Dynamical coupling of intrinsically disordered proteins and their hydration water: comparison to folded soluble and membrane proteins

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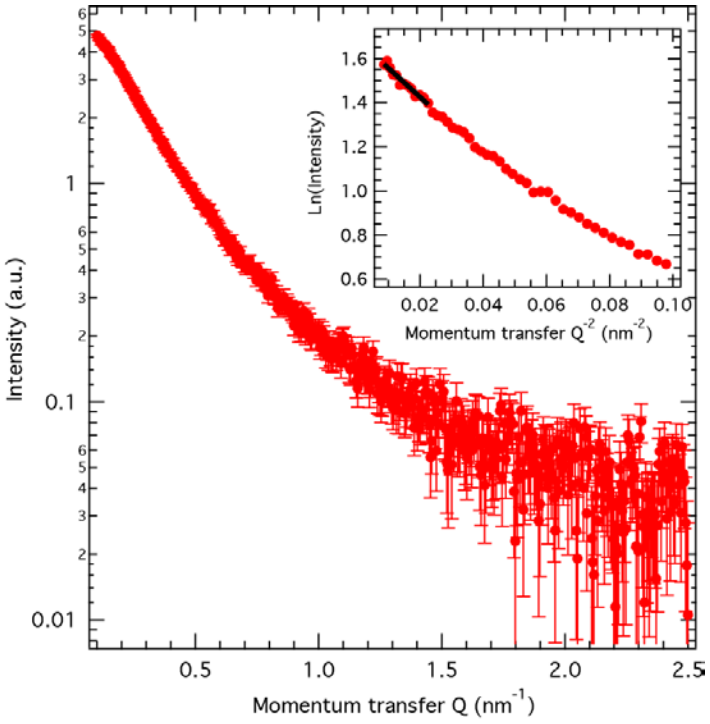
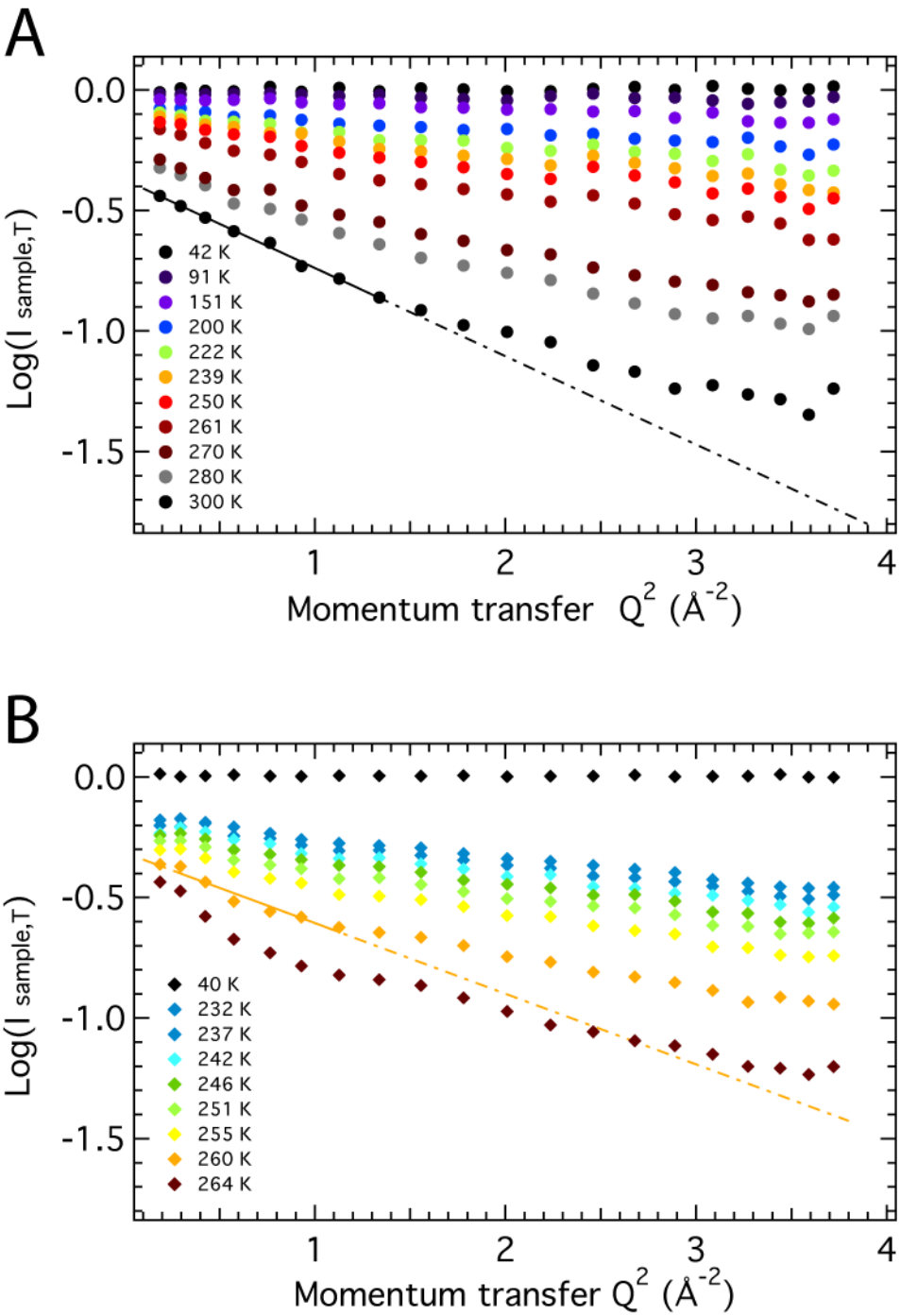
Supporting Material

