Getting better data diffraction: on-line crystal dehydration

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Despite the success of macromolecular X-ray crystallography (MX) and enormous advances in the field, one of the major hurdles still to be bypassed is the availability of well-diffracting crystals. As the goals of the MX projects become more challenging, with an increasing number of membrane proteins and huge macromolecular complexes being studied, large solvent content and loose packing of the molecules are becoming more frequent and the resulting diffraction quality of the crystals is often insufficient to achieve structural solution.

There are a number of post-crystallisation treatments that have been described so far to improve X-ray data including soaking with different compounds, cross-linking, crystal annealing and dehydration to mention a few examples. Among them, dehydration is one of the most frequently reported methods to have beneficial effects on diffraction. Although crystal dehydration can be performed manually in a step-wise and time-consuming fashion, currently there are devices that can perform the same treatment with finer control of the dehydration process. Added to this, such devices are coupled with data collection to provide a direct monitoring of the dehydration effect on the diffraction quality of the crystal.

Adaptable to a variety of synchrotron beamlines, the HC1 device developed at the EMBL Grenoble is currently in operation at synchrotron sources world-wide (ESRF, DLS, MAX-lab, CLS, and BESSY). The HC1 device is fully portable and easy to install on a standard beamline without disturbing any of the other equipment (Sanchez-Weatherby et al., 2009). It requires minor input from the end user and its GUI-oriented architecture allows a continuous monitoring of the progress of the experiment. In spite of being in its infancy, on-line crystal dehydration with the HC1 has proven to be a powerful means to extract the most of crystals, with the possibility of freezing dehydrated crystals for later data collection on site (Russi et al., 2011). To give an account of the capabilities of the HC1, a selected set of remarkable outcomes from the device under operation at the ESRF since 2009 will be presented in the talk.

Sanchez-Weatherby, J., M.W. Bowler, J. Huet, A. Gobbo, F. Felisaz, B. Lavault, R. Moya, J. Kadlec, R.B.G. Ravelli, and F. Cipriani, 2009. Improving diffraction by humidity control: a novel device compatible with X-ray beamlines. Acta Cryst. D 65: 1237-1246.

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