UC RIVERSIDE Chemical and Environmental Engineering

CEE Seminar Speaker

DANIEL WOLDRING

Assistant Professor
Department of Engineering and Material Science
Michigan State University

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MACHINE LEARNING COMES TO THE RESCUE FOR PROTEIN ENGINEERING TASKS

Predicting how drugs will interact with membrane transporters is an essential step in developing safe and effective therapies. In this talk, I will explore how machine learning, particularly our graph neural network (HOLIgraph), can shed light on inhibitory properties of diverse ligands targeting organic anionic transporting polypeptides (OATPs). By comparing what we learn from simply looking at drug structures and protein sequence information to the richer insights gained by incorporating high-resolution cryoEM data, we demonstrate that deeper structural context of protein-drug interactions can dramatically enhance predictive accuracy. Our molecular interaction–based GNN approach not only reproduces known binding pockets within OATPs but also identifies key amino acid residues shaping ligand specificity. This holistic view of drug-transport interactions could shine new light on better predictions of drug-drug interactions and more rational drug design, empowering researchers and clinicians alike to make informed decisions about new therapeutics.

BIOGRAPHY

Dr. Woldring is an Assistant Professor in the Department of Chemical Engineering and Materials Science at Michigan State University, where he integrates engineering principles with advanced machine learning to tackle challenges in protein therapeutics and diagnostics. Leading a team of four graduate students, two postbacs, and six undergraduates, he combines high-throughput wet lab experiments with computational modeling to pioneer new strategies in protein engineering. Among his lab's signature projects are HOLI-graph, which elucidates membrane transporter specificity—especially regarding OATP1B1—and EvoSeq, an approach harnessing protein evolution data to refine AI-driven models. This synergy has yielded 15 peer-reviewed articles and preprints in the past five years.

Dr. Woldring is certified in Mental Health First Aid, reflecting his dedication to fostering a supportive, collaborative environment for emerging scientists. His laboratory currently holds two PI-led grants: an NIH-NIAID R21 focused on rational monoclonal antibody discovery against carbohydrate antigens in neuroblastoma, and a USDA-NIFA award employing deep learning and directed evolution to help fruit trees detect bacterial pathogens. Through these initiatives, Dr. Woldring aims to translate fundamental protein engineering discoveries into cutting-edge therapeutics, ultimately improving outcomes for patients – and plants!