RMN y reconocimiento molecular. Interacciones carbohidrato-proteína

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Molecular recognition by specific targets is at the heart of the life processes. In recent years, it has been shown that the interactions between proteins (lectins, enzymes, antibodies) and carbohydrates mediate a broad range of biological activities, from fertilization, embryogenesis, and tissue maturation, to pathological processes. The elucidation of the mechanisms that govern how sugars are accommodated in the binding sites of these receptors is currently a topic of interest. Thus, the determination of the structural and conformational factors and the physicochemical features which govern the molecular recognition of these molecules is of paramount importance. This presentation is focused on the application of standard and state-of-the-art NMR methods both from the ligand and receptor's perspective (especially chemical shift perturbation analysis, Saturation Transfer Difference, and trNOESY experiments) to the study of molecular recognition processes between a variety of polypeptides of biomedical interest and carbohydrate-based molecules, drugs and inhibitors. Lectins, antibodies, and enzymes, both wild type and mutants, have been used as receptors with the final aim to know and to evaluate the relative importance of polar (hydrogen bonding, electrostatic interactions) and non polar (van der Waals, CH-π) forces in the molecular recognition process. As examples, structural and conformational details of glycan recognition by different domains will be shown, with special emphasis in the application of novel 19F- and paramagnetic-based NMR methodologies.