SASSIE Tutorial

Small Angle Scattering: Structural Biology and Soft Matter Workshop

ACA Meeting

July 25, 2015

This tutorial will cover the basic features of the SASSIE-web online simulation and analysis tool for the modeling of biomolecular structures using small angle scattering data. Topics covered will include:

- Monte Carlo simulation of an intrinsically disordered protein to create an ensemble of protein structures
- Calculation of the theoretical scattering from protein models
- Comparison of theoretical and experimental scattering data
- Minimization of the structures that best fit the experimental scattering data.

During the tutorial, we will go through the SASSIE Quick Start guide, which covers the above topics by going through a specific example. If time permits, we will cover advanced topics in the above areas or other SASSIE modules depending on participant interest. No software needs to be installed on your computer to run SASSIE. However, a modern HTML5 compatible web browser with Javascript enabled such as Chrome, Firefox, Opera or Safari is required.

Due to the limited time available for this tutorial, it is strongly suggested that you register and log in, as well as familiarize yourself with some basic concepts, prior to the tutorial. These concepts will be used, but will not be covered in detail, during the tutorial. Instructions on how to register and log in can be found on the Basic Usage page. This page also describes the layout of the main web page and how the modules work. Also described are the Session Manager and the Job Manager. Please familiarize yourself with these concepts prior to the tutorial if possible.

To view the generated structure ensemble, you will need to be familiar with a molecular viewing program that can display both PDB and DCD files. VMD is one such viewer (click here to download) and a quick VMD tutorial is provided. VMD or another suitable viewing program does not need to be installed on your computer. However, you can do all of the exercises in the Quick Start guide without it.

There will not be time to cover basic MD methods, including how to build all-atom starting structures. Those who would like additional information, including a link to a previous weeklong MD summer school that covers these topics, can find it here. In this case, the SASSIE lectures
and labs refer to an earlier standalone version of SASSIE. Lectures and labs from a recent short course that used SASSIE-web can be found here.