BrownDye: Software for Performing Brownian Dynamics on Biological Molecules

Abstract:
One of the main challenges of computational biology is predicting the rate constants of association and dissociation of large molecules. In order to make the computations feasible, simplifying assumptions are made that still allow essential features of the physical process to be captured. Discussion will include current and upcoming features of the software as well as the physics and algorithms involved.

Thursday, May 7, 2015
2:00 PM
AP&M 5829