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1-Deoxy-D-xylulose-5-phosphate reductoisomerase (DXR)

DXR is an enzyme of the MEP pathway (nonmevalonate pathway) of isoprenoid precursor biosynthesis. It interconverts 1-deoxy-D-xylulose 5-phosphate (DXP) and 2-C-methyl-D-erythritol 4-phosphate (MEP). Initial SEC-SAXS experiments showed a stable dimer of DXR in solution. DXR contains two long flexible loops which are not present in any homolog. With EOM we modeled these flexible loops in solution.

<u>HlyA</u>

Hemolysin A (HlyA) is a Repeats In Toxins (RTX) toxin secreted by uropathogenic E. coli and strongly influences the course of urinary tract infections. HlyA lysis several cell types like erythrocytes, epithelial cells and leukocytes but the exact virulence mechanism is still not understood. Initial SAXS data with the shorter constructs of HlyA showed a different folding state, depending on the chosen buffer, but further optimizations are needed.

NADP-ME

We are analyzing proteins from *Zea mays* (maize) that are involved in a biochemical pathway called C4 photosynthesis. Here, we found that a gene duplication of the ancestral gene coding for the plastidic NADP-dependent malic enzyme (NADP-ME) allowed for subfunctionalization of the two resulting proteins. These proteins are termed nonC4-NADP-ME for the protein that kept the original function and C4-NADP-ME for the protein that was recruited to fulfill a function in C4 photosynthesis. The goal is to clarify the oligomeric status of different mutant versions of nonC4-NADP-ME (WT versus mutations) compared to the C4-NADP-ME. Initial SAXS experiments showed that both proteins primary forms a tetramer in solution. Further investigations are needed to proof buffer or concentrations effects on the oligomeric state.

ABC Transporter NsrFP

The ABC Transporter NsrFP conferring resistance in *S.agalactiae*. Since the transporter and NSR which are part of the nsr operon confer resistance against nisin and other lantibiotics it is important to understand the resistance mechanism to find a solution against the increasing resistant bacteria strains. The extracellular domain (ECD) of the NsrFP Transporter was first analyzed in SAXS. Initial evaluations of the experimental SAXS data of NsrFP solubilized in LNMG showed a stable Transporter in solution, but further adjustments of the Detergents are needed.

The Src-homology 3 domain of phosphatidyl-inositol-3-kinase (SH3)

Structural information on amyloid fibrils is crucial for the understanding of their formation mechanisms and for the rational design of amyloid inhibitors in the context of protein misfolding diseases. The Src-homology 3 domain of phosphatidyl-inositol-3-kinase (PI3K-SH3) is a model amyloid system that plays a pivotal role in our basic understanding of protein misfolding and aggregation. SH3 is a stable protein in neutral pH and unfolds under acid pH (~2.5). After heating up the fibrillation starts. Initial SAXS experiments showed that SH3 is a stable monomer at neutral pH and starts unfolding under acetic pH. Furthermore, this unfolding process is time and buffer dependent. Further investigations of these process are needed.

SecYEG

The Sec-pathway consists of the most prominent SecYEG heterotrimeric protein translocating channel, the ATPase SecA and the Foldase SecB. SecA is important because it contacts the translocon and supports the necessary powerstrokes required for protein translocation through SecYEG by ATP hydrolysis. Initial SAXS data of SecYEG reconstituted in Nanodiscs showed a clear difference in comparison to the empty nanodisc.