SAXS-guided structure and ensemble refinement using explicit-solvent MD simulations. Recent developments and remaining challenges

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The interpretation of the SAS data by computational methods is complicated by the low information content of the data, by scattering contributions from the hydration layer and excluded solvent, and by unknown systematic errors. Explicit-solvent MD simulations may help to overcome such challenges because they add physical information to the low-information experiential data. Specifically, modern force fields may help to identify energetically reasonable conformations during structure refinement, and they provide an accurate description of the hydration layer and of the excluded solvent. After a brief introduction to MD-based SAXS data interpretation, recent developments are presented with some focus on Bayesian methods, maximum-entropy refinement, and intrinsically disordered proteins.