

POWDER DIFFRACTION METHODS IN MACROMOLECULAR CRYSTALLOGRAPHY

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Despite the fact that protein crystallography has been subject to the availability of good quality single crystals, recent reports on the refinement and solution of small protein structures from powder data establish the validity of this technique as a complementary probe. Rapid precipitation of polycrystalline samples and acquisition of superior quality synchrotron X-ray powder diffraction data permit the in-situ exploration of crystal growth, radiation damage, time and temperature effects as well as drug/protein interactions [1]. In the present case, issues which are going to be discussed are: **(a)** structure refinement of selected proteins [1, 2] **(b)** determination of microstructural characteristics (size/strain) from powder data [3] **(c)** successful cryocooling for dramatic reduction of radiation damage **(d)** preparation of heavy atom derivatives and **(e)** high throughput automated data collection (robotic sample changer) leading to the construction of phase diagrams [3]. In the present work, we aim in establishing the full potential of powder diffraction technique in the research of macromolecular systems by careful assessment of various instrumental configurations and recent progress in data analysis.

[1] Von Dreele, R. B. (2005). *Acta Cryst.* **D61**, 22-32. [2] Margiolaki I. et al. *Acta Cryst.* **D61**, 2005, (In Press); See also: ESRF Scientific Highlights, 2004, p. 24. [3] Basso S. et al. (In Preparation).