Poster Presentation

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Application of maximum entropy method to neutron protein crystallography

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Hydrogen atoms or hydrogen bonds play important roles in protein functions. Neutron diffraction is very powerful tool to detect hydrogen atoms. However it is often obtained rather poor resolution data compared with X-ray data due to weak neutron source intensity and large incoherent scattering from hydrogen atoms. The maximum entropy method (MEM) is noble method to obtain high resolution electron or nuclear density distribution from even limited number of diffraction data. The MEM has been applied to not only X-ray data of small molecules but also those of proteins. For the application to neutron data, so far, only small molecules are reported. When preliminary application of the MEM to 1.1 Å resolution partially deuterated neutron protein data (Protein Data Bank ID : 4fc1) is carried out, most of hydrogen and deuterium atoms are observed (Fig. 1). Since this resolution is unusually high, it is of interest that ability of the MEM for usual or low resolution data. In this paper, effects of resolution and data quality for the MEM are examined. Large deuterated crystals are necessary for neutron experiment to reduce incoherent scattering from hydrogen atoms and to improve data resolution. However deuterated condition is not usual for biomolecules. If no deuteration is need for low resolution data by using the MEM, it would be able to observe biomolecules as they are.

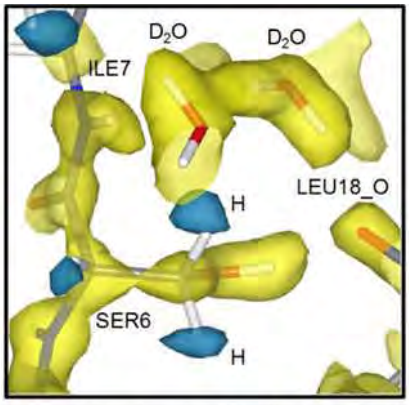

Fig. 1 Nuclear density distribution by MEM with an isosurface level of +/– 1.5 fm/Å^3.

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