Contribution ID: **155** Type: **Poster**

Modeling of small-angle scattering data from proteins with modifications

Monday, 17 September 2018 17:45 (15 minutes)

For the analysis of solution small-angle scattering data of proteins a wide selection of software such as Crysol [1] exists. In the strict sense they are only designed for pure protein structures. Many proteins, however, come with modifications such as fatty acids, glycosyl groups [2] and bile acids [3].

In a few cases such modifications could be accurately modeled together with their underlying protein structure. E.g. for PEGylated hemoglobin, where the electron density of PEG and hemoglobin are very similar, a bead model for the protein and its modification could be successfully applied [4]. An analytical description of the scattering of the PEG chains (Gaussian chain model) worked well, too [5].

However, modifications often differ significantly from proteins with regard to their electron density and hydrophobicity and cannot always be modeled analytically. To account for the different specific density between the modification and the protein we implemented a model in the freely available "Will It Fit?" framework [6] which allows using different scaling factors for the displaced volumes of the modification- and protein-related atoms. The poster will give an overview on the modeling of proteins with modifications and show first results on solution SAXS data.

[1] J.Appl.Cryst. **28** 768 (1995)
[2] Biophys.J. **96** 153 (2009)
[3] Biochem. **43** 5987 (2004)
[4] Biophys.J. **94** 173 (2008)
[5] Langmuir 2015 **31** 8402 (2015)
[6] J.Appl.Cryst. **46** 1894 (2013)

Primary authors: Dr SCHMIELE, Martin (Niels Bohr Institutet, Københavns Universitet); Mr DREYER, Lasse Sander (Niels Bohr Institutet, Københavns Universitet); Dr BROK, Erik (Niels Bohr Institutet, Københavns Universitet); Dr SMITH, Gregory Neil (Niels Bohr Institutet, Københavns Universitet); Prof. ARLETH, Lise (Niels Bohr Institutet, Københavns Universitet)

Presenter: Dr SCHMIELE, Martin (Niels Bohr Institutet, Københavns Universitet)

Session Classification: Poster session 1

Track Classification: P3 Structure and dynamics in life sciences