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Title: Chapter 4: Cross-correlation in Biomolecules

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Abstract:

This chapter focuses on the methods used to quantitatively measure auto- and cross-correlated cross-relaxation relaxation rates in biomolecules and interpret these rates in terms of structure and dynamics. A theoretical description of average Liouvillian theory is presented in the beginning, to set the stage for understanding various experiments used to measure cross-relaxation in biomolecules. A series of multidimensional experiments to measure CSA-dipole, dipole-dipole, and CSA-CSA cross-correlations in large biomolecules such as proteins are discussed. Cross-correlated nuclear spin relaxation rates provide rich information about slow correlated motions as well as fast and slow internal motions in proteins. The next part of this chapter deals with motional models used to quantify cross-correlations. The model-free formalism and correlated internal motions are described in detail. A highlight of this chapter is an overview of the different cross-correlation parameters that can be obtained from dynamics studies. Several examples of applications of measurements of cross-correlation rates are then described, with special attention to proteins, nucleic acids and ligand-binding studies. The chapter concludes with a description of the famous TROSY experiments in biomolecules, which are based on CSA-dipole and dipole-dipole cross-correlations

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