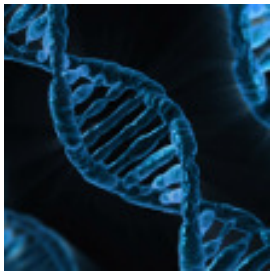

Contribution ID: **47** Type: **Oral presentation**

Contributed talk 1 - Exploring protein association pathways with time-resolved SAXS and SANS

Monday 4 June 2018 13:55 (20 minutes)

Protein performs its biological functions by interacting with other proteins. Protein complexes, which are formed as a result of these interactions, consist of two or more components that associate along specific pathways - protein association pathways. The association pathway from monomer to oligomer is critical in a range of biological processes and thus it is of a vital importance to elucidate both atomic-resolution structures of intermediates along the pathway as well as the structure of the final state. Although considerable progress has been made in using experimental and computational techniques to determine start and final structural states, we have a limited understanding of what happens in between.
By enabling both time resolution and structural detail Time-Resolved Small Angle X-ray/Neutron Scattering (TR-SAXS/TR-SANS) is uniquely suited to interrogate complex self-assembly reactions and to provide a molecular understanding of self-assembly pathways. However, the analysis of such data is complicated because scattering arises from a mixture of many components, the information content in each spectrum is limited and there is no framework for simultaneous analysis of data from different data sources. The similar problem is faced when resolving conformational ensembles from small angle scattering data.
To overcome this problem we develop a method that combines a computational structural modeling (which delivers atomic-resolution structures) with experimental data (which provides information about the population of different states). The method applies Bayesian probabilistic model to analyze scattering data from mixtures of oligomeric species, allows for a modeling large structural ensembles, can be used to assess uncertainty of all parameters and minimizes over-fitting. Our software is developed to meet high software standards and will become available to ESS users from the early stage of operation.

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Session Classification: Dynamics of Intrinsically Disordered Proteins

Track Classification: Dynamics of intrinsically disordered proteins