

CONTENTS

Contributors

ix

1. Bioinformatics Tools to Identify and Quantify Proteins Using Mass Spectrometry Data

1

So young Ryu

1. Introduction

2

2. MS Data

2

3. Protein Identification

5

4. Protein Quantification

12

5. Conclusion

15

Acknowledgments

15

References

15

2. Unraveling Oxidation-Induced Modifications in Proteins by Proteomics

19

Carolina Panis

1. A Very Brief Introduction to Oxidative Stress and Redox Homeostasis

20

2. Proteins as Targets of Oxidative Modification

21

3. Redox Proteomics: The Comprehensive Study of Oxidation-Induced Protein Damage

25

4. The Use of Proteomics for Mapping the Redox Homeostasis Network: Lessons from Cancer Research

29

5. Perspectives and Conclusions

33

References

33

3. Role of Proteomics in Biomarker Discovery: Prognosis and Diagnosis of Neuropsychiatric Disorders

39

Suman Patel

1. Summary

40

2. Commonly Used Methods for Proteome Characterization

42

3. Proteomics and Biomarker

46

4. Diagnosis of Neuropsychiatric Disorders

50

5. Proteomics of Neuropsychiatric Disorders

55

6. Strength, Weakness, and Future Challenges: Biomarker Discovery

66

7. Concluding Remarks

67

References

68

4. On the Use of Knowledge-Based Potentials for the Evaluation of Models of Protein-Protein, Protein-DNA, and Protein-RNA Interactions	77
Oriol Fornes, Javier Garcia-Garcia, Jaume Bonet, and Baldo Oliva	
1. Introduction	78
2. Knowledge-Based Potentials	80
3. Modeling of Protein Interactions Using Templates	82
4. Modeling Interactions of Proteins Using Docking	85
5. Prediction of Protein-Binding Regions	93
6. Characterization of Transcription Factor-Binding Sites	98
7. Adapting Split-Statistical Potentials for Protein-DNA Interactions	105
8. Conclusions	109
Acknowledgments	110
References	110
5. Algorithms, Applications, and Challenges of Protein Structure Alignment	121
Jianzhu Ma and Sheng Wang	
1. Introduction	122
2. Structural Alphabet	124
3. Protein Pairwise Structure Alignment	130
4. Protein MSA	155
5. Conclusions and Perspectives	167
References	170
6. Application of Evolutionary Based <i>in Silico</i> Methods to Predict the Impact of Single Amino Acid Substitutions in Vitelliform Macular Dystrophy	177
C. George Priya Doss, Chiranjib Chakraborty, N. Monford Paul Abishek, D. Thirumal Kumar, and Vaishnavi Narayan	
1. Introduction	178
2. Materials and Methods	183
3. Results	188
4. Discussion	263
5. Conclusion	263
Acknowledgments	264
References	264

7. Current State-of-the-Art Molecular Dynamics Methods and Applications	269
Dimitrios Vlachakis, Elena Bencurova, Nikitas Papangelopoulos, and Sophia Kossida	
1. Introduction	270
2. The Role of Computer Experiments in Modern Science	272
3. Brief History of Computer Molecular Simulations	274
4. Physics in MD	276
5. Algorithms for MD Simulations	278
6. Computational Complexity of MD Simulations and Methods to Increase Efficiency	281
7. High-Performance Parallel Computing	285
8. General-Purpose Computing Using Graphics Processing Units	288
9. Software for MD Simulations	290
10. Force Fields for MD	293
11. Current Limitations of MD	307
12. Conclusions	308
Acknowledgments	309
References	309
8. Intrinsically Disordered Proteins—Relation to General Model Expressing the Active Role of the Water Environment	315
Barbara Kalinowska, Mateusz Banach, Leszek Konieczny, Damian Marchewka, and Irena Roterman	
1. Introduction	316
2. Definition of the Fuzzy Oil Drop Model	317
3. Results	324
4. Discussion	339
5. Conclusions	343
Acknowledgments	344
References	344
9. Conformational Elasticity can Facilitate TALE-DNA Recognition	347
Hongxing Lei, Jiya Sun, Enoch P. Baldwin, David J. Segal, and Yong Duan	
1. Introduction	348
2. Methods	350

3. Results	352
4. Discussion	360
Acknowledgments	363
References	363
10. Computational Approaches and Resources in Single Amino Acid Substitutions Analysis Toward Clinical Research	365
C. George Priya Doss, Chiranjib Chakraborty, Vaishnavi Narayan, and D. Thirumal Kumar	
1. Introduction	366
2. Computational Methods in SAP Analysis	371
3. Database Resources for SAPs	374
4. Molecular Phenotypic Effect Analysis	375
5. Sequence Information Analysis	376
6. Computational Methods for Structure Determination	377
7. Docking	380
8. Types of Docking	391
9. Molecular Dynamics	393
10. Concluding Remarks	396
Acknowledgments	399
References	399
Author Index	425
Subject Index	461