May external alignment be described by a single tensor? Quinine as a test study

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Residual Dipolar Couplings (RDCs) are more and more becoming a complementary tool to NOEs and scalar couplings for the stereochemical analysis of small organic compounds. This analysis is mainly done by determination of the alignment tensor **A**, a symmetric 2nd rank traceless matrix which encodes rotational probability distribution.

If the studied compound shows several populated conformers in solution, the average RDCs will depend both on populations and a particular alignment tensor for each conformer.

$$< D_i^{red} >= \sum_{j=1}^{N} p_j r_{ij}^T A_j r_{ij}$$

Since the number of independent couplings will be in most cases relatively scarce, the above equation will be undetermined. However, we hypothize that for molecules in which different conformers show a similar global shape, the above equation can be aproximated by the use of a single alignment tensor.

$$< D_i^{red} >\approx \sum_{j=1}^{N} p_j r_{ij}^T A r_{ij}$$

To test this hypothesis we have chosen the quinine molecule since it presents a small conformational space (eight low energy conformers) showing all of them a similar shape. Quinine was aligned in PELG and the RDCs measured by recording 13C coupled 1D spectra. Alignment tensor components and populations were simultaneously determined by least-squares fitting on DFT optimized structures. Results indicate that conformational space is mainly largely dominated by two conformers. Further experiments are being carried out to validate the single tensor hypothesis.

[1] Thiele, C. M. *Concepts in Magnetic Resonance Part A* **2007**, *30A*, 65-80.

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