Supporting information

A convenient way to apply TRAMITE to predict the residual dipolar coupling between two coupled nuclei P and Q is by using the expression¹:

\[ D_{PQ}^{r}(\theta, \phi) = \frac{\gamma_P \gamma_Q \mu_{2h}}{16\pi^2 I_{PQ}} A_{\alpha}^{PQ} \left\{ 3 \cos^2 \theta - 1 + \frac{3}{2} R \sin^2 \theta \cos 2\phi \right\}, \]  

where \( A_{\alpha}^{PQ} = \frac{1}{3} \left( A_{zz}^{PQ} - (A_{xx}^{PQ} + A_{yy}^{PQ})/2 \right) \) is the unitless axial component of the alignment tensor \( D \) (whose components are expressed in Hz), \( R \) is the rhombicity defined by \( A_r^{PQ} / A_{\alpha}^{PQ} \), with \( A_r^{PQ} = \frac{1}{3} \left( A_{xx}^{PQ} - A_{yy}^{PQ} \right) \), and the remaining constants have their usual meanings. Because \( D \) is traceless, \( A_{\alpha}^{PQ} = 2 A_r^{PQ} \). \( \theta \) is the angle formed between the P–Q interatomic vector with the z axis, and \( \phi \) is the angle between the projection on the x–y plane of the vector P–Q with the x axis. TRAMITE lets one calculate all the variables within the brackets in equation [1] according with the two conditions explained in the communication, followed by scaling the axial component \( A_{\alpha}^{PQ} \) by standard fitting procedures.

The figure shows the results obtained for another five biomolecules.

![Figure 1](image-url)

**Figure 1.** Correlations among experimental \(^1D_{PQ}\) values and predicted with TRAMITE. (A) \(^1D_{CH}\) and (B) \(^1D_{NH}\), from the NMR models 1 and 9, respectively, of Ubiquitin deposited in the PDB.² (C) \(^1D_{NH}\) from the NMR model 1 of Cyanovirin-N deposited in the PDB.³ (D) \(^1D_{CH}\) from Lewis A trisaccharide.⁴ (D) \(^1D_{CH}\) from LNF-3 pentasaccharide.⁵ The (●) symbols correspond to the prediction for the individual structure from a MC simulation⁴ with the best \( \chi \) value, while the (○) are obtained from averaging the first 9 structures with individual \( \chi \) values lesser than 3.
References