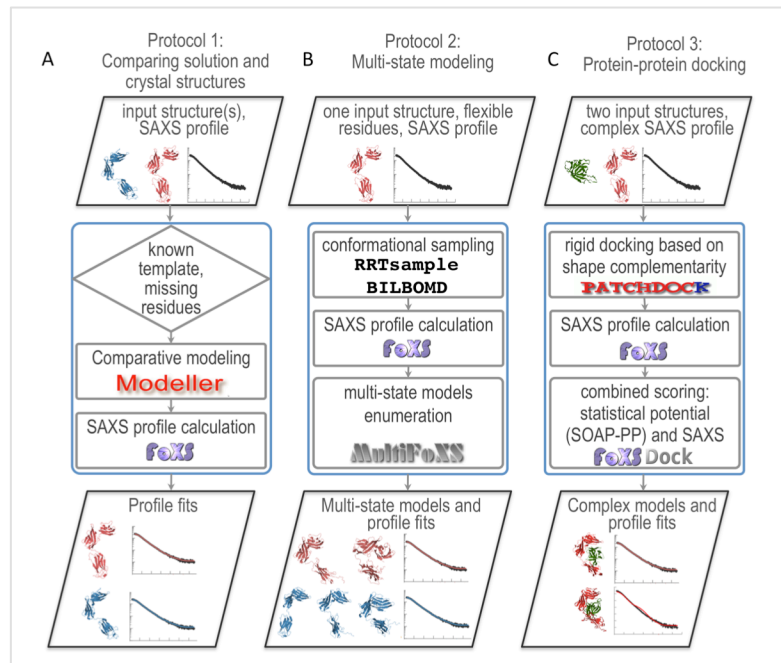


Modeling Structure and Dynamics of Protein Complexes with SAXS Profiles

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In this tutorial we will learn how to use three protocols using web servers or software packages for modeling atomic structures based on SAXS profiles.

The first protocol is for comparing solution and crystal structures including modeling of missing regions and determination of the oligomeric state. We will be using FoXS for SAXS profile calculation and fitting, as well as MODELLER for addition of missing regions. The second protocol performs multi-state modeling by finding a set of conformations and their weights that fit the SAXS profile starting from a single-input structure. We will be using Rapidly exploring Random Trees (RRTs) or high-temperature Molecular Dynamics (BilboMD) for sampling possible conformations, and MultiFoXS for multi-state modeling. The third protocol, FoXSDock, is for protein-protein docking based on the SAXS profile of the complex. We will be using PatchDock for docking, as well as FoXS and statistical potential for combined scoring. The methods are available as web servers or standalone programs in the IMP package.



Web servers:

<https://modbase.compbio.ucsf.edu/foxs/index.html>

<http://modbase.compbio.ucsf.edu/multifoxs/>

<http://sibylys.als.lbl.gov/bilbomd>

<https://modbase.compbio.ucsf.edu/foxsdock/>

<http://bioinfo3d.cs.tau.ac.il/PatchDock/>

IMP download: <https://integrativemodeling.org/download.html>

The tutorial files are available from:

<http://www.cs.huji.ac.il/~dina/software.html>