Protein Powder Diffraction: why Bother?

Christopher Gilmore, Wei Dong, *Department of Chemistry, University of Glasgow, Glasgow, UK.* E-mail: chris@chem.gla.ac.uk

This discussion of powder protein powder diffraction looks at what is currently achieved with small molecule powder data, and low resolution single crystal protein crystallography and asks what techniques from these areas can be translated into the world of protein powders:

1. Qualitative PXRD: Pattern matching - can we classify and match patterns using the full pattern profile and not just the peaks as in the SNAP-1D [1] and PolySNAP [2] computer software, and can this information be used as an aid to crystallization?

2. Quantitative PXRD: Can we identify components in powders in a quantitative mode using full powder profiles as used in the SNAP-1D/PolySNAP software?

3. Unit Cells with protein PXRD: Can we index poor quality patterns? Can using the full profile help? What about brute force methods using grid computing techniques?

4. Single crystal low resolution protein diffraction can give the molecular envelope; can this be achieved with powder data?

All these issues will be discussed with examples where possible.

[1] Gilmore C.J., Barr G., Paisley J., *J. Appl. Cryst.,* 2004, **37***,* 231-242. [2] Barr G., Dong W., Gilmore C.J., *J. Appl. Cryst,* 2004, **37**, 243-252. [3] Von Dreele R.B., *Acta Cryst.,* 2005*,* **D61**, 22-32. [4] Gilmore C.J., Wright J., Fitch A., *Transactions of the Amer. Cryst. Assocn.,* 2002*,* **37,** 113-123.

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