Joseph P Fernandez

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Data Scientist | *Computational Chemist* | *Predictive Modeling Expert*

Current Employment

Post Doctoral Research Fellow, University of Cincinnati (2022 – Present)

- Research Fellow in the Procter & Gamble Digital Accelerator at University of Cincinnati, College of Engineering and Applied Science
- Developing advanced simulation and data analytics pipelines to predict the behavior of biodegradable polymers, applying principles of computational chemistry and large-scale data processing.
- Leveraging predictive modeling and machine learning approaches to reduce experimental costs and accelerate sustainable materials research for consumer applications.

Education

The Ohio State University (2017 – 2023)

Ph.D., Organic Chemistry Division of the Chemistry Graduate Program

- Research Focus: Computational Chemistry
- Areas of Expertise: molecular modelling, predictive modelling, quantitative data analysis, drug discovery, enzyme-ligand interaction analysis, organic mechanism elucidation, statistical thermodynamics
- Technical Skills: applications in quantum mechanics (*Gaussian*) and molecular dynamics (*Schrödinger, AMBER, AutoDock*), high throughput data analysis (*python, pandas, numpy, matplotlib, Jupyter, rdkit*), and HPC (*Unix, bash*)

The Ohio State University (2007 – 2011)

B.A., Chemistry *with Honors in the Arts and Sciences*

B.A., Philosophy *with Honors in the Arts and Sciences*

Research Experience

Post Doc Fellow, P&G Digital Accelerator @ UC (2022 – Present)

- Engineered data-driven docking and molecular dynamics (*Schrödinger*) pipelines to analyze microbial enzymes and polymeric substrates, informing predictive biodegradation models in wastewater systems.
- Developed and optimized predictive polymer biodegradation model (*python, Jupyter*) that achieved an $R^2 > 0.8$ on OECD 301B data for over 100 natural and synthetically functionalized polymers, decreasing experimental iteration time.
- Implemented advanced Markov chain algorithms to extend the biodegradation model's predictive power, enabling robust simulation of metabolite distributions under diverse polymer compositions.
- Built and deployed a Streamlit based web application to democratize model usage, accelerating R&D workflows by replacing labor-intensive physical testing with instant model-driven predictions.
- Produced technical documentation and internal publications on proprietary predictive modeling methodologies, capturing organizational IP and fostering cross-functional knowledge sharing.

Graduate Research Associate, The Ohio State University (2017 – 2022)

Dissertation Advisor: Dr. Christopher Hadad

- Leveraged advanced computational chemistry simulations to model and predict physical properties of novel organic molecules and complex biochemical systems, optimizing research insights with HPC environments (Unix, Bash).
- Designed and analyzed novel therapeutics targeting organophosphorus poisoning of acetylcholinesterase using high-throughput binding energy calculations, advancing computational drug discovery pipelines.
- Developed innovative Python-based workflows for binding energy analyses and data visualization, streamlining the screening of compound libraries and enhancing structure-activity insights.
- Elucidated organic reaction mechanisms via free energy calculations and transition state theory, reducing experimental effort by accurately predicting reaction outcomes and guiding synthesis strategies.

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

PI: Dr. Michael Caligiuri

- Central collection, processing, storage, and characterization of tissue samples and derivatives (plasma, serum, DNA, RNA, protein) from patients with any hematologic malignancies.

Awards & Honors

John S. Swenton Award for Outstanding Teaching (2021)

- Recognized as the top graduate teaching associate for excellence in classroom instruction, demonstrating advanced communication, presentation, and problem-solving abilities.

Grants & Fellowships

GAANN Fellowship (2019)

- Awarded by the U.S. Department of Education to support advanced training and research in computational chemistry, including high-throughput analysis and data-intensive methodologies.

Graduate Enrichment Fellowship (2017 – 2018)

- Provided immersive funding to pursue interdisciplinary graduate research, fostering the development of specialized computational and analytical skills in organic chemistry.

Teaching Experience

The Ohio State University

Staff Teaching Associate (2011 – 2013, 2016 – 2017)

Graduate Teaching Associate (2017, 2018, 2021)

- Developed new instructional materials and laboratory experiments, mentoring undergraduate teaching assistants to ensure consistent and high-quality course delivery.
- Instruct (virtual and in person) and grade regular coursework

- General Chemistry I&II, Organic Chemistry I&II, Computational Chemistry, Spectroscopy of Organic Compounds

Publications

Sahraeian, T.; Kulyk, D. S.; **Fernandez, J. P**.; Hadad, C. M.; Badu-Tawiah, A. K. Capturing Fleeting Intermediates in a Claisen Rearrangement Using Nonequilibrium Droplet Imbibition Reaction Conditions. Anal. Chem. 2022, 94 (43), 15093–15099. https://doi.org/10.1021/acs.analchem.2c03268.

Scott, S.; **Fernandez, J. P**.; Hadad, C. M.; MacKay, A. "Molecular Docking as a Tool to Examine Organic Cation Sorption to Organic Matter" Environ. Sci. Technol. 2022, 56(2), 951 – 961, doi:10.1021/acs.est.1c06147

Wolfson, E. R.; Schkeryantz, L.; Moscarello, E. M.; **Fernandez, J. P**.; Paszek, J.; Wu, Y.; Hadad, C. M.; McGrier, P. L. "Alkynyl-Based Covalent Organic Frameworks as High-Performance Anode Materials for Potassium-Ion Batteries" ACS Appl. Mater. Interfaces 2021, 13(35), 41628 – 41636, doi: 10.1021/acsami.1c10870

Gunther, M. J.; Pavlović, R. Z.; **Fernandez, J. P**.; Zhiquan, L.; Gallucci, J.; Hadad, C. M.; Badjić, J. D. "Stereo- and Regioselective Synthesis of Molecular Baskets" J. Org. Chem. 2019, 84(7), 4392 – 4401, doi:10.1021/acs.joc.9b00330 \

Parkin, S. R.; Coldren, W. H.; **Fernandez, J. P**.; Hadad, C. M.; Behrman, E. J. "Polymorphism, Crystal Packing, Twinning, and Molecular Conformations in 5'-Halo-5'-deoxyguanosines and a Hydrate of the Pseudo-halide Analogue, 5'-Azido-5'-deoxyguanosine" Crystal Growth & Design. 2018, 18(11), 6995 – 7005, doi:10.1021/acs.cgd.8b01162

Presentations

Fernandez, J.P.; Franjesevic, A.J.; Coldren, W.H.; Nosseir, O.; Zhuang, Q.; Hadad, C.M. Molecular Conformations in the Active Site of Organophosphorus-Aged Acetylcholinesterase: Insights into the Rational Development of Nerve Agent Countermeasures*. Selected Oral Presentation* at the Gordon Research Conference: Detection, Countermeasures, and Prevention of Chemical and Biological Threats; Ventura, CA; March 2019

Service

- Ohio-5 SURE Mentor (2021)
- Industry Day Host (2018)
- Prospective Student Host (2017,2018)

Professional Affiliations

- American Chemical Society

Additional Technical Skills

- Microsoft Office, LLM, ChatGPT, ML/AI, Web Development, Graphics Processing

Hobbies & Interests

- Proud husband and father of four children, raising goats and chickens on a rural homestead
- Avid distance runner, fantasy reader, and eternal optimist