

Preface

more advanced users can
biology, making it useful
the field. We have tried
of relevant theoretical and
apters, particularly in Part
topic to the next and be
computational studies of bio-
that the individual parts as
anical details can be found
serve as a useful reference
physics and biochemical

account of computational
We hope that it will serve
leic acids, and biological
continue to be revealed.
l with, collaborated with,
ltidimensionality of those
pecial thanks to Professor
ost important, for supply-
ndation for our scientific
directly to the creation of
our friends and family.

Oren M. Becker
Alexander D. MacKerell, Jr.
Benoît Roux
Masakatsu Watanabe

Contents

Foreword Martin Karplus *iii*

Preface *vii*

Contributors *xi*

Part I Computational Methods

1. Introduction 1
Oren M. Becker, Alexander D. MacKerell, Jr., Benoît Roux, and Masakatsu Watanabe
2. Atomistic Models and Force Fields 7
Alexander D. MacKerell, Jr.
3. Dynamics Methods 39
Oren M. Becker and Masakatsu Watanabe
4. Conformational Analysis 69
Oren M. Becker
5. Treatment of Long-Range Forces and Potential 91
Thomas A. Darden
6. Internal Coordinate Simulation Method 115
Alexey K. Mazur
7. Implicit Solvent Models 133
Benoît Roux
8. Normal Mode Analysis of Biological Molecules 153
Steven Hayward
9. Free Energy Calculations 169
Thomas Simonson

10. Reaction Rates and Transition Pathways 199
John E. Straub
11. Computer Simulation of Biochemical Reactions with QM-MM Methods 221
Paul D. Lyne and Owen A. Walsh

Part II Experimental Data Analysis

12. X-Ray and Neutron Scattering as Probes of the Dynamics of Biological Molecules 237
Jeremy C. Smith
13. Applications of Molecular Modeling in NMR Structure Determination 253
Michael Nilges

Part III Modeling and Design

14. Comparative Protein Structure Modeling 275
András Fiser, Roberto Sánchez, Francisco Melo, and Andrej Šali
15. Bayesian Statistics in Molecular and Structural Biology 313
Roland L. Dunbrack, Jr.
16. Computer Aided Drug Design 351
Alexander Tropsha and Weifan Zheng

Part IV Advanced Applications

17. Protein Folding: Computational Approaches 371
Oren M. Becker
18. Simulations of Electron Transfer Proteins 393
Toshiko Ichiye
19. The RISM-SCF/MCSCF Approach for Chemical Processes in Solutions 417
Fumio Hirata, Hirofumi Sato, Seiichiro Ten-no, and Shigeki Kato
20. Nucleic Acid Simulations 441
Alexander D. MacKerell, Jr. and Lennart Nilsson
21. Membrane Simulations 465
Douglas J. Tobias

Appendix: Useful Internet Resources 497

Index 503