Structure Determination of Organic Molecules Using Residual Dipolar Couplings

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The determination of relative configuration by nuclear magnetic resonance is often complicated by either absence of NOE data and/or ^{3}J coupling data, remoteness of the stereocenters or conformational equilibria.

The recently reintroduced residual dipolar couplings[1] provide complimentary information to these convential nmr restraints. In order to demonstrate the utility of residual RDCs for organic structure determination we have applied this methodology to a problem, which is comparable to the determination of relative configurations, namely the differentiation and assignment of diastereotopic protons in strychnine, which can also readily be solved by conventional methods [2].

The second application that will be shown is the determination of the relative configuration of an α-methylene-γ-butyrolactone. For this substance conventional nmr spectroscopic means fail due to the existence of conformational equilibria such that both possible diastereoisomers are in line with the experimental data (^{3}J and NOE). Using RDCs, however, it is possible to unambiguously assign the relative configuration (in this case to be *trans*).[3]

The third application, that will be shown, is the determination of the conformation of a photoswitchable organocatalyst. [4] The catalytically inactive species showed some pseudo-background reactivity, the reason for which was determined by a conformation determination using RDCs.

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