An Error Analysis of Relative Stereochemistry determinations via Residual Dipolar Coupling NMR

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Nuclear Magnetic Resonance (NMR) is a common technique used to determine the two-dimensional structure of molecules. However, some molecules have important three-dimensional structures that determine their biological and chemical properties. One such property is stereochemistry where a molecule can have two orientations that are mirror images; this creates two otherwise structurally identical molecules called enantiomers. Two enantiomers have nearly identical properties and are generally indistinguishable by NMR. If there are two or more atoms in a molecule exhibiting chirality, then there are four or more possible diastereomers that can be distinguished using Residual Dipolar Coupling (RDC) NMR. The three-dimensional structure of a molecule can be determined using RDC NMR and the correct diastereomer can be identified using this technique. In my work, I have developed a measure of merit for the assignment of relative stereochemistry using RDC NMR that is expressed as a percent certainty. This measure of merit was used to analyze factors currently thought to affect the accuracy of the assignment of structures.