

# ***Cosolvent Sites-Based Discovery of Mycobacterium Tuberculosis Protein Kinase G Inhibitors***

*Sabahudin Redzic Chemistry Senior Seminar*

A rampant problem in the realm of infectious diseases would be the prevalence of antibiotic resistant disease strains that arise from improper and insufficient drug protocols. Tuberculosis (TB), caused by the bacterium *Mycobacterium tuberculosis* (Mtb), would be an example of just such phenomena plaguing the world today. In this article, scientists addressed the issue by targeting the kinase PknG which in addition to being vital to the pathogenicity of TB contained an ATP binding pocket that allowed for greater selectivity by competing ATP inhibitors. The researchers ran mixed solvent molecular dynamics simulations to find potential ligand-PknG interactions, scaffold docking simulations to narrow potential target compounds, binding affinity estimations to verify chosen scaffolds, and radioactive ATP assays to document inhibition of Mtb. The compounds identified as inhibitors of PknG in this article may serve as lead compounds for the development of new anti-TB drugs which may aid in combatting the aforementioned rise in antibiotic-resistant strains.