Abstract:
Infectious diseases represent a global health dilemma. Millions of new infections are noted each year which result in millions of deaths. A race has been established between the causative bacteria and drug discovery efforts to see how quickly new therapeutics can be evolved (let alone approved by the relevant regulatory agency) as compared to the geographic spread of disease as well as drug-resistant strains. We have chosen to leverage computational techniques such as machine learning with medicinal chemistry and mechanistic biology to seed the discovery of novel therapeutics for infections from *Mycobacterium tuberculosis* and *Staphylococcus aureus*. Representative programs will be discussed that have led to new strategies to identify drug-like small molecule antibacterials through Bayesian approaches, evolve them with medicinal chemistry heuristics and Bayesian models, and study their intrabacterial metabolism.