# ISPyBB extensions for membrane proteins

D. Molodenskiy, D. Franke, H. Mertens & D. Svergun

European Molecular Biology Laboratory, Hamburg Outstation, Notkestrasse 85, D-22607 Hamburg, Germany, **dmolodenskiy@embl-hamburg.de**

The application of small-angle X-ray scattering (SAXS) to structural investigations of transmembrane proteins in detergent solution has become increasingly popular in the last few years [1]. However, its widespread use is hampered by two main obstacles: presence of free micelles of detergent in solution and formation of detergent corona around the hydrophobic region of the protein. To overcome these problems it is possible to i) use online combination of size-exclusion chromatography (SEC) with SAXS and ii) model geometrical shape of the detergent corona by utilizing the ab initio programs MONSA [2] and MEMPROT [3]. Therefore, it is important to develop a data analysis pipeline, facilitating determination of the main SAXS parameters and reconstruction of low resolution models of membrane proteins from the optimized solution. Automated analysis pipelines [4, 5] may be supported in this by integrating the additional data about membrane proteins and detergent systems into the ISPyB (Information System for Protein CrystallographY Beamlines) data system for SAXS [6]. The pipeline may then communicate with ISPyB via dedicated services to retrieve the a-priori information and to submit the analysis results. The ISPyB is currently deployed at EMBL Hamburg (https://ispyb.embl-hamburg.de/ispyb/security/logon.do), ESRF (https://ispyb.esrf.fr/ispyb/security/logon.do) and Diamond Light Source (https://ispyb.diamond.ac.uk/).

The ISPyB extension can be described as follows:

a) Organization of the storage of raw and processed SAXS data from SEC-SAXS runs, as well as complementary data from UV, RI, RALS and MALS. Development of an appropriate graphical user interface (GUI).

b) Calculation and storage of electron density of a protein on base of amino-acid sequence in FASTA format.

c) Implementation of an “Add Additives” button for detergents. Electron density for head/tail group and the buffer is pre-computed from the chemical components.

d) Implementation of a pipeline for automated modelling using the programs MONSA and MEMPROT. Display of the automated analysis results.

e) Modification of automated analysis pipeline: if electron densities are available, then run MONSA instead of DAMMIF. If high resolution *a prior* structure is available in addition to electron density values, then run MEMPROT.

The ISPyB activity is conducted in the frame of WP5 of iNEXT project.

**References**

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