GRANT MCCONACHIE

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EDUCATION

Boston University, Boston, MA 2022 – Expected 2027
PhD, Biomedical Engineering | GPA: 3.93/4.00 | Advisor: Dr. Brian DePasquale

Oregon State University, Corvallis, OR 2016 – 2020
BS, Bioengineering | GPA: 3.85/4.00 | Summa Cum Laude

THESIS PROJECTS

Improve odorant-receptor interaction predictions using foundation models for underexplored *Aedes aegypti* receptors.

- Developed deep learning models to predict odor binding to mosquito olfactory receptors using high-dimensional protein-small molecule data and high-performance computing (HPC).
- Built multimodal low-rank adapted foundation models with PyTorch and HuggingFace frameworks.
- Contributions culminated in various posters and a manuscript currently available on biorXiv and under review at ICLR 2026.

GNN models for assessing the impact of individuality on collective dynamics in schooling fish.

- Developed custom graph neural network (GNN) models for latent graph inference to model collective dynamics of *Danionella translucida*.
- Implemented models using PyTorch and PyTorch Geometric frameworks.
- Work currently under review for presentation at COSYNE 2026.

Design novel GNN foundation models that exploit metabolic organization to generate olfaction specific odorant embeddings.

- Engineered multiple GNN foundation models incorporating pretext tasks tailored to capture olfactory-specific molecular features.
- Exploited metabolic pathway organization to inform embeddings, aiming to enhance molecular representations for downstream olfactory prediction tasks.

EXPERIENCE

Post Baccalaureate Fellow 2021 – 2022
National Cancer Institute | Frederick, MD

- 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 2019 – 2020
Oregon State University | Corvallis, OR

- 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.

SKILLS

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

POSTERS, PUBLICATIONS, AND TALKS

Low rank adaptation of chemical foundation models generates effective odorant representations
bioRxiv 2025. Paper.
Grant D. McConachie, Emily Duniec, Florence Guerina, Meg A. Younger, Brian DePasquale.

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.

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.

HONORS AND AWARDS

National Science Foundation Graduate Research Fellowship (NSF GRF).
Awarded a 5-year fellowship, worth $159,000 in funding, 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.

SERVICE

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

Reviewer
Reviewer for ICLR (2025), NeurIPS (2025), ICLR (2026), COSYNE (2026)