

CONTENTS

SIGNIFICANCE OF COMPUTATIONAL BIOLOGY

Computational Biology Opportunity and Challenges for the Future	1
John C. Wooley and Matesh N. Varma	
Overview of Significant Challenges in Molecular Biology Amenable to Computational Methods	11
Robert M. Glaeser	

INITIAL PHYSICAL AND CHEMICAL STUDIES

Basic Physical and Chemical Information Needed for Development of Monte Carlo Codes	21
Mitio Inokuti	
Interactions of Low-Energy Electrons with Condensed Matter: Relevance for Track Structure	33
R.H. Ritchie, R.N. Hamm, J.E. Turner, and W.E. Bolch	
Electron Emission Resulting from Fast Ion Impact on Thin Metal Foils: Implications of These Data for Development of Track Structure Models	49
R.D. Dubois and C.G. Drexler	
Direct Ionization of DNA in Solution	65
J.H. Miller, W.E. Wilson, and R.H. Ritchie	

TRACK STRUCTURE CODE DEVELOPMENT

Charged-Particle Transport in Biomolecular Media: The Third Generation	77
M. Zaider, A. Fung, and M. Bardash	

Track Structure, Chromosome Geometry, and Chromosome Aberrations	93
David J. Brenner, John F. Ward, and Rainer K. Sachs	
Monte Carlo and Analytic Methods in the Transport of Electrons, Neutrons, and Alpha Particles	115
Randall S. Caswell and Stephen M. Seltzer	
PITS: A Code Set for Positive Ion Track Structure	137
W.E. Wilson, J.H. Miller, and H. Nikjoo	
Monte Carlo Track-Structure Calculations for Aqueous Solutions Containing Biomolecules	155
J.E. Turner, R.N. Hamm, R.H. Ritchie, and W.E. Bolch	

COMPARISON OF TRACK STRUCTURE CODES

Comparison of Various Monte Carlo Track Structure Codes for Energetic Electrons in Gaseous and Liquid Water	167
Hooshang Nikjoo and Shuzo Uehara	
A Comparison between Two Monte Carlo Codes on Determination of Transient Chemical Yields	187
R.N. Hamm, J.E. Turner, and A. Chatterjee	
An Attempt to Modify the MOCA Water-Vapor-Ion Code to Simulate Liquid Phase	195
S.B. Curtis, J.B. Schmidt, and W.E. Wilson	

MODELING OF BIOLOGICAL EFFECTS

Three Statistical Technologies with High Potential in Biological Imaging and Modeling	199
Moshe Fridman and J. Michael Steele	
Monte Carlo Approach in Assessing Damage in Higher Order Structures of DNA	225
Aloke Chatterjee, James B. Schmidt, and William R. Holley	
A Nucleosome Model for the Simulation of DNA Strand Break Experiments	243
Michel Terrissol and Ekkehard Pomplun	

A Computational Approach to the Relationship between Radiation Induced Double Strand Breaks and Translocations	251
William R. Holley and Alope Chatterjee	
Index.....	261