

SAS of membrane proteins: the data we have, what modelling would we need?

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Proteins are polymers that fold in a well-defined 3D structure, which can be determined by X-ray diffraction to atomic resolution, given well-diffracting crystals are available. To allow their biological function however, a certain flexibility can be allowed: in the majority of cases, the protein oscillates between two extreme conformations.

I will present two examples of membrane protein systems that we study by SANS. Indeed, membrane proteins need to be handled in detergent to avoid precipitation. We have determined conditions in which bound detergent and free micelles can be completely matched, the SAS data being thus exclusively produced by the studied protein.

The first example is a bacterial protein, SpNox, composed of a unique polypeptide chain, folded in two independent domains, linked by a linker. The atomic structure of a homologous protein is available, but the SANS data shows a larger object. We suspect flexibility between the two domains.

The second example is another bacterial protein, BmrA. This protein is formed by the combination of two polypeptide chains, and the structure of homologues have been determined in different conformations depending on the type of ligand it is incubated with. Are those structures crystallisation artefacts or do they exist in solution? Are they artefacts due to protein manipulation in detergent, or do they also exist when the protein is embedded in a membrane? Also, what is the structure of the protein when it is not incubated with any ligands? Probably an equilibrium between the different conformations...