Laura McDonnell

### Undergraduate Honors Student

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## Education

*B.Sc.*, BIOCHEMISTRY MAY 2024 (EXPECTED)

Certificate: Fundamentals of Programming GPA: 3.9

Temple University, Philadelphia, PA

## Research

[CARNEVALE GROUP](https://carnevalelab.org/), TEMPLE UNIVERSITY AUG 2023 – PRESENT

**Project**: Application of machine learning (ML) to elucidate protein structure-function relationships

• Trained a custom variational autoencoder ML model on datasets of protein domain sequences to generate novel proteins in order to evaluate model efficacy

• Optimized model training hyperparameters to improve performance

[BORGUET GROUP](https://sites.temple.edu/borguet/members/), TEMPLE UNIVERSITY MAY 2021 – MAY 2023

**Project**: Spectroscopic study of molecular interactions with UiO Metal-Organic Frameworks (MOFs)

Primary Project: Investigating diffusion of water within UiO MOFs

• Determination of binding site distribution and binding energies of adsorbed H2O on a UiO-67 MOF using Temperature-Programmed Desorption Mass Spectrometry (TPD-MS)

• Characterization of key H2O-MOF interactions tracked over time using Fourier-Transform Infrared Spectroscopy (FT-IR)

Secondary Project:Probing and analyzing catalytic sites on metal-organic frameworks

• Identification of acidic and basic sites on UiO-67 MOFs by tracking FT-IR of adsorbed acetonitrile

• Determination of the strength and prevalence of Lewis acid defect sites at various activation temperatures using CD3CN as a probe molecule

## Work Experience

MATHEMATICS TUTOR OCT 2021 – PRESENT

TEMPLE UNIVERSITY

• Worked with students to teach and strengthen mathematical concepts ranging from algebra to calculus and proofs

COMPUTATIONAL CHEMISTRY INTERN JUNE 2023 – AUG 2023

CONIFER POINT PHARMACEUTICALS, LLC.

**Project**: Designing and optimizing therapeutic drugs *in silico*

• Conducted an independent inhibitor development project using Schrödinger’s Maestro software. Workflows included molecular docking screenings, MM-GBSA free energy calculations, and QSAR modeling

• Utilization of Python scripting to parse and extract data from large libraries

## Publications

1. Anomalous Infrared Intensity Behavior of Acetonitrile Diffused into UiO-67

 R.P. McDonnell, V.S.D. Devulapalli, T.H. Choi, **L. McDonnell**, I. Goodenough, P. Das,

 N.L. Rosi, J.K. Johnson, E. Borguet, *Chemistry of Materials* **2023** *35* (21), 8827-8839

 DOI: [10.1021/acs.chemmater.3c00639](https://pubs.acs.org/doi/full/10.1021/acs.chemmater.3c00639)

2. Effect of Pore Size on H2O Diffusion into UiO-6x Metal-Organic Frameworks

 **L. McDonnell**, R.P. McDonnell, V.S.D. Devulapalli, N.L. Rosi, E. Borguet,

 To be submitted to *J. Chem. Phys.*

## Presentations

1. In Situ Infrared Study of Acetonitrile Diffusion into UiO-67 Metal-Organic Frameworks

**L. McDonnell,** E. Perkins, R.P. McDonnell, V.S.D. Devulapalli, I. Goodenough, P. Das,

N.L. Rosi, E. Borguet

Eastern US YCC Partnership Research Symposium and Chemistry Career Expo, August 5, 2021.

1. Effect of Thermal Activation on Acetonitrile Diffusion into UiO-67 Metal-Organic Frameworks

**L. McDonnell,** E. Perkins, R.P. McDonnell, V.S.D. Devulapalli, I. Goodenough, P. Das,

N.L. Rosi, E. Borguet

College of Science and Technology Undergraduate Research Symposium, Temple University, Philadelphia, PA, November 5, 2021.

1. Probing Thermally Activated Defects in UiO-67 Metal-Organic Frameworks Using Temperature-Programmed

**L. McDonnell,** E. Perkins, R.P. McDonnell, V.S.D. Devulapalli, I. Goodenough, P. Das,

N.L. Rosi, E. Borguet

TAFDV Virtual Student Poster Session and Business Meeting, January 26, 2022.

1. Optimizing a Latent Variable-Based Generative Model for Protein Sequences

**L. McDonnell,** J. Lamanna, M.E. Mowlaei, P. English, X. Shi, V. Carnevale

College of Science and Technology Undergraduate Research Symposium, Temple University, Philadelphia, PA, November 17, 2023.

## Professional Activities

Member of American Chemical Society (ACS) 2023 – Present

Member of Society for Molecular Biology & Evolution (SMBE) 2023 – Present

## Technical Skills

PROGRAMMING Python • Java • R • PyTorch • Bash

COMPUTATIONAL Maestro • VMD • PyMol • Chimera • BLAST

SCIENTIFIC SOFTWARE ChemDraw • IGOR • LabVIEW • LaTeX

ULTRA-HIGH VACUUM (UHV) SYSTEMS

 • Temperature-programmed techniques (e.g., TPD-MS, TP-IR)

 • UHV chamber operation and maintenance

## Honors

TEMPLE UNIVERSITY HONORS PROGRAM AUG 2020 – PRESENT

DEAN’S LIST (GPA > 3.75) FALL 2020, SPRING 2021, FALL 2021, SPRING 2022, SPRING 2023

DEAN’S SCHOLARSHIP RECIPIENT AUG 2020 – PRESENT

TAGGART ENDOWED SCHOLARSHIP RECIPIENT AUG 2023 – PRESENT