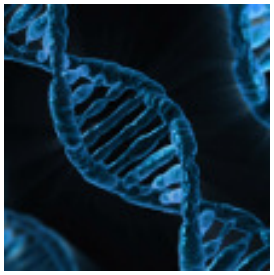

Contribution ID: **50** Type: **Oral presentation**

Contributed talk 2 - Structural characterization of intrinsically disordered protein micelles

Monday 4 June 2018 14:15 (20 minutes)

To obtain a molecular understanding of IDPs, a combined approach of experiments and simulations is useful. Recently we have shown that a coarse-grained model based on the primitive model, that has been used for modelling polyelectrolytes for over 30 years, works well for a range of IDPs where electrostatics governs the intra- and intermolecular interactions [1]. However, some IDPs have the tendency to self-associate into oligomers, also known as micelles. To simulate the self-associating proteins, further development of the model is performed, using the saliva protein Statherin as model system. For this purpose, Statherin has been characterized by small-angle x-ray scattering and the effect of protein concentration, salt and temperature have been investigated. Preliminary Monte Carlo simulation results follow the experimental trends at lower protein concentrations and provide further insight into shape and polydispersity.

[1] C. Cragnell, E. Rieloff and M. Skepö, J. Mol. Biol., 2018, https://doi.org/10.1016/j.jmb.2018.03.006

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