Interpretation of SAXS data using MD simulations: Detergent micelles and ion cloud of charged proteins

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Small-angle X-ray scattering (SAXS) is an experimental technique used to study biomolecules under near-native conditions. As the information content of the experimental data is low, methods that integrate the data with accurate computational models are urgently required. In recent years, all-atom molecular dynamics (MD) simulations have developed to a increasingly popular and reliable tool for interpreting SAXS experiments and and, more general, for gaining atomic-level insights into biomolecules. [1]

Detergent micelles are often employed as a membrane mimics to solubilize membrane proteins. Accurate information about the size and shape of micelles is important for the stability of protein- detergent complex. We show how MD can be combined with the SAXS data to derive temperature- dependent atomic models of monodisperse micelles. [2]

The ion cloud around charged proteins influence the radius of gyration (Rg) of the protein, complicating the interpretation of experimental SAXS data. In order to quantify this effect, we compared SAXS curves calculated from all-atom MD simulations with the experimental data. Furthermore, we developed a tool for a fast and accurate prediction of the ion cloud effect on Rg. [3]

Our current work is focusing on using multiple-replica MD coupled to SAXS data, following the maximal entropy principle, in attempts to study polidisperse micelles. In addition, we aim to expand available analytic models for the prediction of SAXS curves of micelles and to understand the influence of micelle shape fluctuations on SAXS curves.

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