

## Poster Presentation

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#### *The use of workflows for macromolecular crystallography experiments at the ESRF.*

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The high performance of modern synchrotron facilities means there is an increasing reliance on automated data analysis and collection methods. The EMBL and ESRF are actively involved in designing and implementing such automated methods. However, as these methods are evolving there is also a need to continually integrate newer and more sophisticated data analysis and collection protocols with experimental control. This integration often poses a challenge, requiring a high level software environment to automatically coordinate beamline control with data acquisition and analysis. This is why we have extended the Eclipse RCP version of the workflow tool Passerelle into a user friendly GUI for experiment design by scientists and programmers [1], which is now part of the Data Analysis WorkbeNch (DAWN) collaboration (<http://www.dawnsci.org>). The execution of several complex workflows using this technology are now fully integrated in the new version of MxCuBE [2] and deployed on the ESRF macromolecular crystallography beamlines. Here, I will present their current implementation and the data quality improvements that can be achieved. In particular we have developed automated crystal re-orientation workflows that can improve the success of ab initio phasing experiments and help mitigate against radiation damage effect [3]. Other protocols implemented include a 3D diffraction based centring routine, a dehydration protocol and the automated measurement of a crystals radiation sensitivity. Lastly I will present our future plans for other new advanced diffraction based workflow routines, including automated crystal screening and data collection protocols.

[1] Brockhauser, S., Svensson, O., Bowler, M. W., et al., *Acta Cryst. D68*, 975-984 (2012)., [2] Gabadinho, J., et al. *J. Sync. Rad.* 17, 700-707 (2010)., [3] Brockhauser, S., Ravelli, R. B. G., & McCarthy, A. A. *Acta Cryst. D69*, 1241-1251 (2013).

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