

## NMR Spectroscopy: A Valuable Tool in the Weaponry of Medicinal Chemistry

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Medicinal Chemistry constitutes a branch of Chemistry aiming in the design and synthesis of novel drugs to treat major diseases. 2D NMR Spectroscopy has especially become a valuable tool in the hands of Medicinal Chemists since the majority of drugs are organic compounds of low molecular weight (<1000) or peptides (<5000).

The first step after the synthesis of potential pharmaceutical products is their structure elucidation. To fulfill this aim 2D NMR spectroscopy has offered a tremendous help. It is not an exag-

geration to say that 2D NMR spectroscopy aids not only the Medicinal Chemists to characterize the new products but also Pharmaceutical technologists providing information about polymorphism of drug powders and of drugs in tablets. The synthetic drugs must have pharmacokinetics that prohibit their toxicity. NMR spectroscopy has its contribution on this aspect by studying drug metabolism through analysis of biological fluids. Its coupling with liquid chromatography offers the separation and characterization of metabolic products (LC-NMR).

NMR has many applications in the Medicinal Chemistry. NOE effect allows to study the conformations of drug molecules in many environments that simulate the biological ones. The conformation of the molecule is related to its bioactivity. NMR permits to comprehend on the stereoelectronic parameters that govern the bioactivity of drug molecules and therefore to design and synthesize novel drugs with optimized pharmacological profile. This rationale design minimizes the synthetic compounds to be prepared and the man power to be involved.

*In vitro* NMR spectroscopy has been developed and HSQC (Heteronuclear Single Quan-

tum Coherence) experiment offers the possibility to study the binding of a drug in the active site. Thousands of molecules can be tested and new molecules can be developed through this approach. Recently *in vivo* NMR has been applied using the same experiment but in a real biological environment.

*In conclusion*, NMR spectroscopy constitutes a valuable tool in Medicinal Chemistry and offers new avenues in the adventurous research trip towards the discovery of novel drugs that will ameliorate the suffering of humanity from undesired diseases.

