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NMR of Proteins and Small Biomolecules

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Preface

Nuclear Magnetic Resonance (NMR) is one of only a few scientific techniques that have been widely applied in many different areas such as physics, chemistry, biology and medicine. Today, NMR plays a crucial role in structure-function studies of organic and inorganic compounds and of large biomolecules, particularly proteins and DNA. In medicine it is one of the most important imaging techniques available to physicians and it also has extensive applications in pharmaceutical research. In this special issue of NMR of Proteins and Small Biomolecules, review chapters cover a wide-range of topics on some of the latest developments in NMR techniques and their applications.

A review of recent developments in structure-based drug discovery begins this volume by showing how combining 1D and 2D NMR techniques with molecular docking can efficiently screen and identify novel "druggable" leads. The success of such an approach relies on the selection of worthwhile therapeutic targets; presumably proteins that are critical in particular diseases. In that context, studying protein-ligand interactions with NMR techniques that have unique powers for the study of weak protein-ligand interactions, as described in chapter 2, followed by the use of residual dipolar coupling approaches, reviewed in chapter 3, may be essential. Chapter 4 is dedicated to the study paramagnetic metalloproteins, giving an overview of paramagnetic NMR and ^{13}C directly detected protonless NMR spectroscopy. Since NMR is especially powerful for the study of proteins dynamics, more recent developments in transverse relaxation dispersion experiments, which have extended the range of NMR relaxation studies to the milli-micro second timescale, are illustrated in chapter 5. Solid and liquid state NMR techniques for studying membrane proteins represent another "hot" area of contemporary research. Chapters 6 and 7 systematically describe these approaches. This volume concludes with chapter 8, a review of the considerable sensitivity enhancement attainable in magnetic resonance spectroscopic imaging (MRSI) through the use of dynamic nuclear polarization transfer. This non-invasive technique can be applied to the measurement of metabolites *in vivo* to allow early diagnosis and assessment of diseases in personalized medicine.

I hope that the reviews of these unique topics in NMR techniques and their applications as presented in this volume NMR of Proteins and Small Biomolecules are informative and fun to read; and I thank all the authors who made this project possible.

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