GRANT MCCONACHIE

PHD CANDIDATE

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Boston, MA, USA
LinkedIn | Github | Website

EXPERIENCE

PhD Research

Boston University, Boston, MA | 2021 - Present

- Conducting research with Dr. Brian DePasquale, exploring graph neural networks and large language models to model protein-small molecule binding for olfaction and collective behavior.
- Training deep learning models to predict odor binding to mosquito olfactory receptors using high-dimensional protein-small molecule data and high-performance computing.
- Developing dynamic graph neural network models to predict temporal aspects of glassfish collective behavior using keypoint data.
- Awarded the NSF GRF, worth $159,000 in funding, for pioneering research applying machine learning to decipher mosquito olfactory processing.
- Presented research posters at 4 high-profile conferences — See "Poster and Publications" below — showcasing advancements in machine learning for olfactory processing.

Post Baccalaureate Fellow

National Cancer Institute, Frederick, MD | 2020 - 2021

- Worked as an Automation Engineering Technician for the Frederick National Lab for Cancer Research.
- Developed software and automation scripts to enhance workflow efficiency in a high-throughput lab focused on discovering novel drug candidates from natural products.
- Developed a RESTful API, using flask, to control 6 automated chromatography machines, reducing manual workload by 90% and improving productivity.

Research Assistant

Oregon State University, Corvallis, OR | 2019 - 2020

- Conducted research with Dr. Cory Simon to leverage mathematics, machine learning, statistical mechanics, and computer simulations to understand porous material.
- Aided in projects that used machine learning and data collection techniques to predict adsorption properties of metal organic frameworks (MOFs).
- Co-authored a paper published in the *ACS Chemistry of Materials* journal.

Intern

Capstone Surgical Technologies, Troy, MI | Jun 2019 – Sep 2019

- Interned at a surgical device startup, contributing to research, development, and regulatory processes.
- Worked with NX 3D modeling software and developed a neural network in Python using TensorFlow.
- Assisted in evaluating potential shortcomings of emerging biotechnologies.
- Performed FDA regulatory work to support compliance efforts.

EDUCATION

Boston University

PhD Biomedical Engineering
2021 – Present

Oregon State University

BS Bioengineering
Summa Cum Laude (3.85/4.0)
2020

SKILLS

- PyTorch
- JAX
- Python
- MATLAB
- Cluster computing (SGE)
- API development
- GNNs
- Self-supervised learning
- Transformers (Huggingface)
- Multimodal models
- LoRA

OPEN-SOURCE CONTRIBUTIONS

Optax

Added a normalized temperature scaled cross entropy loss (NT-XENT) to DeepMind's optimization library Optax.

REVIEWED FOR

ICLR 2025

POSTERS AND PUBLICATIONS

Learning the Language of Smell: Foundation Models for Protein-Odor Interactions.
Frontiers in NeuroAI Symposium 2025, Kempner Institute, USA. Poster.
Grant D. McConachie, Emily Duniec, Florence Guerina, Meg A. Younger, Brian DePasquale.

Improved Odor-Receptor Interaction Predictions via Self-Supervised Learning.
NAISys 2024, Cold Spring Harbor Laboratory, USA. Poster.
Grant D. McConachie, Emily Duniec, Meg A. Younger, Brian DePasquale.

A Graph Neural Network Self Supervised Learning Approach to Generate a Meaningful Chemical Latent Space for Olfactory Tasks.
AChemS 2024, FL, USA. Poster.
Grant D. McConachie, Meg A. Younger, Brian DePasquale.

Graph neural network guided *in silico* deorphanization technique for olfactory receptors.
COSYNE 2024, Lisbon, Portugal. Poster.
Grant D. McConachie, Meg A. Younger, Brian DePasquale.

Screen for New Antimicrobial Natural Products from the NCI Program for Natural Product Discovery Prefractionated Extract Library.
ACS Infectious Diseases 2023. Paper.
Lucero Martínez-Fructuoso, S. J. Ryan Arends, Vitor F. Freire, Jason R. Evans, Sean DeVries, Brian D. Peyser, Rhone K. Akee, Christopher C. Thornburg, Rohitesh Kumar, Susan Ensel, Gina M. Morgan, Grant D. McConachie, Nathan Veeder, Leonard R. Duncan, Tanja Grkovic**,** Barry R. O'Keefe

National Cancer Institute (NCI) Program for Natural Product Discovery: Exploring NCI-60 Screening Data of Natural Product Samples with Artificial Neural Networks.
ACS Omega 2023. Paper.
Jason R Evans, Rhone K Akee, Shaurya Chanana, Grant D. McConachie, Christopher C. Thornburg, Tanja Grkovic, Barry R. O'Keefe

Recommendation System to Predict Missing Adsorption Properties of Nanoporous Materials.
Chemistry of Materials 2021. Paper.
Arni Sturluson, Ali Raza, Grant D. McConachie, Daniel W. Siderius, Xiaoli Z. Fern, Cory M. Simon

TEACHING EXPERIENCE

Linear algebra - Teaching Assistant
Boston University, Boston, MA | Spring 2025

Graduate level intro to machine learning - Teaching Assistant
Boston University, Boston, MA | Spring 2024

Chemical process dynamics and simulation - Learning Assistant
Oregon State University, Corvallis, OR | Spring 2020

HONORS AND AWARDS

National Science Foundation Graduate Research Fellowship (NSF GRF)
Awarded a 5-year fellowship to support my PhD research in applying state of-the-art AI tools to gain an understanding of how the olfactory system encodes information.

Quantitative Biology & Physiology (QBP) Trainee
Recipient of a prestigious 2-year training grant, supporting PhD candidates in computational biology and related fields.