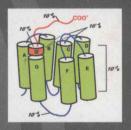
## MODERN MAGNETIC RESONANCE

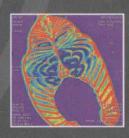
EDITOR: GRAHAM A. WEBB

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Applications in Chemistry, Biological and Marine Sciences









## Modern Magnetic Resonance

Part 1: Applications in Chemistry, Biological and Marine Sciences

Graham A. Webb (Ed.)
Royal Society of Chemistry, London, UK



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### Modern Magnetic Resonance

Part 1

Part 1: Applications in Chemistry, Biological

and Marine Sciences

Part 2: Applications in Medical and

**Pharmaceutical Sciences** 

Part 3: Applications in Materials Science and

**Food Science** 

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#### **Preface**

It is a great pleasure for me to Introduce the handbook of Modern Magnetic Resonance, MMR. The various techniques which comprise MMR derive essentially from three sources, all of which were produced by physicists. To-day they are widely used by scientists working in many diverse areas such as chemistry, biology, materials, food, medicine and healthcare, pharmacy and marine studies.

The first source of MMR studies is nuclear magnetic resonance, NMR. This provides details on the relative positions of nuclei, i.e. atoms, in a molecule. Consequently NMR provides structural information on samples which may be in the solid, liquid or gaseous state. Nuclear relaxation data yield dynamic information on the sample and the topology of the dynamic processes if the sample is undergoing a molecular change. Thus high and low resolution NMR studies provide information on all interesting aspects of molecular science. The protean nature of NMR is reflected in its many applications in chemistry, biology and physics which explore and characterize chemical reactions, molecular conformations, biochemical pathways and solid state materials, to name a few examples.

Magnetic resonance imaging, MRI, is the second source of MMR data. MRI provides a three-dimensional image of a substatuce, and is consequently widely employed to assess materials both *in vitro* and *in vivo*. The importance of MRI studies in many areas of science and

medicine is shown by the recent award of the Nobel Prize to Lauterbur and Mansfield.

The third source of MMR results is due to electron spin resonance, ESR. This is a technique for detecting unpaired electrons and their interactions with nuclear spins in a given sample. Thus ESR data are often used to complement the results of NMR experiments.

Taken together NMR, MRI and ESR comprise the field of MMR, recent years have witnessed the fecundity of these techniques in many scientific areas. The present three volumes cover applications in most of these areas. Part 1 deals with Chemical Applications, Biological and Marine Sciences. Medical and Pharmaceutical Sciences are covered in Part 2. Part 3 provides examples of recent work in the Materials Science and Food Science.

I wish to express my gratitude to all of the Section Editors and their many contributors for their hard work and dedication in the creation of MMR. My thanks also go to Emma Roberts and the production staff at Kluwer, London, for their assistance in the realization of these volumes.

Royal Society of Chemistry Burlington House Piccadilldy London, W1J OBA G.A.WEBB February 2005

#### Foreword to Application in Chemistry

Magnetic resonance has continued to be an emerging technique, to be applied to almost all fields of pure and applied sciences, including chemistry, physics, biology, materials science, medicine, etc. during past 60 years since its discovery. The applications in chemistry of this volume covers advanced studies on chemical aspect of magnetic resonance spectroscopy and imaging dealing with the state-of-the-art developments of new techniques together with those of basic concepts and techniques, consisting of 93 articles which are grouped to 25 chapters. They are alphabetically arranged for convenience of readers: amyloids, chemical shifts and spin coupling constants, fibrous proteins, field gradient NMR, host-guest chemistry,

imaging, inorganic materials and catalysis, lipid bilayers and bicelles, membrane-associated peptides, membrane proteins, new developments, NOE and chemical exchange, NQR and ESR, organometallic chemistry, paramagnetic effects, protein structures, polymer structure, polymer dynamics, polymer blends, quantum information processing, residual dipolar couplings and nucleic acids, solid state NMR techniques, structural constraints in solids, and telomeric DNA complexes. The section editors are grateful to contributors to this section for their fine contributions.

