LAUFER CENTER
FOR PHYSICAL AND QUANTITATIVE BIOLOGY

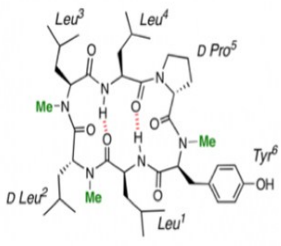
Seminar 2015

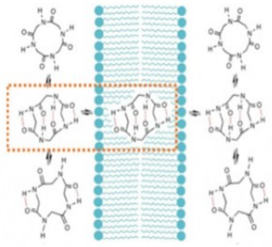
Emerging challenges for computer-aided drug design: macrocycles and allosteric modulators

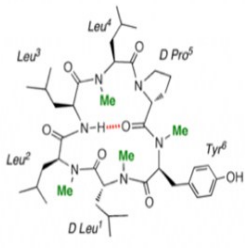
Matt Jacobson
Department Pharmaceutical Chemistry
University of California, San Francisco

Challenges in drug discovery, such as inhibiting protein-protein interfaces or increasing enzyme activity, have motivated my group to explore potential roles for computational chemistry beyond those addressed by docking, QSAR, and other widely used methods. I will discuss two of our efforts, to facilitate computer-aided design of (1) macrocycles, an emerging class of therapeutics intermediate between small-molecule and protein therapeutics; and (2) allosteric modulators, where the challenge is to optimize not just potency of binding but also achieve the desired modulation of function (activation or inhibition). Our computational approaches utilize all-atom simulations, guided by thermodynamic principles.

Research interests are in the areas of computational structural biology and computer-aided drug design.







Friday October 9, 2015

2:30 PM

Laufer Center Lecture Hall 101

Host: Markus Seeliger

Refreshments following seminar

Laufer Hub 110

For a disability related accommodation, please call 631-632-5400

Stony Brook University