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 [1] and performed a 15K nPX analysis of concanavalin A structures, then a 15K to 293K comparison [2]. This latter study [2] 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 the nPX developments [3] 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.

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