

## **Development of a High-throughput Structure Determination Pipeline at BM14**

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The basic operations to be performed for the collection of MAD and SAD data from protein crystals are well established and have been implemented successfully at beamlines across the world. There is now, however, intense activity aimed at revolutionizing the possibilities via a series of improvements, centered around (i) the mechanical aspects of automation, improved precision and improved visualization and (ii) the software aspects of automation and integration.

BM14 is a tunable bending magnet beamline at the ESRF operated by the UK research councils in collaboration with the EMBL Grenoble outstation. A high-throughput pipeline for structure determination by SAD and MAD phasing is being developed through our participation in the BBSRC e-science project e-HTPX ([www.e-htpx.ac.uk](http://www.e-htpx.ac.uk)).

An overview of the hardware and software implemented at BM14 for automation of macromolecular data collection will be presented. In particular, software developments which allow the user to keep track of the sample from their home lab to and from the beamline, as well as management of experimental data acquired, through the development of an easy to use beamline Laboratory Information Management System (LIMS) will be described. Our experiences in the use of SAD phasing with naturally occurring light atoms, such as sulphur and manganese, and their application for use in a high-throughput structure determination pipeline are summarized.

**Keywords: MAD phasing, automation, LIMS**