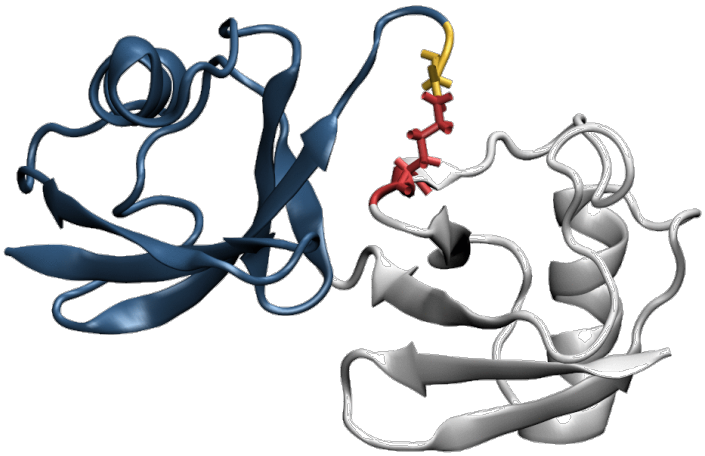
AUC 2017

SASSIE Software to Model AUC & SAS Data Using Atomistic Ensembles From Molecular Simulations

July 25, 2017



Molecular simulation is an important technique to analyze and interpret molecular phenomena across many disciplines. AUC & Small-angle scattering (SAS) utilizing either light or neutron sources are valuable methods to characterize shape, interactions, and properties of many soft-matter systems. Modeling of AUC & SAS data is often done using analytical functions and/or dummy-ball (DB) models. While these methods are simple, they have proven to be quite robust and have allowed for a tremendous expansion of AUC & SAS studies to a wide variety of systems. Atomistic modeling can be used to interpret AUC & SAS data and inherently provides structural and atomic interactions that are unavailable using analytical or DB models. In addition, atomistic models can allow the use of experimental and computational constraints on the experimental data. The goal of

this introductory course is to use modern simulation methods and software tools to predict and analyze AUC & small-angle scattering data of biological systems. The bulk of the course will introduce SASSIE, a software framework designed to facilitate the use of atomistic modeling to interpret AUC & scattering data. The course will involve a mixture of lectures and examples with student lessons. Examples will involve various protein and DNA molecules, as well as their complexes. The emphasis will be on structure building, ensemble molecular simulation, calculation of AUC & scattering profiles, and comparison to experimental data.

NOTE: Files to carry out the labs are no longer available below. Please see more recent courses for updated labs and files.

Tuesday 7/25/2017

Session 1

Time	Lead	Activity	File
9:00 - 9:30	DWW	Lecture: Simulation & SASSIE Overview	lecture_1
9:30 - 9:45	DWW	Interactive Session: PDB & Participant Backgrounds	---
9:45 - 11:00	DWW	SASSIE-web Quick Start	lab_V.pdf

Session 2

Time	Lead	Activity	File
11:30 - 13:30	DWW	SASSIE-web Workflows	lab_VI.pdf

Session 3

Time	Lead	Activity	File
14:30 - 14:45	DWW	Lecture: Advanced SASSIE-web	lecture_2
14:45 - 16:30	DWW	Advanced SASSIE-web	lab_VII.pdf

Session 4

Time	Lead	Activity	File
17:00 - 17:20	DWW	Interactive Session: Participant Projects and Modeling Requirements	---
17:20 - 19:00	DWW	Extra time for Participant Projects & Advanced Simulation	---

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