Karanveer Brar

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Education

University of Toronto **Toronto, ON**

HBSc in Chemistry, Mathematics & Statistics Minor *Sept. 2025 – June 2029*

- **Relevant Coursework:** Introductory Inorganic Chemistry I, Chemistry: The Molecular Science, Calculus I & II, Linear Algebra I, Introduction to Computer Science

Research Experience

The Matter Lab **Toronto, ON**

Undergraduate Research Intern | Supervised by Marcel Müller *Feb. 2026 – Present*

- Curated a lanthanide(III) binding dataset from 5 sources, recovering missing ligand structures via PubChem formula search with descriptor matching, removing radical and conflicting entries, and imputing fingerprints with confidence-weighted KNN, with feature engineering from Morgan fingerprints, RDKit descriptors, and metal properties.
- Developed a stacked tensor-network kernel machine and LightGBM model tuned with Optuna and validated by ligand-grouped 10-fold CV to prevent leakage, plus a contrast model trained on within-ligand targets to isolate metal-to-metal selectivity from overall affinity.
- Applied SHAP analysis to quantify metal versus ligand feature contributions, then screened candidate ligands across the 4f series, ranking by neighbor-margin selectivity and adjacent-pair separation factors and requiring agreement between measured, out-of-fold, and predicted values.
- Built a DEAP genetic algorithm for inverse design of selective ligands, using reaction-based fragment mutations and a fitness combining affinity, selectivity gap, synthetic accessibility, structural-alert penalties, and a Fairchem UMA 3D strain filter.

Laboratory Experience

General Chemistry Laboratory | Department of Chemistry **Fall 2025 – Present**

- Executed multi-step wet chemistry protocols including gravimetric and volumetric quantitative analysis, acid-base and redox titrations, and solvent-based organic compound extractions.
- Performed quantitative analyses by potentiometry, UV/visible and infrared spectrophotometry, flame atomic spectrometry, and ion chromatography, preparing standard solutions and calibrating instrumentation according to standard operating procedures.
- Synthesized, isolated, and purified target compounds, analyzing purity and structure using spectroscopic methods and documenting step-by-step procedures in a formal research-grade laboratory notebook.
- Applied statistical methods to identify sources of error, propagate uncertainty, and assess matrix interferences, generating publication-standard technical reports that contextualized experimental deviations from theoretical thermodynamic and kinetic models.

Extracurriculars

Mathematics Union **Toronto, ON**

Vice President of Academic Affairs *May 2026 – Augest 2026*

- Launched registration systems for the mentorship program and fall Colloquium series, collecting 16+ mentor/mentee sign-ups and 3 speaker submissions.
- Designed promotional posters and materials for academic events to increase undergraduate engagement.
- Supported coordination of fall Colloquium events, assisting with logistics for seminars featuring student and faculty speakers.

Physics Student Union (PhySU) **Toronto, ON**

First-Year Representative (PHY131/132) *Oct. 2025 – May 2026*

- Elected to represent over 300 first-year physics students, liaising directly with the physics department faculty to advocate for improvements in course delivery, assessment structures, and learning resources.
- Coordinated 5+ academic workshops and peer study sessions (averaging 40+ attendees per event) designed to bridge gaps in first year foundational physics.
- Synthesized student feedback surveys into actionable proposals, collaborating with student councils to resolve systemic academic concerns through active faculty engagement.

Technical Skills

Programming & Frameworks: Python (NumPy, pandas, PyTorch, scikit-learn, LightGBM, Matplotlib), Java, Bash/Shell scripting, GitHub

Computational Chemistry & ML: ORCA (DFT, single-point calculations, geometry optimization), SLURM HPC Cluster scheduling, RDKit (SMILES, descriptors, fingerprints, 3D conformer generation), Fairchem/UMA, Optuna (Bayesian Tuning), SHAP (Model Interpretability), DEAP (Genetic Algorithms)

Experimental Chemistry: Quantitative titration, gravimetric analysis, potentiometry, UV/Vis and IR spectrophotometry, flame atomic spectrometry, ion chromatography, liquid-liquid extraction, recrystallization, analytical data error propagation, chemical safety protocol

Certifications & Safety: WHMIS 2015, Ontario Basic Health & Safety Awareness, Standard First Aid CPR (Exp. Dec. 2026)