Tetsuo Asakura, Hazime Saitô and Isao Ando

# Color Plate Section

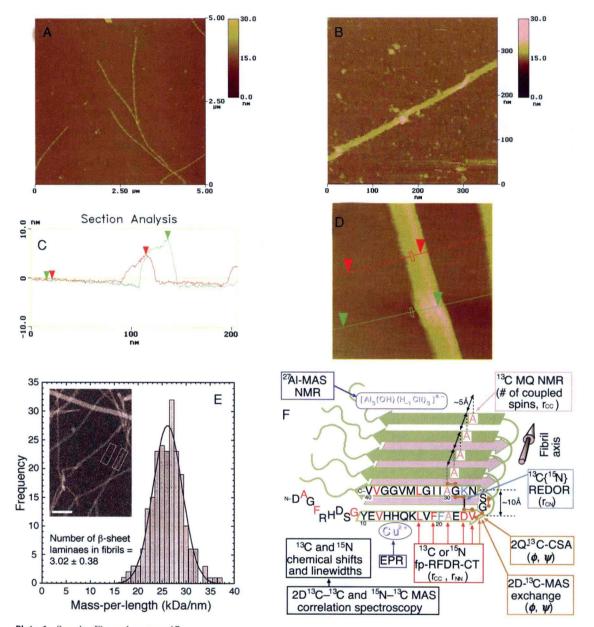


Plate 1. See also Figure 1 on page 17.

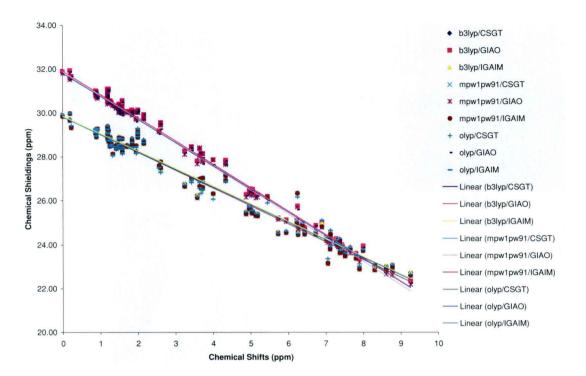


Plate 2. See also Figure 2 on page 53.

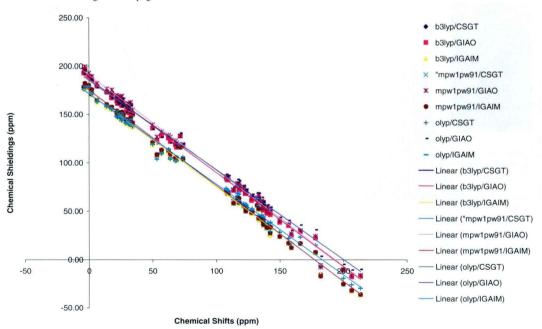


Plate 3. See also Figure 3 on page 54.

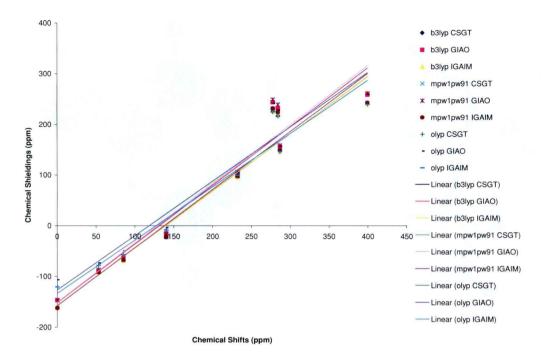


Plate 4. See also Figure 4 on page 55.

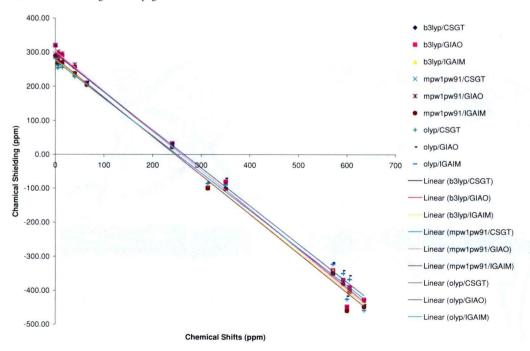
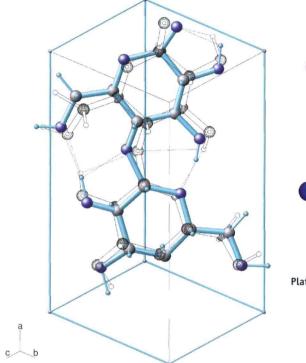
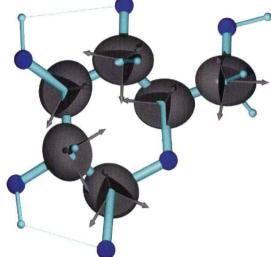


Plate 5. See also Figure 5 on page 56.





