EMBL is constructing an integrated facility for structural biology at PETRA III (http://petra3.desy.de), the new third generation synchrotron at DESY in Hamburg. At the center of the facility will be three beamlines for life science applications. Two beamlines (MX1, MX2), will cover a wide range of challenging applications in macromolecular crystallography, while the third beamline (BioSAXS), will provide excellent conditions for small angle X-ray scattering on solutions of biological macromolecules. All major components have been purchased and the construction work is progressing. On the BioSAXS beamline, we expect ‘first beam’ during the summer of 2010; the first crystallography beamline should start operation in autumn of 2010.

### Figure 1
Schematic view of the EMBL beamlines on PETRA III. All three beamlines receive X-rays from U29 undulators (light grey boxes), and will be tunable using a ‘PETRA III’ double crystal monochromator with a Si-111 crystal (black boxes) as the first optical element. On the crystallographic beamlines, Si-311 crystals (medium grey boxes) will also be available for spectroscopic applications. On the BioSAXS and MX2 beamlines the addition of multilayer monochromators (blue boxes) and white beam mirrors (red boxes) is planned at a later stage for high-flux and ‘pink-beam’ applications. On all three beamlines the focusing elements will consist of adaptive X-ray mirrors in KB-configuration (green boxes). The focusing mirrors will be located at different positions between the X-ray source and the sample (red crosses) thereby producing the desired beam properties at the sample position.

The **X-ray optics** of the three beamlines are designed such, that the uniquely low emittance of the PETRA III storage ring is translated into optimum beam properties for different applications (Figure 1). For the **BioSAXS beamline**, a **virtually parallel X-ray beam** is foreseen – this is obviously only possible with a relatively large focal size. At the other extreme, for achieving the best conditions for **micro-**
crystallography on beamline MX2, focal sizes of less than 5 micron are planned – again such small focal spots can only be achieved by accepting a relatively large beam divergence. The optical parameters for the second crystallographic beamline, MX1, are chosen to be in between those of the other two beamlines providing a compromise between focal spot size and beam divergence – this beamline will offer optimum conditions for resolving many diffraction orders (i.e. for large unit cells and/or high resolution data collection) on small crystals. All three beamlines will be tunable over a wide wavelength range to optimize the collection of anomalous signals.

The main application of the BioSAXS beamline will be small-angle X-ray scattering experiments on solutions of biological macromolecules. Robotized liquid handling will allow experiments to be performed with smaller sample amounts than those presently used, and with reduced cycling times between samples. Other sample environments will be available on request. To extend the range of applications into non-solution experiments, EMBL has formed a partnership with the GKSS who will be in charge of 15% of the beamtime on the BioSAXS beamline. GKSS is contributing a highly flexible and automatized vacuum flight tube that will allow quick changing of the sample-to-detector distance and, if needed, also the detector. A PILATUS 2M pixel-array detector to be placed on the BioSAXS beamline was delivered in January 2010 and is currently being commissioned.

Both crystallographic beamlines will be equipped with high-precision multi-axis diffractometers and state-of-the-art detectors. At present, we have already assembled a substantial part of one of the future PETRA III endstations on the EMBL Wiggler beamline BW7A on the DORIS storage ring. This prototype consists of an MD2 diffractometer including a mini-kappa goniostat and a RAYONIX 225HE mosaic CCD detector integrated in the TINE control system and controlled by the user via an adapted version of the ESRF-developed mxCube graphical user interface. This prototype setup was successfully used for data collection by the participants of the M2M crystallography workshop that took place at EMBL-Hamburg in November of 2009.

For the automatic mounting of crystals the ‘MARVIN’ sample changer will be used. The MARVIN-system was developed in-house at EMBL Hamburg. It is based on an industrial 6-axis robot and features a large capacity cryogenic dewar (150 SPINE pins) and cycle times of less than 30 seconds. A prototype of this system is available on the EMBL beamline BW7B at DORIS. The system underwent successful intense stress-testing last autumn, whereby for example one single crystal was mounted, automatically centred in the X-ray beam, exposed to X-rays, and dismounted more than 50 times without any detectable ice formation or change in diffraction quality of the sample.

The beamlines will be complemented by facilities for biological sample preparation and characterization comprising various biophysical techniques. These facilities will be located in laboratories situated in a newly constructed extension of the PETRA III experimental hall in the immediate vicinity of the beamlines (Figure 2). The construction of the building is near to completion – in fact, the EMBL@PETRA3 team has already moved into the offices in the new building in March. The laboratories should start operation before the summer. Most notably, the high capacity high-throughput crystallization facility (http://www.embl-hamburg.de/facilities/htpx/) currently located on a different part of the DESY Campus, will be moved into the extension building to also be in close vicinity of the beamlines. Unfortunately, this will result in an interruption of the crystallization services later this year – please check the website of the facility for an up-to-date schedule.
Figure 2: 3D-CAD rendering of the EMBL beamlines at PETRA III. The BioSAXS beamline is located in sector 8, the two macromolecular crystallography beamlines, MX1 and MX2 in sector 9 of PETRA III. The laboratories for sample preparation and characterization are situated in an annex building to the PETRA III experimental hall, here indicated in green.

Building on the success of the existing computing services such as Auto-Rickshaw (http://www.embl-hamburg.de/Auto-Rickshaw/) and ATSAS on-line (http://www.embl-hamburg.de/ExternalInfo/Research/Sax/atsas-online/), on-site data evaluation and structure determination will be enabled by a state-of-the-art computing infrastructure.

We are working hard to greet the first ‘friendly users’ to our new beamlines in 2010 – we’ll keep you posted here and elsewhere. If you have ideas on how to challenge the new beamlines, please contact us at petra3(at)embl-hamburg.de.