
CONTENTS

Preface	ix
1 INTRODUCTION	1
1.1. Biochemistry: Studies of Life at the Molecular Level	1
1.2. Computer Science and Computational Sciences	5
1.3. Computational Biochemistry: Application of Computer Technology to Biochemistry	6
References	9
2 BIOCHEMICAL DATA: ANALYSIS AND MANAGEMENT	11
2.1. Statistical Analysis of Biochemical Data	11
2.2. Biochemical Data Analysis with Spreadsheet Application	20
2.3. Biochemical Data Management with Database Program	28
2.4. Workshops	31
References	40
3 BIOCHEMICAL EXPLORATION: INTERNET RESOURCES	41
3.1. Introduction to Internet	41
3.2. Internet Resources of Biochemical Interest	46
3.3. Database Retrieval	48
3.4. Workshops	52
References	52
4 MOLECULAR GRAPHICS: VISUALIZATION OF BIOMOLECULES	53
4.1. Introduction to Computer Graphics	53
4.2. Representation of Molecular Structures	56
4.3. Drawing and Display of Molecular Structures	60
4.4. Workshops	69
References	70

5	BIOCHEMICAL COMPOUNDS: STRUCTURE AND ANALYSIS	73
5.1.	Survey of Biomolecules	73
5.2.	Characterization of Biomolecular Structures	80
5.3.	Fitting and Search of Biomolecular Data and Information ...	87
5.4.	Workshops	98
	References	103
6	DYNAMIC BIOCHEMISTRY: BIOMOLECULAR INTERACTIONS	107
6.1.	Biomacromolecule–Ligand Interactions	107
6.2.	Receptor Biochemistry and Signal Transduction	111
6.3.	Fitting of Binding Data and Search for Receptor Databases ...	113
6.4.	Workshops	119
	References	121
7	DYNAMIC BIOCHEMISTRY: ENZYME KINETICS	123
7.1.	Characterization of Enzymes	123
7.2.	Kinetics of Enzymatic Reactions	126
7.3.	Search and Analysis of Enzyme Data	133
7.4.	Workshops	140
	References	144
8	DYNAMIC BIOCHEMISTRY: METABOLIC SIMULATION	147
8.1.	Introduction to Metabolism	147
8.2.	Metabolic Control Analysis	152
8.3.	Metabolic Databases and Simulation	153
8.4.	Workshops	160
	References	162
9	GENOMICS: NUCLEOTIDE SEQUENCES AND RECOMBINANT DNA	165
9.1.	Genome, DNA Sequence, and Transmission of Genetic Information	165
9.2.	Recombinant DNA Technology	169
9.3.	Nucleotide Sequence Analysis	171
9.4.	Workshops	179
	References	181

10	GENOMICS: GENE IDENTIFICATION	183
10.1.	Genome Information and Features	183
10.2.	Approaches to Gene Identification	185
10.3.	Gene Identification with Internet Resources	188
10.4.	Workshops	204
	References	207
11	PROTEOMICS: PROTEIN SEQUENCE ANALYSIS	209
11.1.	Protein Sequence: Information and Features	209
11.2.	Database Search and Sequence Alignment	213
11.3.	Proteomic Analysis Using Internet Resources: Sequence and Alignment	221
11.4.	Workshops	228
	References	230
12	PROTEOMICS: PREDICTION OF PROTEIN STRUCTURES	233
12.1.	Prediction of Protein Secondary Structures from Sequences ..	233
12.2.	Protein Folding Problems and Functional Sites	236
12.3.	Proteomic Analysis Using Internet Resources: Structure and Function	243
12.4.	Workshops	264
	References	266
13	PHYLOGENETIC ANALYSIS	269
13.1.	Elements of Phylogeny	269
13.2.	Methods of Phylogenetic Analysis	271
13.3.	Application of Sequence Analyses in Phylogenetic Inference ..	275
13.4.	Workshops	280
	References	284
14	MOLECULAR MODELING: MOLECULAR MECHANICS	285
14.1.	Introduction to Molecular Modeling	285
14.2.	Energy Minimization, Dynamics Simulation, and Conformational Search	287
14.3.	Computational Application of Molecular Modeling Packages ..	296
14.4.	Workshops	311
	References	313
15	MOLECULAR MODELING: PROTEIN MODELING	315
15.1.	Structure Similarity and Overlap	315
15.2.	Structure Prediction and Molecular Docking	319

15.3. Applications of Protein Modeling 322

15.4. Workshops 337

References 340

APPENDIX **343**

1. List of Software Programs 343

2. List of World Wide Web Servers 345

3. Abbreviations 353

INDEX **357**