

Liam Haas-Neill

Toronto, Canada

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Computational Biophysicist | Machine Learning Researcher | Python Developer

QUALIFICATION SUMMARY

PhD in computational biophysics with extensive experience in Python, data analysis, and machine learning. Experienced in biomolecular simulations and developing pipelines for analyzing protein structural and dynamics data. Published protein science researcher with a strong background in interdisciplinary problem-solving and collaboration with cross-functional teams. Experienced with developing machine learning models for automating workflows. A lifelong learner, eager and excited to continue learning new skills, hone existing skills, and apply them to solving new problems.

EDUCATION

PhD in Physics
MSc in Physics
HBSc in Physics

University of Toronto, Toronto, 2025
University of Toronto, Toronto, 2018
University of Toronto, Toronto, 2017

RELEVANT PROFESSIONAL EXPERIENCE

Machine Learning Researcher

RWDI – Independent Contractor, 2025 – Current

My role was to automate engineer workflows using predictive modelling including both regression, classification tasks, and heuristics.

- Led initiatives to preprocess, clean, and engineer features from large datasets using Python.
- Collaborated with cross-functional teams (engineering, product management, software developers) to identify key pain points in workflows to be automated.
- Designed and implemented machine learning pipelines, leveraging frameworks such as PyTorch, scikit-learn, and xgboost.
- Research and development of methods for machine learning of 3D structures of buildings

Computational Biophysicist - Graduate Researcher

University of Toronto, Toronto, 2017-2025

My work involved performing simulations on high performance computing systems, analyzing biomolecular simulations in python, and communicating findings in scientific journals

- Designed and executed large-scale molecular simulations to study protein dynamics in diseases such as cancer and HIV
- Specific focus on protein-protein interactions in the context of disease mutations and on protein-polymer interactions and their effect on protein structure and dynamics
- Developed Python scripts for analysis protein structure & dynamics data from simulations
- Published 3 peer-reviewed articles, including in *Nature Communications* and *Protein Science*, showcasing impactful research findings
- Collaborated with interdisciplinary teams of biologists, chemists, and physicists to cross-validate simulation and experimental results
- Developed visualizations of protein structure, and structural analyses to clearly communicate research findings

KEY SKILLS

Programming: Python, NumPy, Pandas, Matplotlib, C++, Linux, Windows, HPC

Biotechnology: Molecular dynamics simulations, MDAnalysis (Python), MDTraj (Python), BioPython, SwissModel, Modeler, Homology Modeling, Visual Molecular Dynamics (VMD), ChimeraX, CHARMMGUI, Multiple Sequence Alignment, GROMACS

Machine Learning: Sci-kit Learn, Keras, PyTorch, Azure AI

SELECTED PUBLICATIONS

1. **Haas-Neill L**, Meneksedag-Erol D, Chaudhry A, Novoselova M, Ashraf QF, de Araujo ED, et al. (2025). The structural influence of the oncogenic driver mutation N642H in the STAT5B SH2 domain. *Protein Science*. <https://doi.org/10.1002/pro.70022>
2. **Haas-Neill, L.**, Joron, K., Lerner, E., & Rauscher, S. (2025). PEG-mCherry interactions beyond classical macromolecular crowding. *Protein Science*. <https://doi.org/10.1002/pro.5235>
3. Joron, K., Viegas, J.O., **Haas-Neill, L.** et al (2023). Fluorescent protein lifetimes report densities and phases of nuclear condensates during embryonic stem-cell differentiation. *Nature Communications*. <https://doi.org/10.1038/s41467-023-40647-6>
4. **Haas-Neill, L.**, Meneksedag-Erol, D. et. Al (2024). An all-atom view into the disordered interaction interface of the TRIM5 α PRYSPRY domain and the HIV capsid. *bioRxiv*. <https://doi.org/10.1101/2024.12.06.627233>

CONFERENCES

Biophysical Society Annual Meeting: 2019, 2020, 2023, 2024
Biophysical Society of Canada Annual Meeting: 2019, 2020, 2023
World Association of Theoretical and Computational Chemists (WATOC): 2020
PyCon: 2019

ACADEMIC AWARDS, HONORS, AND SCHOLARSHIPS

Biophysical Society of Canada Poster Award	2022
E. F. Burton Fellowships in Physics	2021
Faculty Of Arts and Science Program-level Fellowship	2021
Dr. James A. & Connie P. Dickson Scholarship In Science & Mathematics	2015, 2017
C. L. Burton Scholarship for Mathematics and Physical Sciences	2016
Howard Ferguson Provincial Scholarship	2013, 2015, 2016
Fletcher-clark Scholarships in Science And Economics	2015
University of Toronto Entrance Scholarship	2013

OTHER INTERESTS

Piano, singing, music production, volleyball, running, weightlifting, canoeing, camping, hiking