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Contribution ID: 23

Type: poster contributions

Modeling of flexible biomolecular complexes in solution small-angle scattering

We outline a modeling scheme for calculating the scattering profiles from complex biological samples, such as multi-domain membrane proteins with intrinsically disordered regions and embedded in phospholipid nanodiscs. The scheme bases itself on a hybrid of classical form factor based modeling and the well known spherical harmonics-based formulation of small-angle scattering amplitudes.

We demonstrate the utility of this modeling scheme through a recent example of a structural model of the growth hormone receptor membrane protein in a nanodisc. We investigate how the scattering profiles from the complex would appear under different scattering contrasts. For each contrast situation we discuss what structural information is contained and the related consequences for modeling of the data.

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