Explicit Atom Deuterium Contrast Matching for Small Angle Neutron Scattering on Biomolecular Systems

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The contrast variation method is a powerful technique for determining the structure of individual components in systems containing components with different scattering length density, ρ . By changing the scattering length density of the target solute or the solvent, specific solute scattering contributions can be emphasized. The contrast variation technique has been widely used in small angle neutron scattering (SANS) due to the large difference between the scattering lengths of hydrogen and its isotope, deuterium. In general, contrast variation methods have focused on matching out the bulk contribution of the solute, but not how contrast affects the scattering at specific scattering vectors, **q**, which are associated with specific structural distances. We present, SCOMAP-XD, a 3D structure-based explicit atom deuteration workflow to calculate the bulk contrast match points and investigate **q**-dependent contrast effects with SASSENA, an explicit atom SANS calculator.
Our method combines empirical models to understand deuterium incorporation at both the exchangeable and non-exchangeable hydrogen sites, due to hydrogen-deuterium exchange and bacterial growth in D2O, respectively. It calculates bulk contrast match points within 2.4% solvent D2O accuracy for several biomolecular systems and contrast conditions. The method is readily applicable to a variety of systems and provides a foundation to investigate specific **q**-dependent contrast matching.