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In-house X-ray single crystal diffraction as a tool for efficient synchrotron data collection

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Abstract content

The benefits of synchrotron X-ray diffraction experiments are many, but involve traveling and many logistic issues. For macromolecule crystallographers there is a significant risk that the samples taken to the beamlight are salts or low-resolution diffracting crystals. Several technologies are available to screen crystals, from simple such as dye exclusion, smashing the crystal, X-ray equipment to diffract directly over the crystal plate, etc. However, availability of a single crystal diffractometer makes a difference in terms of the learning experience and opportunity to collaborate with chemists and biologists as well. CIAD has been awarded a diffractometer with a high-intensity microsource Cu-Kα, goniometer with kappa geometry, low temperature system and a CMOS detector. After several months of continuous operation, protein crystals have been diffracted up to 1.6 Å and more than a dozen small molecule structures have been determined. Graduate courses in structural biology (CIAD) and supramolecular chemistry (Universidad de Sonora) will benefit as practical session will be possible. In the near future, the throughput of new macromolecule structures will increase, either from in-house data collection or from optimized crystallization conditions proved to produce good diffracting crystals to be taken to the beamline. Moreover, the area of small molecule and crystal engineering will start as chemists and material scientists have the opportunity to characterize their materials. Therefore, availability of in-house diffraction does not compete with synchrotron data collection, but makes more focused and efficient the scarce beamline time available

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Summary

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