Molecular envelopes from protein powder diffraction data

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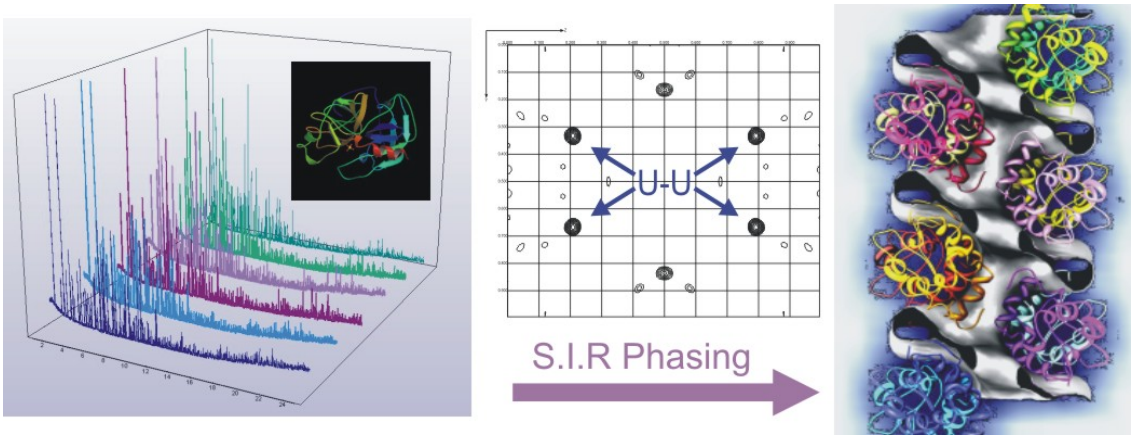
The preparation of single crystals suitable for x-ray analysis is frequently the most difficult step in structural studies of proteins. Recently, an interest has grown for protein powder diffraction, and the method is becoming be well-established in the field of structure refinement and molecular replacement [1,2,3]. However to fully probe the potential of the technique, there is a need to assess the quality of the structural information that can be extracted de novo from powder protein data. With the aid of two examples, it is shown that de novo solution of the crystallographic phase problem can be achieved at low resolution using microcrystalline powder samples via the single isomorphous replacement method. With synchrotron radiation and optimised instrumentation, high-quality powder patterns have been recorded from which it was possible to generate phase information for structure factors up to 6 Å resolution. pH- and radiation-induced anisotropic lattice changes were exploited to reduce the problem of overlapping reflections, which is a major challenge in protein powder diffraction. The resulting data were of sufficient quality to compute molecular envelopes of the protein molecule and to map out the solvent channels in the crystals, which are essential structural data for the characterization of microcrystalline proteins as novel mesoporous materials. The possible improvements of the method, for example using Multiple Isomorphous Replacement, are discussed.



References

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