Redesigning Drug Design

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Drug design lags far behind other engineering disciplines in lacking predictive, quantitative models that allow small-molecule therapeutics to be designed, rather than fortuitously discovered. While many challenges exist to building these models, our laboratory uses cycles of computational predictions coupled to experimental measurements to rapidly generate data that can be used to improve rigorous, quantitative approaches to small molecule design based on alchemical free energy calculations. In this talk, we will describe how this process can be done cheaply and in a fully automated manner by inverting the drug discovery problem, and describe our first few steps toward this goal.