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Why can't we engineer drugs on a computer? And what can be done about it?

The design of airplanes, bridges, chemical plants, and computer chips is aided significantly by modern computational tools. Design of novel molecules, however, is done primarily by trial-and-error. A prime example is the pharmaceutical industry, where the complexity of biomolecular interactions has greatly limited our ability to model and design effective small molecule drugs. This means drug design has remained somewhat of a black art, relying on many ad hoc assumptions and on the

intuitive insights of experienced medicinal chemists.

What are the barriers that must be overcome in order to model drug-ligand binding affinities, solubilities, partitioning into delivery formulations and polymorph stabilities effectively? Is there a hope to change the process of designing drugs with high efficacy, good bioavailability and a specific mode of action from a trial-and-error art to a nanoscale engineering process using high-quality, reliable modeling?

In my talk, I will discuss the barriers above, some of the successes that are emerging in the field, and describe research in the Shirts group on modeling the noncovalent interactions of small molecules with sufficient reliability and efficiency to have a place in the modern pharmaceutical workflow. In particular, I will discuss approaches we are developing to predict binding affinities of small molecules to proteins, and to

Wednesday Seminar Series