

## POWDER DIFFRACTION STUDIES OF POLYCRYSTALLINE PROTEIN

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Although historically powder diffraction was primarily a tool for phase identification, recently advances in instrumentation and software have allowed it to probe the structures of increasingly complicated molecular systems including proteins (1). We have been investigating the feasibility of the use of powder diffraction to investigate protein structure using the high resolution powder diffraction beamline, ID31, at the ESRF.

The use of cryocrystallography is standard practice in the field of single-crystal protein diffraction to reduce radiation damage during the long scans required to obtain the highest-resolution data. It had previously been reported that protein powder diffraction under cryoconditions results in a loss of crystallite quality (2), and this provided the impetus for our study on the use of cryoprotectants to maintain data quality under these conditions.

Several different protein systems were examined with various symmetries and unit cell sizes. It would appear that powder diffraction would not be an ideal tool for structural studies of large proteins since the high angle data become indistinguishable from the background due to the problem of powder averaging. On the contrary, for small proteins with a molecular mass of less than 20kD, high quality data can be collected using synchrotron radiation with a resolution limit of around 3Å. Indexing and Rietveld refinement can also be achieved routinely in favourable cases using the popular powder diffraction software packages CRYSFIRE and GSAS (3).

### References

(1) R. B. Von Dreele, P. W. Stephens, G. D. Smith and R. H. Blessing  
*Acta Cryst.* (2000) **D56**, 1549-1553; R. B. Von Dreele, *Acta Cryst.* (2001). **D57**, 1836-1842.

(2) J. Wright  
*Acta Cryst.* (2002). **A58** (Supplement), C213.

(3) Available from CCP14: <http://www.ccp14.ac.uk>