Frontier TPS 13A Biological Small Angle X-ray Scattering Beamline

During the past ten years, biological small-angle X-ray scattering (BioSAXS) beamlines were built in nearly all advanced synchrotron facilities worldwide. The impact of BioSAXS beamlines on the research of structural biology has been well demonstrated with the fruitful results published in high-impact journals. To follow this trend, a dedicated, state-of-the-art bio-SAXS/WAXS beamline at TPS (**TPS 13A**) was proposed by Ming-Daw Tsai and Meng-Chiao Joseph Ho in 2014, which develops into a joint project between the NSRRC and Academia Sinica.

This dedicated TPS BioSAXS beamline will outperform the current SAXS beamline, **TLS 23A1**, and aim for advanced bio-structural researches. There are four major operation modes for the new beamline, including :

1. High flux mode for integrated measurements of SAXS/WAXS/UV-Vis-absorption/Refractive-index/Multi-angle-light-scattering (MALS) with an online high-performance liquid chromatography (HPLC) instrument, suitable for exploring biomacromolecular solution structures of a wide length scale and structural kinetics down to microsecond time scale.
2. Ultra SAXS (USAXS) mode for resolving hierarchical structures of bio-machinery assembly up to 1-μm length scale.
3. Anomalous SAXS (ASAXS) mode for metal or mineral distributions (including calcium) in bio organelle or drug carriers.
4. Microbeam SAXS/WAXS (μSAXS) mode for structural mapping of the textures or specific infected cells in natural/synthetic bio-tissues, organelles, or biomaterials.

With these features, the frontier TPS BioSAXS beamline will cover both the needs of academic research and bio-industrial applications.

With a IU24 undulator as the source of 4–23 keV X-rays, the major beamline optical system (**Fig. 1**) contains integrated double crystal/multilayer monochromators (DCM/DMM) for options of high energy resolution mode ($\Delta E/E = 1.5 \times 10^{-4}$) and high flux mode (~$5 \times 10^{14}$ photon/s) at the sample position for time-resolved structural studies. This is followed by a beam focusing system with vertical focusing (VFM), horizontal focusing (HFM), and vertical deflection (VDM) mirrors, located 30 m, 30.6 m and 33 m from the photon source, respectively. The focus point of the K-B system of the high flux mode is set to the end of experimental hutch at ca. 52 m for a maximum sample-to-detector distance of ~12 m.

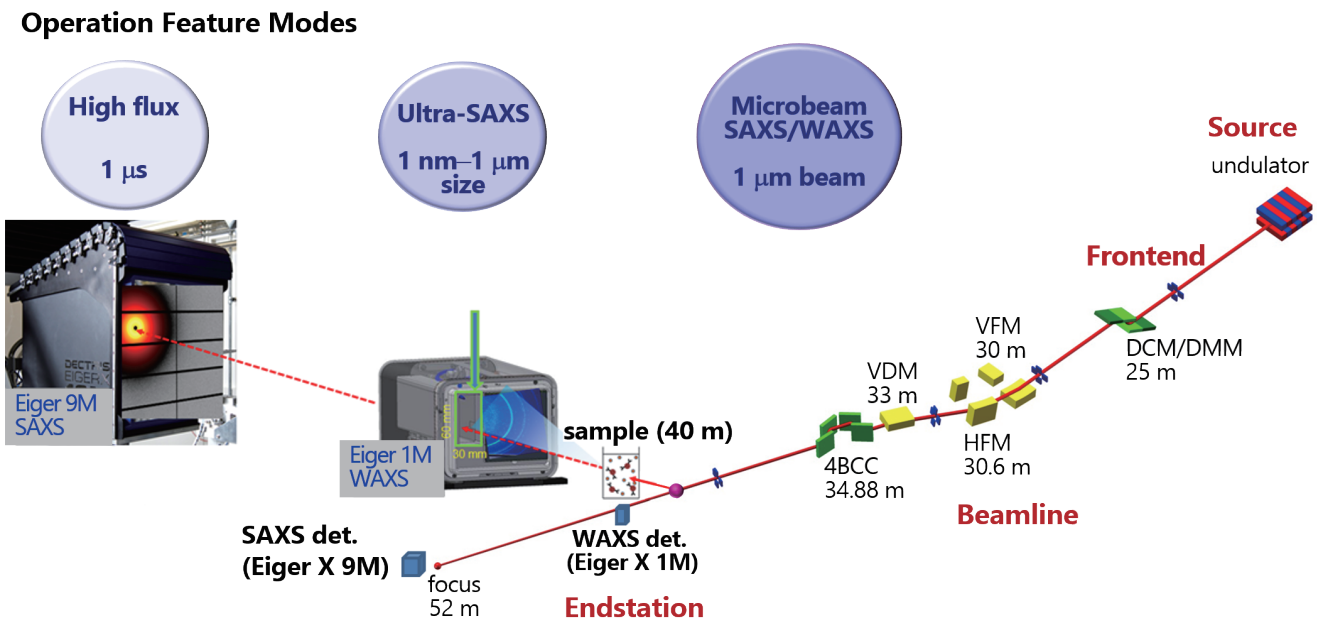

Fig. 1: **TPS 13A**-BioSAXS beamline layout, with the feature operation modes indicated.

