

Preface

Fundamental research in chemical and biological sciences has witnessed significant advances in recent years with the boundary becoming blurred between the two rival, traditional disciplines. Concomitantly, rapid development of interdisciplinary research techniques in support of such advances is taking place at regular intervals. In addition, taught courses delivered at universities are being designed to equip the younger generation with knowledge and skills needed to pursue interdisciplinary research.

A sound knowledge of the biomolecular structure aided by appropriate bioanalytical techniques is indispensable to elucidate the mechanism of action of biological macromolecules and their function at large. The present book intends to provide a good introduction and understanding on a range of biomolecular and bioanalytical cum biophysical techniques and is primarily aimed at the advanced undergraduate (years 3 and 4) and MSc students who are fresh to research. Nowadays, short-term research projects (team and/or individual based) form an essential component of the taught curriculum and make a sizeable contribution towards assessment in modern Chemistry and Biology courses. Hence, it is important that prospective research students acquire sufficient background and skills in various research techniques before graduating. The book should also be suitable for those contemplating an advanced postgraduate (PhD) and postdoctoral research career in Chemistry, Biochemistry, Biophysics and Pharmaceutical Chemistry in academia and industry.

The book is research focused, interdisciplinary and comprehensive with a broad selection of topics drawn from contemporary Chemistry and Biology research, in a single volume. The order of chapters and the depth of coverage make the book well balanced and well connected with a gradual, smooth flow of information and increasing knowledge. It attempts to bridge the gap between introductory core material taught in years 1 and 2 undergraduate levels and advanced research texts; thus prior knowledge of the former is expected to derive a complete understanding of the present book.

In many ways, the present book is the first of its kind with an international team of authors of considerable teaching and research experience, each contributing a single chapter on a specific technique of her/his expertise. The format of each chapter is broadly similar with greater emphasis on experimental procedures accompanied by case studies rather than theory. Obviously, it is not possible to elaborate on every technique in critical detail but they are sufficient to provide the necessary background and detailed experimental procedures to afford the reader a good understanding of the various techniques before applying them. Further, each chapter is accompanied by a selection of books recommended for further reading and a comprehensive list of references pertinent to the technique discussed. The suitability of the book as lecture material will depend on the intended learning objectives and outcomes of the taught course as determined by the lecturer.

The book is broadly organised into five parts after a short, important chapter on Health and Safety (H&S). In addition to common laboratory safety, safety in a research laboratory requires additional knowledge of chemical and biohazards and risks associated with special techniques and high end equipment.

The first part covers Chapters 2 to 5 on Chemoinformatics, Bioinformatics, Gene expression analysis and Proteomics. These chapters describe the computational tools available to search relevant databases for molecules with the likelihood of biological activity or placing sequence data (DNA, RNA, proteins) in a

biological context or design experiments for the cloning or analysis of genes expressed in eukaryotic cells or compare the proteomes of different biological samples.

The next set of chapters (6 to 8) covers Protein expression and purification, Chromatography and separation techniques in Biology and Synthetic methodology in chemical biology describe in detail the recombinant genetic and synthetic methods used for the preparation of proteins and small peptide molecules, respectively, and the various chromatographic methods used for the separation and purification of such molecules.

The subsequent set of chapters (9 to 12) covers Mass spectrometry, Analytical ultracentrifugation, Light scattering, Reaction kinetics in Biology and Isothermal titration calorimetry form the core analytical techniques for characterisation of biomacro molecules through the measurement of mass-to-charge ratios of gas phase ions, the quantitative determination of molecular size and shape and determination of the steady-state kinetic parameters of enzymes and the investigation of biomolecular interactions to define the thermodynamics of binding in order to understand basic biological processes. Prior knowledge about these properties of a biomolecule should provide the basis for its three-dimensional structure determination.

Chapters 13 to 15 on Molecular Spectroscopy (Infra-red, Raman, Fluorescence, Circular dichroism spectroscopies) discuss how molecular vibrations manifested by distinct IR and Raman spectral bands can be correlated with functional groups and their role in biomedical research, application of a number of specific steady-state fluorescence-based techniques to analyse the structures, associations and conformations of biological macromolecules and determination of protein secondary structure using circular dichroism.

Finally, the last four comprehensive chapters (16 to 19) on Biomolecular structure determination (X-ray, NMR and Cryo-TEM, Molecular Simulation) describe the (i) determination of the high resolution structures of proteins and their complexes in the crystalline state (X-ray), (ii) determination of the three-dimensional structure and conformational analysis of DNA in the solution state (NMR), (iii) visualisation at atomic resolution of a wide range of macromolecular complexes in frozen hydrated form (Cryo-TEM) and (iv) the physical basis of computer modelling and principles of molecular simulations to extract structural and thermodynamic quantities.

I hope the book will prove a useful text for students, researchers and lecturers alike.

A book of this type involving a number of different techniques would not have been possible without the valuable contribution and continued support of all the authors and I remain very grateful to them. I also thank the numerous reviewers with their helpful comments and corrections on different chapters. During the course of my academic career, I had the privilege of teaching Biophysical Chemistry to undergraduate and postgraduate students, of varying backgrounds, mostly at the University of Manchester, UK, and benefited from their comments and criticisms. I am also grateful to the former postgraduate (PhD and MPhil) members of my research group whose enthusiastic support gave me the impetus to develop ideas for this book project. Finally, I thank Wiley (UK) for their interest and support throughout.

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