572.833 MOL

CONTENTS

1. Overview	1
2. The Energetics of Nucleotide Ionization in Water-Counterion Environments	18
3. Parameterization and Simulation of the Physical Properties of Phosphorthioate Nucleic Acids	41
4. Crystallographic Studies of RNA Internal loops	56
5. Hydrogen-Bonding Patterns Observed in the Base Pairs of Duplex Oligonucleotides	77
6. Structure and Stability of DNA Containing Inverted Anomeric Centers and Polarity Reversals	92
7. Conformational Analysis of Nucleic Acids: Problems and Solutions	106
8. NMR Structure Determination of a 28-Nucleotide Signal Recognition Particle RNA with Complete	
Relaxation Matrix Methods Using Corrected Nuclear Overhauser Effect Intensities	122
9. Molecular Modeling of DNA Using Raman and NMR Data, and the Nuclease Activity of 1,10-	
Phenanthroline-Copper Ion	150
10. Three-Dimensional NOESY-NOESY Hybrid-Hybrid Matrix Refinement of a DNA	
Three-Way Junction	167
11. Determination of Structural Ensembles from NMR Data: Conformational Sampling and Probability	
Assessment	181
12. NMR Studies of the Binding of an SPXX-Containing Peptide from High-Molecular-Weight Basic N	uclear
Proteins to an A-T Rich DNA Hairpin	195
13. Thermodynamics of Duplex Formation and Mismatch Discrimination on Photolithographically Synth	hesized
Oligonucleotide Arrays	206
14. RNA Folding Dynamics: Computer Simulations by a Genetic Algorithm	229
15. An Updated Recursive Algorithm for RNA Secondary Structure Prediction with Improved Thermod	lynamic
Parameters	146
16. Modeling of DNA via Molecular Dynamics Simulation: Structure, Bending, and Conformational	
Tansitions	260
17. Molecular Dynamics Simulations on Nucleic Acid Systems Using the Cornell et al. Force Field and	Particle
Mesh Ewald Electrostatics	285
18. Observations on the A versus B Equilibrium in Molecular Dynamics Simu8lations of Duplex	
DNA and RNA	304
19. Modeling Duplex DNA Oliagonucleotides with Modified Pyrimidine Bases	312
20. How the TATA Box Selects Its Protein Partner	329
21. RNA Tectonics and Modular Modeling of RNA	346
22. Hairpin Ribozyme Strucuture and Dynamics	360
23. Molecular Modeling Studies on the Ribosome	369
24. Modeling Unusual Nucleic Acid Structures	379
25. Computer RNA Three-Dimensional Modeling from Low-Resolution Data and Multiple-Sequence	
Information	394
26. Comparative Modeling of the Three-Dimensional Structure of Signal Recognition Particle RNA	405

Author Index	415
Affiliation Index	416
Subject Index	417