MS02-P103 LATE | LONG-WAVELENGTH NATIVE SAD PHASING AT BL13-XALOC

ENABLED BY THE PRESENCE OF AN HELIUM CONE

Calisto, Barbara (ALBA synchrotron, Barcelona, ESP); Gil-Ortiz, Fernando (ALBA Synchrotron, Cerdanyola del Vallès, ESP); Carpena, Xavier (ALBA Synchrotron, Cerdanyola del Vallès, ESP); González, Nahikari (ALBA Synchrotron, Cerdanyola del Vallès, ESP); Álvarez, José María (Alba Synchrotron, Cerdanyola del Vallès, ESP); Valcárcel, Ricardo; Ávila, José (Alba Synchrotron, Cerdanyola del Vallès, ESP); Villanueva, Jorge (Alba Synchrotron, Cerdanyola del Vallès, ESP); Juanhuix, Judith (Alba Synchrotron, Cerdanyola del Vallès, ESP); Boer, Roeland (Alba Synchrotron, Cerdanyola del Vallès, ESP)

The MX beamline BL13-XALOC (ALBA synchrotron, Barcelona, Spain) possesses a high-intense collimated beam and allows tailoring the beam size to the size of the sample, most commonly micrometer-sized crystals, by defocusing the beam thus minimizing the scattering background.

Native phasing for determining crystal structures of novel macromolecules is a very promising technique as it exploits the small anomalous signal from naturally occurring elements (atomic number < 20). In particular, measuring the anomalous signal from sulfur at long wavelengths is very appealing because the macromolecules or the crystals need no further derivatization. However, at long wavelengths, X-ray absorption by air and sample dramatically hinders data collection. To partially overcome the air absorption drawback at BL13-XALOC we designed and commissioned a removable Helium Cone (HeC) consisting on a fixed-size chamber filled with helium gas. Comparison of data collected on tetragonal crystals of Hen egg white lysozyme at 2.7 Å (respective energy 4.6 keV) in absence or presence of the HeC highlights the benefit of measuring data for S-SAD phasing in a helium-enriched atmosphere and its most striking effect is observed in the S-substructure determination. The fully-automatic crystal structure determination of lysozyme collected at 2.1 Å (respective energy 6.0 keV) is also discussed.

For more challenging cases we urge MX beamline users to fully and rationally use the advanced data collection strategies available at BL13-XALOC. These include workflows designed by Global Phasing Ltd, and locally implemented strategies such as inverse-beam, low dose, multiple orientations and multiple crystal averaging.