Proposal Code: MX-1814

Proposal Title: New advances in analysis of challenging systems with SAXS measurements

Experiment: BM29; 1 shift (7 hours); 17 February 2016 / 18 February 2016

Users: Melissa Gräwert, Cy Jeffries

Beamline Performance/ Use of Beamtime:

- There were no technical problems during our allocated beam time and we were able to conduct all our planned measurements. We were very satisfied with the beamline support in advance and are excited about the data we were able to collect.

Preliminary results:

- There were three major objectives that we aimed to achieve with our measurements

  i) Data collection for ongoing User projects for finalizing publications/planning further experiments

  ii) Identification of suitable systems that can be used for future time-resolved measurements at the BioSAXS beamline P12 (EMBL Hamburg @ PETRA III, DESY)

  iii) Collection of data for submission as Bench-Mark proteins in the SASBDB (www.sasbdb.org)

- The following data sets were collected

Sample	# data sets (subtracted data)	Comments/Next Steps
i) User Projects		
DNA origami structures	9	Data being used to support proposal at SLAC
phosphoenolpyruvate carboxylase	9	Data being prepared to include in publication
ii) Systems for Time resolved measurements		
Ferritin — pH induced dissociation and re-association	7	Successful dissociation of Apoferritin into smaller oligomeric states (see Figure 1) System will be used in future experiments
Insulin — ligand prevented fibrillation	9	Data sets collected at different pH's in the presence/absence of scavengers Problems with buffer matching
Catalase— pH vs salt induced dissociation	14	Generation of different dissociation models → further analysis to understand these differences

ADH—ligand binding	2	Detectable conformational changes in Apo and Halo structures → currently generating models for both structures
Carbonic Anhydrase—pH induced unfolding	6	Protein trapped in an intermediate unfolded state → models are being calculated to assess the conformational change
iii) Benchmark proteins		
HSA	3	Data collected on dialyzed samples; Good buffer matching for background subtraction; Derived parameters correspond with literature values; In most cases aggregates are negligible; Data will be submitted to the data bank in due course
Cytochrome C	1	
Myoglobin	1	
ß Amylase	1	
GFP	3	

Figure 1: