MS09-2-6 Modelling Diffuse Scattering in Protein X-Ray Crystallography using Internal Motion Models #MS09-2-6

J. Van Der Horn [1], L. Kroon-Batenburg [1]
[1]Utrecht University - Utrecht (Netherlands)

Abstract
Protein structures obtained through X-ray crystallography represent an average conformation of all protein molecules in a crystal. In reality, proteins are very flexible and dynamic. Even in a crystal, they can adopt many different conformations. Clues about their disorder can be captured during X-ray diffraction experiments, in the form of diffuse scattering. The observed diffuse signal can be attributed to correlated motions on various scales. Here, we make the distinction between rigid-body motions and internal motions, like those of secondary structures and single residues. We devised a model which can selectively simulate various types of internal disorder and calculate the diffuse signals associated with them. It is shown that the primary features of the total diffuse signal be attributed to rigid-body motions, whereas the internal motions mainly affect the contrast of the signal.

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