



Khaled M. Elokely, Ph.D., is a medicinal and computational chemist at the University of Wyoming School of Pharmacy, USA. His research sits at the interface of cheminformatics, structural bioinformatics and medicinal chemistry, with one common goal: making computational predictions in drug discovery trustworthy. One direction treats data as a scientific object in its own right, curating large public bioactivity databases by pharmacological mechanism and assay readout, and building verification-first pipelines that expose silent errors before any model is trained. A second direction reads protein structure as a network, using residue contact networks to explain selectivity across kinase and GPCR families. A third uses molecular dynamics and enhanced sampling to study how receptors and enzymes move between functional states, and how quickly those transitions occur. Across these programs, his group emphasizes reproducibility and open science, releasing auditable tools such as MolScope and Curato-opioid for the wider drug-discovery community.