Neutron protein crystallography (nPX) development: reaching yet higher molecular weight capability

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The unique property of the neutron scattering interaction with deuterium being as strong as C, N, O means that medium resolution crystal structure studies can discern the hydrogenation and hydration of a protein structure. We have used the Institut Laue Langevin (ILL) LAue DIffractometer 'LADI' to compare with Ultra-high resolution X-ray PX to define such details of the lectin concanavalin A (Habash et al 2000 Acta Cryst) and performed a 15K nPX analysis of concanavalin A structures between 15K and 293K (Blakeley et al 2004 PNAS). This latter study also brings time-resolved freeze trapping nPX studies as a potential for the future. New nPX instruments at LANSCE-USA, the ILL, ISIS 2 UK (proposed), SNS-USA (under construction) and SNS-Japan (under construction) will further expand the capabilities including into yet higher molecular weight protein complexes and protein DNA complexes. We will review our contribution to these developments and also we offer new simulations addressing the category of non-crystallographic symmetry cases where we show that even higher molecular weight can be examined in nPX studies of deuterium atom placement.

[1] M P Blakeley, M Cianci, J R Helliwell and P J Rizkallah " Synchrotron and neutron techniques in biological crystallography" Chem Soc Reviews (2004) 548-557.

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