Asymptotic analysis of quasielastic neutron scattering data from human Acetylcholinesterase reveals subtle dynamical changes upon ligand binding

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We report on the application of a new, "model-free" approach to analyzing quasielastic neutron scattering spectra from protein powder samples [1] to previously collected QENS data [2] from the enzyme Human Acetylcholenisterase (hACE) with and without the non-covalently bound inhibitor HuperZine A. Our QENS analysis is based on the fact that the form of the quasielastic line for small frequencies can be directly related to the relaxation of the intermediate scattering function for long times. To account for the multiscale dynamics of proteins, we describe the relaxation by a stretched Mittag-Leffler function, which displays slow power law decay for long times and a broad spectrum of relaxation rates. Using Zwanzig's model for diffusion in a rough potential [3], we translate the relaxation rate spectrum into a distribution of energy barriers of the protein energy landscape of global harmonic form [4]. Our analysis reveals that binding of Huperzine A increases the atomic motional amplitudes and slightly slows down its internal diffusive motions. This can be visualized in terms of a softening and roughening of the potential energy surface. A corresponding normal mode analysis is presented and discussed.

References:

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