

FA5-MS04-P01**Macromolecular Crystallographic Studies and Their Relevance to SESAME.**

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Macromolecular Crystallography is a powerful technique for 3D structural analysis of biological samples (enzymes, proteins, lectins, viruses, etc.). Enzymes are large and complex protein molecules consisting of intertwined chains of amino acids. They are formed within the living cells including microscopic fungi and bacteria. The inability of the plant and animal enzymes to meet current demands such as working in extreme conditions has led to an increasing interest in microbial enzymes. Microorganisms represent an excellent source of enzymes owing to their broad biochemical diversity and their susceptibility to genetic manipulation. In the first phase of our study, alkaliphilic and halo-tolerant *Bacillus* sp. strains were isolated and tested for three industrially important enzymes which are Amylase, Cellulase and Xylanase [1]. The isolated bacterial strains will be cultivated and propagated for enzyme production. Purification of the enzymes will be carried out by classical purification methods. The biochemical properties of the enzymes, such as pH optima and stability, temperature optima and stability, molecular weight, effect of some inhibitors will be determined and be compared to other reported enzymes [2]. In the second phase of our study with relevance to SESAME, after crystallization of the enzymes, the X-ray diffraction experiments (SAD/MAD) will be performed in a short time of period and less costs. This will provide us basic information regarding the structure functions like active site or catalytic domain and possible roles of specific residues in molecule. This will also be of benefit to compare with other enzymes and the possibilities or knowledges for site directed mutagenesis for better enzymes in protein engineering studies. With the SESAME Synchrotron coming online, our research program will become a multidisciplinary facility in which biologists, chemists, physicists and medical scientists will collaborate to carry out the researches in the field of structural biology.

[1] Aygan A., Arıkan B., *International Journal of Agriculture & Biology*, **2008**, 10, 369. [2] Aygan A., Arıkan B., Korkmaz H., Dinçer S., Çolak Ö., *Brazilian Journal of Microbiology*, **2008**, 39, 547.

Keywords: macromolecular synchrotron X-ray crystallography; enzymes

FA5-MS04-P02**EMBL Macromolecular Crystallography Beamlines @ PETRA3 – Hamburg Germany.**

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The European Molecular Biology Laboratory is building an integrated infrastructure for life science applications at PETRA III, the new 3rd generation synchrotron at DESY in Hamburg. Two beam lines will be devoted to macromolecular crystallography and a third beamline to small angle X-ray scattering on solutions of biological macromolecules.

The beam lines target challenging applications in crystallography of large macromolecules and complexes of low availability (including those expressed from natural sources), that are difficult to crystallize and derivatize.

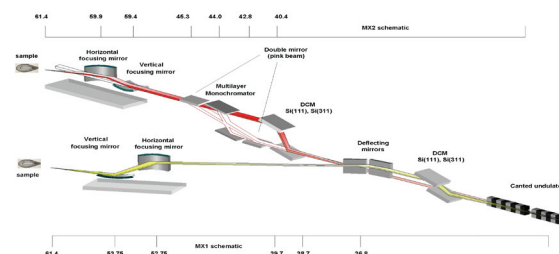
The beamlines will be equipped with state-of-the-art sample handling technologies facilitating high-throughput handling of small samples.

The two MX beamlines will be clustered at one end of the experimental hall using the last straight sector 9. The straight section contains two PETRA-III standard 2-meter undulators with a canting angle of 5 mrad. The optical design of the beam lines has been finalized to achieve sufficient angular and spatial offset between the macromolecular crystallography beam lines.

Beamline MX1 will be tunable over a large energy range (5(4)–17 keV) to allow crystallographic data acquisition at absorption edges of a broad range of elements for experimental phase determination. This beam line will also provide a very low beam divergence (<0.2mrad) and variable focus size (20-100 µm) to adapt to challenging biological projects. Crystallographic information will be complemented by in crystallo spectroscopies.

Beamline MX2 will be tunable (7-35 keV) and optimized for micro-focusing down to <5 µm (1-2 with add-on optics) to allow data acquisition on extremely small crystals of biological macromolecules.

Special applications will be pink beam Laue diffraction and ultrahigh resolution - high energy applications.



Keywords: macromolecular X-ray crystallography; microcrystals; phasing