protein interaction prediction with confidence assessment". In: *AICHE Annual Meeting*. San Diego, CA, Oct. 2024.
- [7] S. Betala, R. Ahmed Barghout, Z. Xu, and R. Mahadevan. "Screening protein sequences generated via conditional diffusion for enhanced fitness using a GNN-based functional predictor". In: *Machine Learning for Computational Biology Conference (MLCB)*. Seattle, WA, Sept. 2024.
- [8] R. A. Barghout, Z. Xu, S. Betala, and R. Mahadevan. "Advances in generative modeling methods and datasets to design novel enzymes for renewable chemicals and fuels". In: *Current Opinion in Biotechnology* 84 (2023), p. 103007. DOI: [10.1016/j.copbio.2023.103007](https://doi.org/10.1016/j.copbio.2023.103007).
- [9] Z. Xu, R. Ahmed Barghout, and R. Mahadevan. "Deep Learning-Based Protein Sequence-to-Function Prediction Framework". In: *Metabolic Engineering Conference (ME15)*. Singapore, 2023.
- [10] R. Ahmed Barghout. "Machine Learning for Kinetic Parameter Prediction in Organisms". In: *Canadian Chemical Engineering Conference*. Vancouver, BC, 2022.
- [11] K. Haddadi, R. Ahmed Barghout, and R. Mahadevan. "KinMod database: a tool for investigating metabolic regulation". In: *Database* 2022 (2022). DOI: [10.1093/database/baac081](https://doi.org/10.1093/database/baac081).
- [12] J. Verrett, R. Qiao, and R. Ahmed Barghout. *Foundations of Chemical and Biological Engineering I*. Vancouver, BC: BCcampus, 2020.

## Academic Community Involvement

- Aug 2023–Jul 2025 **VP Logistics, GradSWE, UofT Faculty of Applied Science**
  - Led GradSWE podcast and executive coordination; secured funding via grant proposals; piloted, planned, and edited 'She Speaks STEM' podcast
- Sept 2023–Apr 2024 **HR Recruitment Team Member, BridgeTO, Toronto, ON**
  - Managed recruitment databases; aligned mentors with at-risk youth; standardized onboarding documentation.
- Apr 2022–Apr 2023 **Mentorship Program Coordinator, CEGSA, UofT**
  - Expanded participation by 33%; introduced Grad-4th Year peer matching; organized social events to strengthen networks.

## Honors and Awards

- Jan 2025 Diran Basmadjian Graduate Scholarship, UofT.
- Dec 2022 & 2023 Rein Otson Memorial Graduate Scholarship, UofT.

- Apr 2021 3MT First Place, UBC CHE Research Day.
- Apr 2021 Short Research Presentation First Place, UBC.
- Apr 2021 Thomas Bennett Scholarship, UBC.
- Dec 2020 UBC International Community Achievement Award.
- Nov 2020 Faculty of Applied Science International Student Scholarship, UBC.
- Oct 2020 Trek Excellence Scholarship for International Students, UBC.
- Apr 2020 CHBE Award in Breakthrough Innovations and Engineering Leadership.