



	Experiment title: Structural and thermodynamical properties of the micelle formation of Statherin: an intrinsically disordered protein	Experiment number: MX-2027
Beamline: BM29	Date of experiment: from: 18 Apr 2018 to: 20 Apr 2018	Date of report: 8 Jan 2020
Shifts: 6	Local contact(s): Bart Van Laer, Mark Tully	<i>Received at ESRF:</i>
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Report:

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Abstract:

Attractive interactions between intrinsically disordered proteins can be crucial for the functionality or, on the contrary, lead to the formation of harmful aggregates. For obtaining a molecular understanding of intrinsically disordered proteins and their interactions, computer simulations have proven to be a valuable complement to experiments. In this study, we present a coarse-grained model and its applications to a system dominated by attractive interactions, namely, the self-association of the salivaprotein Statherin. SAXS experiments show that Statherin self-associates with increased protein concentration, and that both an increased temperature and a lower ionic strength decrease the size of the formed complexes. The model captures the observed trends and provides insight into the size distribution. Hydrophobic interaction is considered to be the major driving force of the self-association, while electrostatic repulsion represses the growth. In addition, the model suggests that the decrease of association number with increased temperature is of entropic origin.