USAXS with an ultra-high collimated beam is achieved with the optics utilizing the DCM of the DCM/DMM monochromators, the same focusing K-B system of the high flux mode, and the four-bounce crystal collimator (4BCC) (comprising two sets of horizontal Si-111 or Si-311 double crystals for even better collimation) selectively moved into the beam path, subsequently the beam is leveled by the same VDM. The measured minimum scattering wavevector, $q = 0.0003$ Å^{-1}, allows for the resolving of length scale up to a few micrometers. A set of high precision, high heat-load slits located at 15.5 m from the IU24 source can provide a virtual source of the microbeam down to 1–10 μm. A unique microbeam at the sample area with a small beam divergence is then achieved with ~1 : 1 demagnification optics, comprising the DCM, the second set of K-B focusing mirrors (VFM2 and HFM2 for a focus at the sample position), the 4BCC, and the VDM (**Fig. 1**). The microbeam mode provides scanning SAXS/WAXS structural mapping capability.

For the detecting system, two area pixel-detectors (Eiger X 9M & 1M) are housed in a 12-m long and 1.5-m diameter vacuum chamber for flexible changes of the sample-to-detector distance and low air-scattering background (**Fig. 2**). For integrative measurements with an online sample purifying environment, an HPLC/SAXS/UV-vis/RI/MALS system (**Fig. 3**) is developed for the beamline.

In summary, the frontier **TPS 13A** BioSAXS beamline provides high flux for time-resolved, simultaneous SAXS/WAXS down to 1 μs for biological structures and structural kinetics, microbeam SAXS/WAXS for structural mapping, and USAXS for hierarchical structural assemblies up to 1 micrometer length scale. With these unique features, the **TPS 13A** BioSAXS beamline provides a new platform to domestic and international users for innovation and breakthrough researches in structural biology. (Reported by U-Ser Jeng)

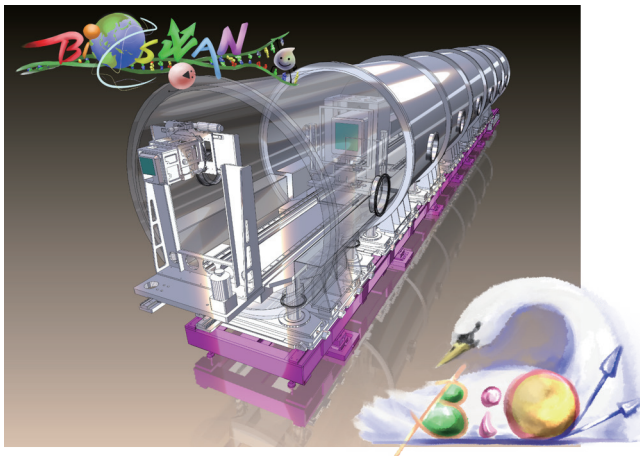

Fig. 2: The feature detecting system of the **TPS 13A** BioSWAN beamline for BIOlogical Small- and Wide-ANgle X-ray scattering.

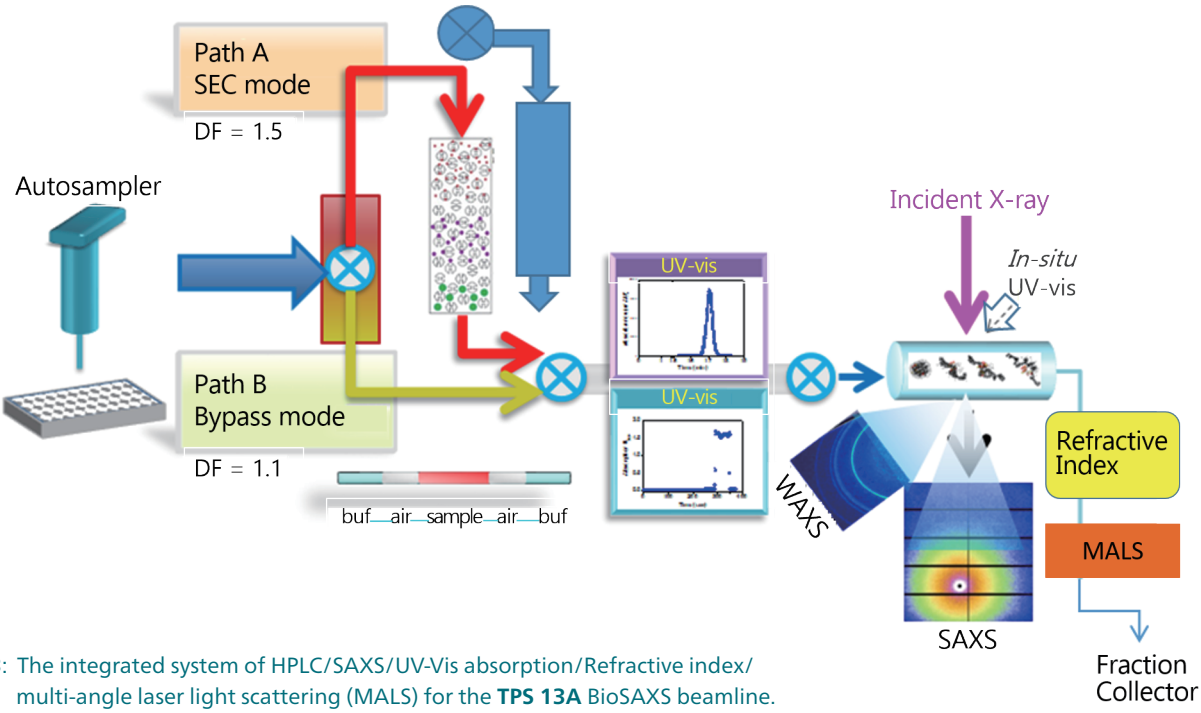

Fig. 3: The integrated system of HPLC/SAXS/UV-Vis absorption/Refractive index/multi-angle laser light scattering (MALS) for the **TPS 13A** BioSAXS beamline.