Abstract:
Increasing computing power has made it possible to study drug-target interactions by means of molecular dynamics simulations. However, the characterization of bound/unbound states and the estimation of binding kinetics from these data remains a challenging task. I will briefly explain how Markov state modeling can be used to estimate drug affinity and binding rates, thereby supporting drug design. In addition, I will demonstrate how this approach can be adapted to compute transition rates in biological switches.

Once the binding kinetics have been estimated, reaction rate equations can be used to describe the time course of concentrations of occupied receptor binding sites. Coupled to a mathematical model that quantifies the ligand’s efficacy, this approach allows to study the potency of a drug and the effect of treatment strategies by computer simulations. I will illustrate this method in terms of a mathematical model for the administration of GnRH analogues in reproductive endocrinology.

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