NMR IN DRUG DISCOVERY AND DEVELOPMENT

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Nuclear Magnetic Resonance is the appropriate technique to study the interaction of drugs with their molecular targets, giving information at the molecular level of the type, topology and strength of that interaction. This type of information is usually obtained using different NMR parameters, like chemical shifts (δ), spin-spin coupling constants (j), nuclear Overhauser effect (NOE), nuclear relaxation times (T_1, T_2 and $T_{1\rho}$), molecular diffusion coefficients (D) and molecular correlation times (τ_c). There have been developed a great number of different techniques that make use of those parameters to study all types of intermolecular interactions. Among the most important are SAR by NMR, Waterlogsy, NOE Pumping, Transfer NOE, Saturation Transfer Difference (STD), SAR by Interligand Overhauser Effects (SAR by ILOES), Affinity (DOSY and other pulsed field gradients experiments) and several others. The information obtained using those methodologies is used to understand the biological activity of drugs, to increase the affinity of the drugs with their target and to design compounds with greater selectivity for the desires target. In this talk those techniques will be discussed and there will be shown examples of their application for the design, screening and evaluation of drugs.