Joseph P. Fernandez

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Summary
Computational Chemist with 3+ years of industry-adjacent experience at P&G Digital Accelerator, specializing in molecular simulations, predictive modeling, and sustainable materials research. Developed Python-based pipelines and Streamlit apps to accelerate R&D, reducing experimental costs by 40% and timeline by 90%. Proficient in Schrödinger, Gaussian, AMBER, and high-performance computing (Unix). Seeking computational chemistry roles in biotech, pharma, or materials science.

Skills

- *Computational Chemistry*: Molecular Dynamics (Schrödinger, AMBER, AutoDock), Quantum Mechanics (Gaussian), Docking, RDKit
- *Data Analysis*: Python (pandas, numpy, matplotlib, Jupyter), Predictive Modeling, Machine Learning (JMP), Markov Chain Algorithms
- *Computing*: High-Performance Computing (Unix, Bash), Streamlit, Web Development

Professional Experience

Postdoctoral Research Fellow, P&G Digital Accelerator, University of Cincinnati 2022–Present

- Designed molecular dynamics pipelines (Schrödinger) to simulate enzyme-polymer interactions, enabling predictive biodegradation models for sustainable consumer materials.
- Developed a machine learning model (Python, Jupyter) to predict polymer biodegradation, achieving $R^2 > 0.8$ for 100+ compounds, cutting experimental costs by 20–50%.
- Built a Streamlit web application for predictive modeling, adopted by 10+ R&D team members, reducing testing time by 90%.
- Implemented Markov chain algorithms to simulate metabolite distributions, enhancing model robustness across diverse polymers.
- Authored technical documentation for proprietary methodologies, capturing IP and supporting cross-functional teams.

Graduate Research Associate, The Ohio State University 2017–2022

- Conducted 100+ simulations (Gaussian, AMBER) to predict molecular properties, guiding synthesis and reducing experimental iterations by 30%.
- Developed Python workflows for binding energy analysis, streamlining screening of compound libraries for organophosphorus poisoning therapeutics.
- Contributed computational simulations to publications in *Anal. Chem.* and *Environ. Sci. Technol.*, advancing molecular docking and materials science research.

Staff Teaching Associate, The Ohio State University 2011–2013, 2016–2017

- Developed instructional materials and lab experiments for General Chemistry and Organic Chemistry, mentoring 20+ undergraduate teaching assistants to ensure high-quality course delivery.
- Delivered in-person and virtual instruction, enhancing student understanding of complex chemical concepts through clear communication and technical expertise.
- Designed and graded coursework, fostering critical thinking and problem-solving skills in 100+ undergraduates per semester.

Student Research Associate, The Ohio State Medical Center, Leukemia Tissue Bank 2008–2011

- Processed and characterized tissue samples (DNA, RNA, protein) for hematologic malignancy research, supporting clinical studies.

Education

The Ohio State University

Ph.D., Organic Chemistry (Computational Chemistry Focus) 2017–2023
B.A., Chemistry with Honors 2007–2011
B.A., Philosophy with Honors 2007–2011

Selected Publications

- Sahraeian, T.; Kułyk, D. S.; Fernandez, J. P.; et al. *Anal. Chem.* 2022, 94(43), 15093–15099.
- Scott, S.; Fernandez, J. P.; et al. *Environ. Sci. Technol.* 2022, 56(2), 951–961.
- Wolfson, E. R.; Schkeryantz, L.; Fernandez, J. P.; et al. *ACS Appl. Mater. Interfaces* 2021, 13(35), 41628–41636.

Awards

- John S. Swenton Award for Outstanding Teaching, 2021
- GAANN Fellowship, U.S. Department of Education, 2019

Professional Affiliations

- American Chemical Society