Interpretation of SAXS/SANS data with explicit-solvent MD simulations

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1. SAXS and SANS predictions from explicit-solvent MD simulations.

Calculation of SAXS/SANS curve from a given trajectory of all-atom MD simulation; comparison of calculated and experimental curve. We will use lbp protein as an example.

- Analysis of the hydration layer

2. SAXS-guided MD simulations, structure refinement against SAXS curves

When the calculated curve is not in agreement with the experimental curve, experimental curve can be introduced as an energetic restraint into the all-atom MD simulation, in order to guide the protein into the conformations that satisfy experimental data. We will demonstrate this on a case of lpb protein as well. We will start the simulation with the closed structure of the protein, and couple the simulation to the experimental curve of the opened state of the protein, do demonstrate the opening of the protein.

3. Ensemble refinement of intrinsically disordered proteins against SAXS data with commitment to the principle of maximum entropy.

In the case that protein "lives" in more than one state, coupling one simulation to the experimental curve can lead to the over-fitting and/or to the unrealistic structure in simulation. In order to avoid this, one can couple the experimental curve to the multiple-replica simulations. We will demonstrate this, using the intrinsically disordered protein and maximum entropy principle.