

Shaurya Seth

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Overview

- Machine learning engineer with experience building and deploying models that outperform human experts in real-world drug discovery pipelines.
- Published researcher with co-authored work in *Nature Chemical Biology* and *Royal Society of Chemistry*, and foundational training under Richard Sutton and Martha White in reinforcement learning.
- Recipient of multiple competitive research awards, including the Alberta Innovates Studentship and GlycoNet Summer Award, recognizing innovation at the intersection of AI and biology.

Experience

48Hour Discovery Inc.

Apr 2023 – Present

Machine Learning Engineer

Edmonton, AB

- Founded and led the company's machine learning team, establishing a pipeline for weekly experimental validation of AI-designed molecules.
- Designed molecular-binding models (XGBoost) that consistently outperformed expert-designed compounds, validated by biochemical assays.
- Processed 5+ terabytes of paired-end Illumina data (FASTQ) using custom barcodes for genomic analysis.
- Built and deployed internal tools (AWS) that became core infrastructure; widely adopted across lab staff.

Research

Reinforcement Learning & Artificial Intelligence (RLAI)

Apr 2021 – Aug 2021

Undergraduate Researcher; Supervisor: Martha White & Adam White (DeepMind)

Edmonton, AB

- Collaborated with leading RL researchers to automate a real-world water treatment plant using reinforcement learning.
- Benchmarked the first predictive agent for the plant by applying Q-learning and SARSA with linear function approximation on sensory data.
- Demonstrated that classical methods outperformed deep RL (e.g., DQN with replay buffers) on key benchmarks, supporting simpler, more interpretable deployment in industrial systems.

Derda Research Group

Apr 2019 – Jun 2021

Undergraduate Researcher; Supervisor: Ratmir Derda & Russ Greiner (Amii)

Edmonton, AB

- Pioneered the first ML project in the glycomics lab, developing a deep learning model (GlyNet) to predict protein-carbohydrate interactions from molecular structure.
- Developed a novel fingerprint encoding for carbohydrates, enabling accurate binding predictions across thousands of protein targets; the resulting multi-output neural network achieved an R^2 of 0.78.
- Published GlyNet in the Royal Society of Chemistry; the model remains in active use today and has enabled successful experimental validations of novel glycan-protein interactions.
- Presented research at major scientific conferences (GlycoNet), communicating technical findings through posters and talks; awarded three competitive undergraduate research scholarships during this time.

Skills

Programming - Python, R, Swift, SQL

Frameworks - PyTorch, scikit-learn, XGBoost, NumPy, Polars, RDKit

Algorithms - Transformers, LLMs, MLPs, CNNs, SARSA, Q-Learning

Education

University of Alberta

Sep 2018 – May 2023

B.Sc. in Physics; GPA: 3.2

Edmonton, AB

- Reinforcement Learning I (CMPUT 397) with Martha White; Grade: A
- Reinforcement Learning II (CMPUT 609) with Richard S. Sutton; Grade: A-

Awards

Alberta Innovates Summer Research Studentship

2021

GlycoNet Summer Award for Undergraduate Students

2021

Undergraduate Research Initiative Stipend

2020

Publications

[1] GlyNet: a multi-task neural network for predicting protein-glycan interactions. *Royal Society of Chemistry*, 2022.

[2] Genetically encoded multivalent liquid glycan array displayed on M13 bacteriophage. *Nature Chemical Biology*, 2021.