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Using polarisation analysis to compare the dynamics of protonated and per-deuterated samples of proteins.

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Neutron scattering data collected from biological systems are mostly analysed with classical approaches; however, it has already been proven for instance that purely quantum-based effects such as tunnel effects can explain the enhancement of information rates in enzyme catalysis. Our approach is to study both a per-deuterated sample of the green fluorescent protein (dGFP) and a fully protonated sample (pGFP) hydrated in D_2 O, in order to evidence signature of quantum effects thanks to the difference of mass of the two isotopes of hydrogen nuclei combined to supposedly equivalent dynamics. However, it quickly raised more fundamental questions about how careful one has to be when analyzing per-deuterated samples.
We performed QENS experiments on the TOF spectrometer IN5 at ILL. We describe the subdiffusive motion of hydrogen atoms in the protein with fractional Brownian dynamics, using a Mittag-Leffler function as relaxation function. It yields a 3-parameter model for dGFP dynamics that catches the importance of the dynamics of water through a heterogeneity parameter (α), the impact of water within the time window with the relaxation time parameter (τ) and the impact of coherent scattering from both water and the protein through the shape of the Elastic Coherent Scattering Factor obtained with the pseudo-EISF parameter (EISF). This corroborates with static studies combined with polarized neutrons carried out on the diffuse diffractometer D7 at ILL. Therefore, in order to correctly compare the dynamics of deuterium to the dynamics of hydrogen it is paramount to access only the incoherent contribution of scattering for our dynamic studies using QENS combined to polarization analysis.
Polarization analysis applied to QENS at 310K and 220K are planned for October on LET spectrometer at ISIS. To our knowledge this is the first time that this type of studies is applied to biological macromolecules, although the interest for polarized neutrons has already emerged.

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