Structure Refinements of Protein-ligand Complex by the Maximum Entropy Method

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It is important to have detailed structural information of protein crystal to understand functions of a protein. Particularly, interaction between protein and ligand molecule is a fundamental aspect of protein crystallography. The experimental techniques of protein crystallography have been very rapidly improved due to, for example, advent of Synchrotron Radiation source. Hence, it becomes rather usual to collect fairly good quality data set for a protein crystal. The analytical techniques for structure determination of protein crystals have also drastically improved. However, the structure refinement method still remains in an old fashion, i. e. Fourier method.

For materials with simple structure, more sophisticated method called the Maximum Entropy Method (MEM)[1] is now commonly used to obtain accurate electron density distributions. In order to demonstrate the ability of MEM for structure refinement in protein crystallography, the complex of ribose-5-phosphate isomerase(Rpi)[2] between both ribose 5-phosphate(R5P) and arabinose-5-phosphate (A5P) are refined by MEM. Isomerization to ribulose-5-phosphate proceed only for R5P but not for A5P. The MEM density maps revealed very clearly the structural differences between Rpi/R5P and Rpi/A5P.

[1] Sakata M., Sato M., *Acta Cryst*., 1990, **A46**, 263. [2] Hamada K. *et al*., *J. Biol. Chem.,* 2003, **278**(49), 49183.

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