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 expression[1]:

$$D^{PQ}(\theta,\phi) = -\frac{\gamma_P \gamma_Q \mu_0 h}{16\pi^3 r_{PQ}^3} A_a^{PQ} \left\{ \left(3\cos^2\theta - 1\right) + \frac{3}{2} R \sin^2\theta \cos 2\phi \right\}, \qquad [1]$$

where $A_a^{PQ} = \frac{1}{3}\left[A_{zz}^{PQ} - \left(A_{xx}^{PQ} + A_{yy}^{PQ}\right)/2\right]$ 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_a^{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, $A_a^{PQ} = 2A_{zz}^{PQ}$. θ is the angle formed between the P–Q interatomic vector with the z axis, and ϕ 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_a^{PQ} by standard fitting procedures.

The figure shows the results obtained for another five biomolecules.

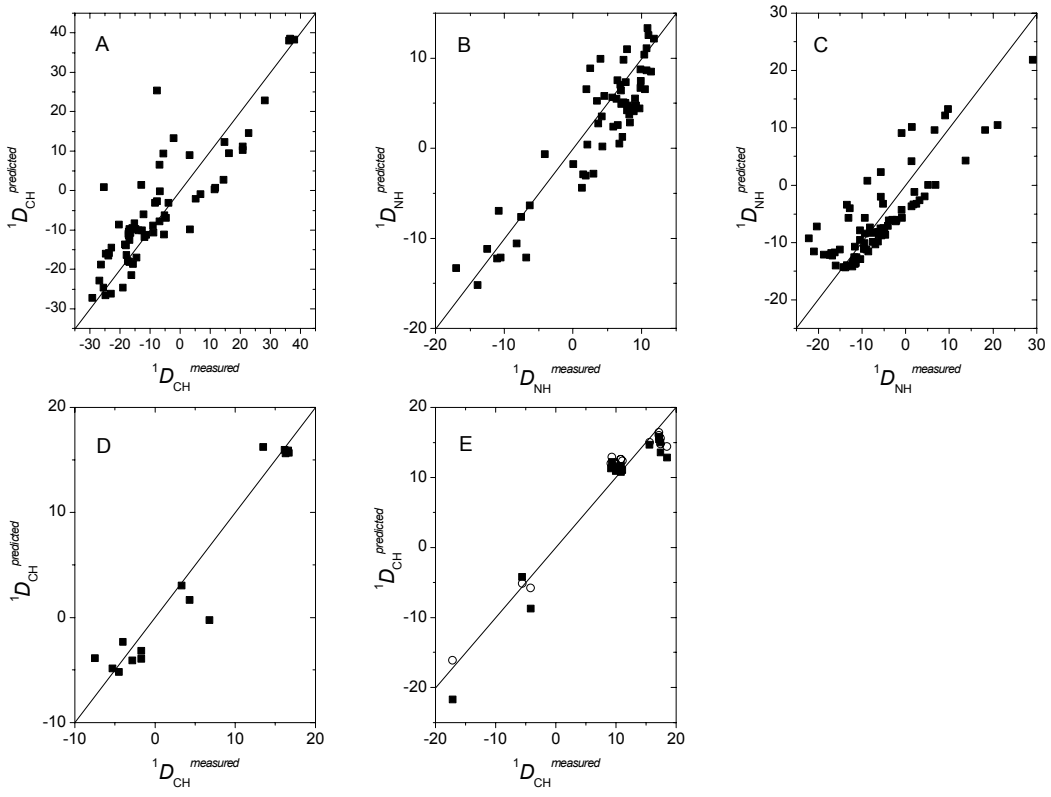

Figure 1. Correlations among experimental $^1D_{PQ}$ values and predicted with TRAMITE. (A) $^1D_{CH}$ and (B) $^1D_{NH,}$ from the NMR models 1 and 9, respectively, of Ubiquitin deposited in the PDB.[2] (C) $^1D_{NH}$ from the NMR model 1 of Cyanovirin-N deposited in the PDB.[3] (D) $^1D_{CH}$ from 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 simulation[4] with the best χ value, while the (○) are obtained from averaging the first 9 structures with individual χ values lesser than 3.

References

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