SAXS intensity profile *I*(*Q*) of H-tau in solution



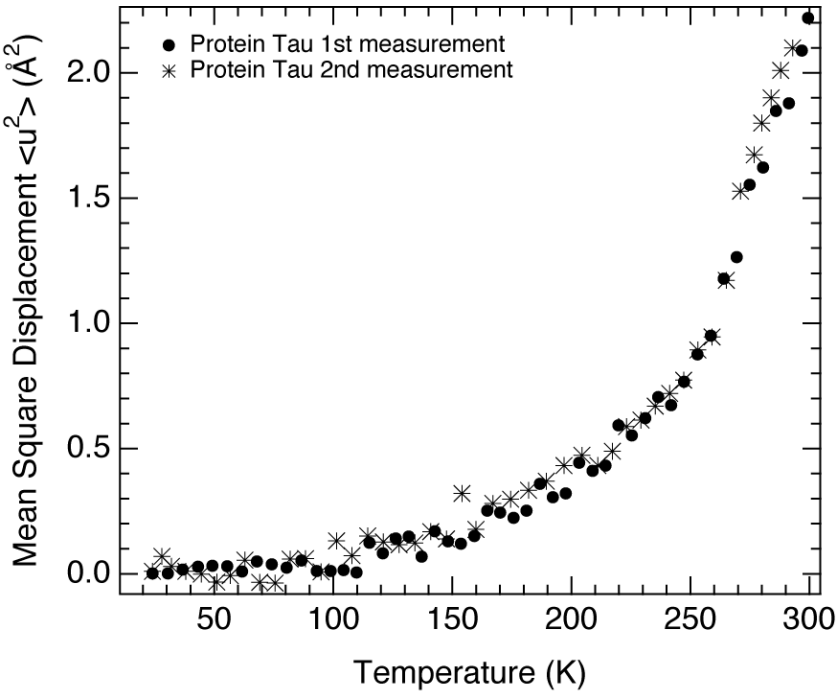
Legend Figure S1: Small angle X-ray scattering curve of H-tau in solution. The inset shows the Guinier fit used for the extraction of R_g.



Legend Figure S2: Logarithmic representation of the normalised intensities (eq. 1 in main text) as a function of Q^2 at various temperatures for H-tau-D_2O (A) and D-tau-H_2O (B). The Q^2 ranges in which MSD were extracted are 0.19 $Å^{-2} < Q^2 < 1.32$ $Å^{-2}$ for the H-tau-D_2O (A) and 0.19 $Å^{-2} < Q^2 < 1.13$ $Å^{-2}$ for D-tau-H_2O (B). They are indicated by solid lines for the highest temperature at which a linear relationship is still observed, *i.e.* 300 K for H-tau-D_2O (A) and 260 K for D-tau-H_2O (B). In (B), ln(I) versus Q^2 is not linear any more at 263 K. Consequently, MSD of D-tau-H_2O are only shown up to 260 K in figs. 1B and 4A of the main text. Broken lines are extrapolations of solid lines.

