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A Plastic Explosive-Degrading Enzyme[1]

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The enzyme nitroreductase catalyzes reduction of high explosives such as TNT and RDX. Although a well-resolved $^{1}H^{15}N$-HSQC is obtained at 37 °C, the HSQC at 4 °C is concentrated between 7.5 and 8.5 ppm and is comprised of sharp overlapped peaks. Thus, it appears that the protein denatures upon cooling. However, the non-covalently-bound FMN cofactor is not released at the lower temperature. Similarly, ultra-violet CD spectroscopy shows that the protein retains essentially full secondary structural content at 4 °C. Thus, it appears that nitroreductase exists as an ensemble of rapidly interconverting loose structures at lower temperature, only adopting a single long-lived structure above 20 °C. Both saturation transfer from water and solvent proton exchange measurements, demonstrate that resonances of the poorly-dispersed spectrum represent protons closer to water, and in faster exchange with it. Thus we propose that the single well-defined structure is favored entropically, by release of water molecules that solvate the protein at 4 °C. We propose that the loosely structured state plays a role in accommodating binding of diverse substrates.

[1]In collaboration with Peng Zhang, University of Kentucky