Electronic Supporting Information (ESI)

Peters et al.

Integrating eq. (1) over Q in the limited range between $Q_{\min}$ and $Q_{\max}$ yields the expression

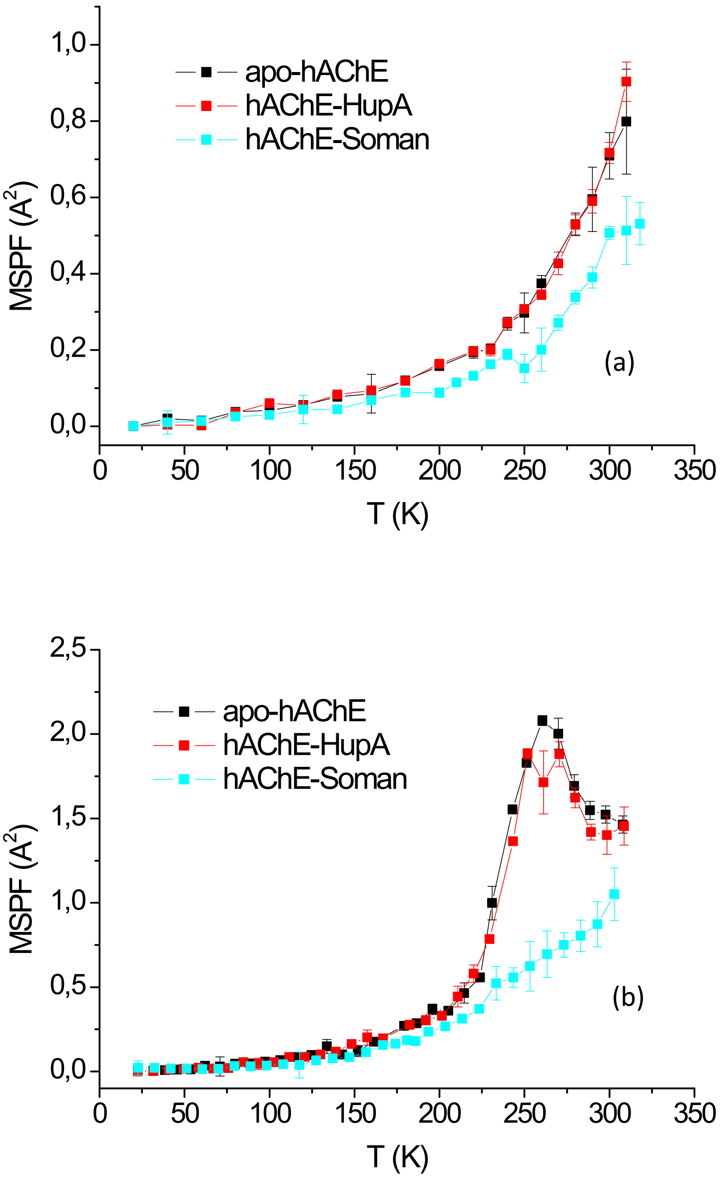
$$S_0 \int_{Q_{\min}}^{Q_{\max}} \exp(-\frac{1}{3}\langle u^2\rangle Q^2)dQ = S_0 \int_{0}^{Q_{\max}} \exp(-\frac{1}{3}\langle u^2\rangle Q^2)dQ - S_0 \int_{0}^{Q_{\min}} \exp(-\frac{1}{3}\langle u^2\rangle Q^2)dQ.$$

We introduce the new variable $t^2 = 1/3 \langle u^2\rangle Q^2$, and transform the integrals into

$$= S_0 \sqrt{\frac{3}{\langle u^2\rangle}} \left\{ \int_{0}^{\sqrt{3/\langle u^2\rangle}\,t_{\max}} \exp(-t^2)dt - \int_{0}^{\sqrt{3/\langle u^2\rangle}\,t_{\min}} \exp(-t^2)dt \right\}.$$

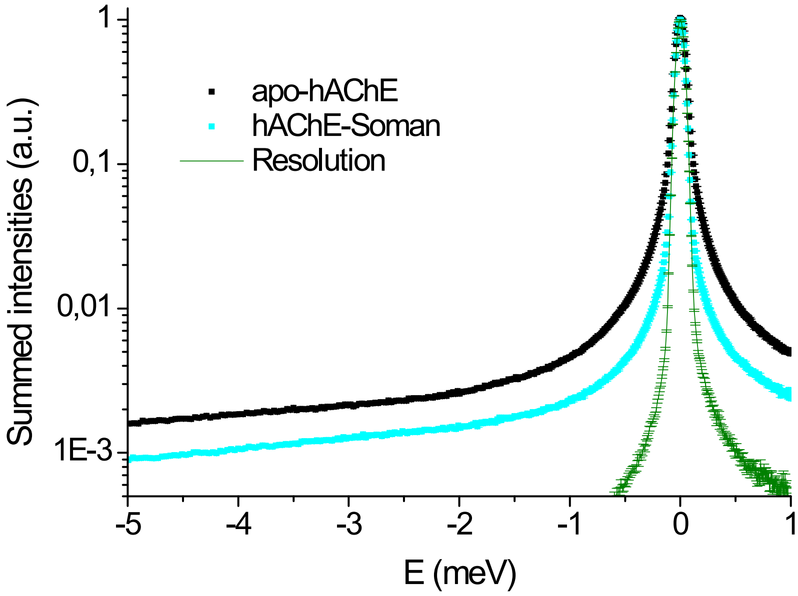
Such integral cannot be calculated analytically, but results in an error function, which can be found in tables (M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions, Dover Publications, 1964):

$$= \frac{S_0}{2} \sqrt{\frac{3\pi}{\langle u^2\rangle}} \{erf(Q_{\max}) - erf(Q_{\min})\}.$$



Supplementary Figure 1 : MSPF extracted from IN6 (a) and IN16 (b) data in the Q-ranges of 0.5 – 1.54 Å^{-1} and 0.55 – 1.8 Å^{-1}, respectively, for the three samples.

Contrary to the MSD, where only a change in slope is seen above 250 K, the MSPF of apo-hAChE and hAChE-HupA decrease above this temperature. This effect is generally attributed to an instrumental resolution effect (Becker, T.; Hayward, J. A.; Finney, J. L.; Daniel, R. M.; Smith, J.C. Biophys. J. 2004, 87, 1436−1444.): if the molecular dynamics grows strongly, it might leave the time window of the spectrometer and appear to tend to a constant value (in case of the MSD) or even decrease as for the MSPF.



Supplementary Figure 2 : Neutron intensities summed over the whole Q-range available on IN6 for the two samples and vanadium, representing the instrumental resolution.