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## **Metainference simulations to interpret small-angle scattering experiments of non-conventional surfactants**

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In the study of soft-matter systems, measurements performed in solution using, e.g., small-angle scattering are very important. Information on the size, shape, and dynamics of the system, can be obtained through modeling of small-angle neutron scattering (SANS) and small-angle x-ray scattering (SAXS) experiments. However, some systems can be challenging to model, due to non-conventional packing or polydispersion. In such cases, molecular dynamics (MD) simulations can help, but often the force fields do not reproduce the correct structural ensemble, or the events happen in a time scale longer than simulation times. Metainference is a Bayesian inference method that enhances the sampling of MD simulations through bias forces that drive the models towards improved agreement with the experiment. The goal is to sample configurations that represent the correct ensemble and, on average, obtain agreement with the experiment. Recently, some of us have extended Metainference to allow using SANS data. Here, we present the first study on surfactant aggregation combining SAXS and SANS Metainference MD simulations. We study Triton X-100, a detergent that has been previously studied in the literature, and for which there is no consensus on the formed micelles' size and shape. This is due to the non-conventional structure of the micelles, which cannot be described by a simple core-shell model, and polydispersion. A polydispersion of aggregates with sizes varying from 3 to 129 molecules is necessary to reproduce the SAXS and SANS spectra simultaneously. Triton X-100 micelles show shapes dependent on their size, with the smaller being rather spherical and the larger being irregular (oblate or triaxial shape). For some sizes, the hydrophobic part shows an onion-like structure. This case study illustrates how Metainference can aid the interpretation of small-angle scattering experiments.

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