Title: A Schrödinger Workshop: A beginners' guide to Structure Based Design

Tools: Maestro, Ligprep, Protein Preparation Workflow, SiteMap, Glide and Ligand Designer

Level: Beginners

Abstract:

If you are interested in learning to navigate the Maestro interface and how to perform design and docking of small molecules, then we will focus on these topics in a 2 hour hands-on workshop designed for beginners to the Schrödinger software.

The main Maestro interface houses all the tools that are required to bring in your starting small molecules and protein system, so that they may be prepared correctly. We will discuss approaches for understanding more about the binding site and its features which will help us think about how a ligand might interact with it. We will explore ligand design in a more automated fashion using the Ligand Designer GUI which facilitates on-the-fly ideation through 'build and dock' workflows. Through the use of embedded libraries of building-blocks, users can modify their initial idea in many intuitive ways: from attachment points on the bound ligand; the free and viable space in the binding site; through to picking specific residues in the protein or specific waters in the binding cavity to guide the design process.

Preparation

Every participant is required to download the Schrödinger license and bring their own laptop. Since we will not go through the basic functionalities of Maestro, we strongly encourage participants to go through our "Getting going with Maestro" online course to learn the basics (requires a free website account):

Getting going with Maestro

Should you wish to prepare further, here are additional resources:

- Ligand Designer (features, highlights, demo videos)
- Maestro, Preparation and Docking
- Small molecule docking