FAST SAXS DATA RECORDING IN SMALL SAMPLE VOLUMES: THE NEW EMBL BIOSAXS BEAMLINE AT PETRA-III

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SAXS is a versatile tool for structural biology studies. It is a unique method for studying structures at low resolution, structural transitions of individual proteins and large macromolecular complexes in solution. The recent novel approaches, in particular, developed at EMBL-Hamburg, tremendously improved resolution and reliability of the technique and significantly enlarged its range of applications and user community. The projected BioSAXS beamline at the upgraded PETRA-III storage ring will allow challenging experiments, which are currently being carried out at the limit of existing SAXS stations in terms of sensitivity and sample consumption. The BioSAXS beamline will combine a high brilliance X-ray beam with low scattering background and energy tunability for anomalous SAXS experiments on biological relevant metals such as Calcium up to Molybdenum. The position of the beamline on a straight section of a 2m canted undulator permits the different modes of operation.

- **Double single crystal monochromator [DCM] mode**
  The DCM mode will be used as standard and allows SAXS experiments in small volumes with a good energy resolution. Also ASAXS will be performed in this configuration.
- **Multilayer monochromator [MLM] mode**
  The high flux of this mode permits time-resolved experiments down to the sub-microsecond level.
- **"Pink beam" mode**
  The use of the raw spectrum of the undulator can be used for ultra high flux experiments such as "few particle" scattering in highly diluted systems. In addition the coherence properties of the X-ray beam can be used.

Beamsizes of 200 x 60 μm^2 and a beam divergence of 40 x 10 μrad^2 will permit SAXS experiments performed on ultra-small sample volumes and high throughput sample screening (HTP mode) in microfluidic lab-on-a-chip systems will be possible. The beamline will further provide a means to characterize complex, potentially flexible macromolecules and mixtures of different oligomeric and functional states, which may not be easily studied by high resolution methods. Cutting-edge experiments, such as kinetic experiments on an ultra-short time scale, anomalous SAXS on biologically relevant atoms/ions, and pilot experiments for future X-FEL applications will become possible. To cope with the large data flow, the expertise of the EMBL SAXS group will also be developed towards an automated data analysis system for on-line construction of structural models, leading to a unique synergy of hardware and software development for SAXS experiments.