# Tianyu Lu

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University of Toronto

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tianyu-lu.github.io · 

tianyu-lu

Research Interests I am interested how machine learning models can generate hypotheses to probe and understand biology, in particular

- Generative models of protein sequence and structure applied to protein engineering
- Connecting wetlab assay development with probabilistic samplers, model-based optimization
- Joints, conditionals, and marginals of *p*(sequence, structure, function)

**PUBLICATIONS** 

Strokach A, **Lu T**, and Kim PM. "ELASPIC2 (EL2): Combining Contextualized Language Models and Graph Neural Networks to Predict Effects of Mutations." Journal of Molecular Biology (2021): 166810.

Conferences

Boucinha A, Kell B, Sheikh F, Diep P, Yeung A, Escobar A, Emond CA, Pierce C, Siddartha K, Chang L, Sadatmousavi P, Stephens S, Lu T, Sajtovich VA. "A framework towards transdisciplinary synthetic biology curricula for heterogeneous undergraduate cohorts." Canadian Engineering Education Association Conference (2021).

**PREPRINTS** 

**Lu T**, Lu AX, and Moses AM. "Random Embeddings and Linear Regression can Predict Protein Function." arXiv preprint arXiv:2104.14661 (2021).

Lu T, and Silva A. "dynUGENE: an R package for uncertainty-aware gene regulatory network inference, simulation, and visualization." bioRxiv (2021).

EXPERIENCE

#### **ProteinQure**

#### Junior Machine Learning Scientist

May 2021 - Present

- Designed an embedding-based kernel for Gaussian process regression for non-canonical peptide property prediction.
- Modeled 3D atom density preferences with 3D-CNNs for a non-canonical amino acid energy function.
- Building sequence, structure, and surface-based property predictors for nanobody design: immunogenicity, solubility, non-specificity, aggregation propensity, target-agnostic binding score.

University of Toronto Research Student

Sep 2020 – April 2021

Supervisor: Prof. Alan Moses

- Modeled gene regulatory network dynamics using neural networks mixed with ODEs.
- Designing gene regulatory networks *de novo* using automatic differentiation through ODE solvers.
- Establish baseline models and datasets protein language model pre-training tasks.

#### **University of Toronto**

Research Student

Aug 2019 - Sep 2020

Supervisors: Prof. Philip Kim, Dr. Pedro Alberto Valiente Flores

- Designing novel protein folds with generative models of protein structures (Transformer, GAN).
- Designing oncoprotein inhibitors using Rosetta and molecular dynamics simulations.
- Implemented code to search the PDB for protein surfaces that mimic DNA.

iGEM Toronto

Co-President Drylab Lead Drylab Member Nov 2020 – Present Apr 2020 – Nov 2020 Apr 2019 – Apr 2020

Supervisor: Prof. Radhakrishnan Mahadevan

- Contributed ML-guided designed plastic-degrading enzyme to BioBrick.
- Working on active learning methods for an iterative drylab-wetlab feedback loop.
- Designed a plastic-degrading enzyme using model-based optimization.
- Quantifying benefits of learned protein sequence embeddings on protein function prediction.
- Analyzing PET catalysis dynamics with molecular dynamics simulations.

### Canadian Synthetic Biology Education Research Group Lead Instructor

**Machine Learning Instructor** 

Supervisors: Patrick Diep, Brayden Kell

- Created code resource on machine learning for protein design and systems biology.
- Presented seven hours of content, covering both classical (Docking, Rosetta, MD) and recent methods (Sequence-to-function models, generative models, representation learning, active learning).

Oct 2021 - Present

Sep 2019 - Oct 2021

• Lead meetings on curriculum development based on pedagogical principles.

#### **EDUCATION**

#### **University of Toronto**

B. Sc. in Bioinformatics and Computational Biology, Computer Science Sep 2018 – Jun 2021 cGPA: 3.94/4.00

#### **McGill University**

Biological, Biomedical and Life Sciences Sep 2017 – May 2018 cGPA: 4.00/4.00

#### **SKILLS**

#### Programming Python, PyTorch, NumPy, Bash

Tools PyMOL, VMD, GROMACS, RosettaScripts, Unix, LATEX

#### **TALKS**

- 1. Accelerating Plastic Recycling with PETase, iGEM Giant Jamboree, Boston, MA, Oct. 2019.
- 2. Recurrent Neural Networks for Protein Design, Ontario iGEM Conference, Guelph, ON, Jul. 2019.

## Awards & Grants

• Skule Endowment Fund (\$5000)	2021
• iGEM Impact Grant (\$3000)	2021
• Institute of Medical Science Grant (\$2000)	2021
• Dean's Student Initiative Fund (\$1000)	2021
• NSERC Undergraduate Research Award (\$6000)	2020
COVID-19 Student Engagement Grant (\$3000)	2020
• iGEM Gold Medal, Best Manufacturing Project Nomination, Boston MA	2019
National Biology Competition, Top 1% (\$3000)	2017
• University of Toronto Entrance Scholarship (\$7000)	2017

#### **INTERESTS**

Frédéric Chopin, cycling, public transport, making things with flour.