**Plate 7.** See also Figure 4 on page 73.

Plate 6. See also Figure 2 on page 72.

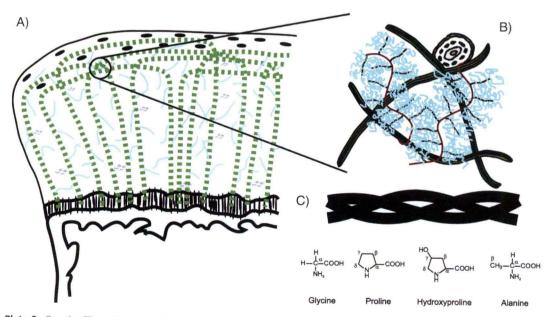
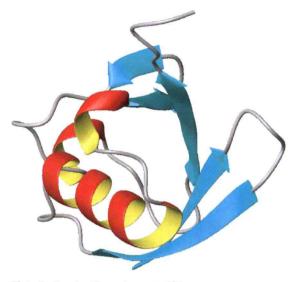


Plate 8. See also Figure 1 on page 84.



**Plate 9.** See also Figure 4 on page 134.

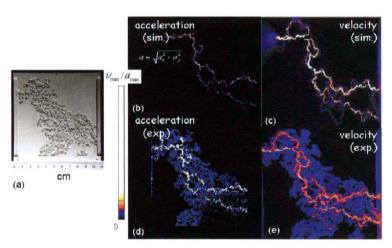
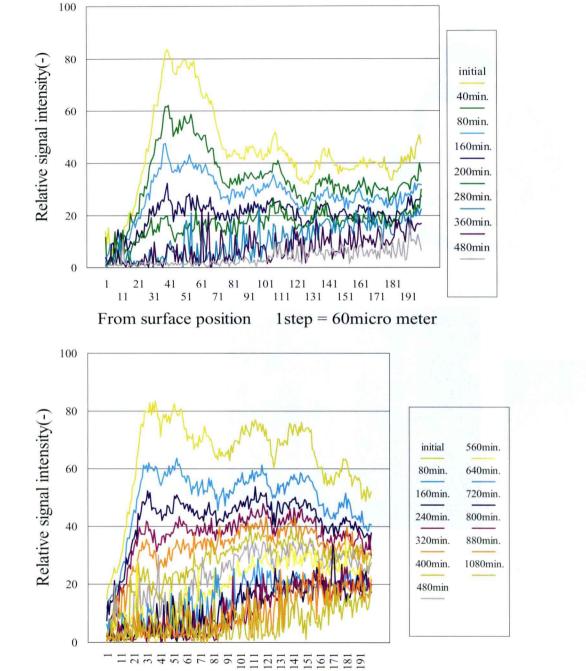


Plate 10. See also Figure 3 on page 157.



From surface position 1 step = 60 micro meter

Plate 11. See also Figure 1 on page 160.

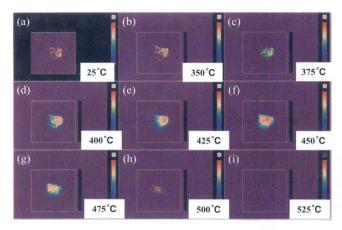


Plate 12. See also Figure 7 on page 166.

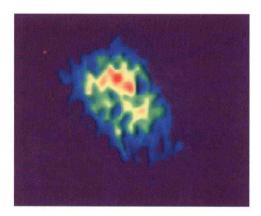


Plate 13. See also Figure 8 on page 166.

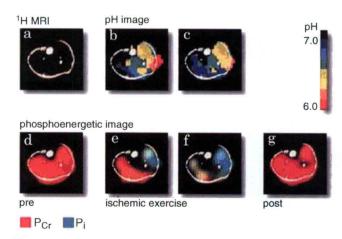


Plate 14. See also Figure 2 on page 171.

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