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MOLECULAR DYNAMICS

APPLICATIONS IN MOLECULAR BIOLOGY

Edited by

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Preface

In the introduction to this series in 'Topics in Molecular Biology' in 1980, great emphasis was placed on the importance of molecular structure for understanding biological phenomena. At that time, the emphasis was on the three-dimensional models determined from experimental methods such as X-ray crystallography; 'more speculative model building and conformational analysis' was mentioned only in passing. In the decade since this was written, the original emphasis on molecular structure has increased with many new structures being solved.

Along with the accumulation of new three-dimensional structures, there has been an awareness that it is not the static picture alone but also the dynamics of macromolecules which is important. Although X-ray crystallography can model some aspects of atomic motion, it has been the extension of computer simulation techniques such as molecular dynamics from physics and chemistry to molecular biology which has provided an overall picture of macromolecular dynamics.

The aim of this book is to review the uses of molecular dynamics and related modelling techniques as applied to biological macromolecules. It is particularly suited for those who have not specialized in simulation techniques. As well as describing applications to proteins, nucleotides and carbohydrates, we have also reviewed the exciting possibilities which emerge from the use of free energy perturbation methods in protein engineering and drug design.

Recently, molecular dynamics has started to play a direct role in the determination of macromolecular structures themselves when simulated annealing protocols are used in combination with experimental data from X-ray crystallography or NMR spectroscopy.

I would like to thank all the authors for their contributions, my colleagues for their advice and David Grist of Macmillan Press for guiding me through the role of volume editor.

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J.M.G.

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