Reproducibility of incoherent elastic neutron scattering on the IN16 spectrometer at the ILL

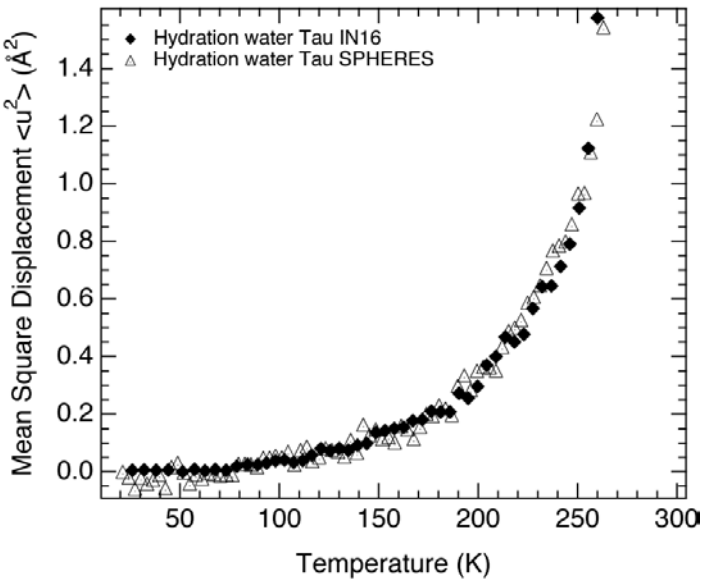
In order to assess the reproducibility of incoherent elastic neutron scattering on IN16, the elastic scan on H-tau-D_2O (0.44 g D_2O / g H-tau) was repeated with the same sample and in exactly the same experimental conditions on IN16. Figure S3 indicates a high degree of reproducibility and gives an idea of experimental and statistical errors involved.



Legend Figure S3: Mean square displacements of H-tau-D_2O (0.44 g D_2O / g H-tau) determined from two independent measurements on IN16. Filled circles correspond to MSD shown in figures 1A and 4A and stars are from the repeated experiment.

Incoherent neutron scattering experiments on the SPHERES spectrometer at FRMII

With the aim of comparing IN16 at ILL (Grenoble, France) with the similar backscattering spectrometer SPHERES ((1); http://www.jcns.info/jcns_spheres; Jülich Centre for Neutron Science at FRMII, Garching, Germany) at FRMII (Garching, Germany), we performed elastic incoherent neutron scattering experiments on SPHERES with the same D-tau-H_2O sample than the one used on IN16. SPHERES is characterized by an energy resolution of 0.6 μeV (FWHM), a wavelength of 6.27 Å and an accessible Q range of 0.2 - 1.9 $Å^{-1}$. The D-tau-H_2O sample was inserted in a Janis Cryostat/Cryofurnace at room temperature and at 135° with respect to the incoming beam. The temperature was lowered to 20 K in 2 hours and elastic scans were performed during temperature raise from 20 K to 300 K at 0.13 K / min. MSD were extracted from normalized intensities in the Q range from 0.2 to 1.22 $Å^{-2}$ as described in the Materials and Methods sections of the main text. Data analysis was carried out with LAMP. Despite slightly different Q-ranges over which MSD were extracted, due to slightly different instrument characteristics (0.2 to 1.22 $Å^{-2}$ on SPHERES and 0.19 to 1.13 $Å^{-2}$ on IN16), results are comparable (figure S4).



Legend Figure S4: MSD of D-tau-H_2O as measured on IN16 (closed diamonds) and SPHERES (open triangles). Data points represented by closed diamonds are the same as those in figure 1B.

Supporting References

1. Wuttke, J., A. Budwig, M. Drochner, H. Kämmerling, F.-J. Kayser, H. Kleines, L. C. Pardo, M. Prager, V. Ossovyi, G. J. Schneider, H. Schneider, S. Staringer, and D. Richter. 2012. SPHERES, Jülich's High-Flux Neutron Backscattering Spectrometer at FRM II. Rev. Sci. Instr. submitted (arXiv:1204.3415v3).