1. Record Nr. UNINA9910555012203321

Titolo	Computation in bioinformatics : multidisciplinary applications / / editors, S. Balamurugan [et al.]
Pubbl/distr/stampa	Hoboken, NJ : , : John Wiley & Sons, Inc., , 2021
ISBN	1-119-65476-9 1-119-65480-7 1-119-65475-0
Descrizione fisica	1 online resource (352 pages)
Collana	Artificial Intelligence and So Computing for Industrial Transformation
Disciplina	570.285
Soggetti	Bioinformatics Computational biology
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Cover -- Half-Title Page -- Series Page -- Title Page -- Copyright Page -- Contents -- Preface -- 1 Bioinfomatics as a Tool in Drug Designing -- 1.1 Introduction -- 1.2 Steps Involved in Drug Designing -- 1.2.1 Identification of the Target Protein/Enzyme -- 1.2.2 Detection of Molecular Site (Active Site) in the Target Protein -- 1.2.3 Molecular Modeling -- 1.2.4 Virtual Screening -- 1.2.5 Molecular Docking -- 1.2.6 QSAR (Quantitative Structure-Activity Relationship) -- 1.2.7 Pharmacophore Modeling -- 1.2.8 Solubility of Molecule -- 1.2.9 Molecular Dynamic Simulation -- 1.2.10 ADME Prediction -- 1.3 Various Softwares Used in the Steps of Drug Designing -- 1.4 Applications -- 1.5 Conclusion -- References -- 2 New Strategies in Drug Discovery -- 2.1 Introduction -- 2.2 Road Toward Advancement -- 2.3 Methodology -- 2.3.1 Target Identification -- 2.3.2 Docking-Based Virtual Screening -- 2.3.3 Conformation Sampling -- 2.3.4 Scoring Function -- 2.3.5 Molecular Similarity Methods -- 2.3.6 Virtual Library Construction -- 2.3.7 Sequence-Based Drug Design -- 2.4 Role of OMICS Technology -- 2.5 High-Throughput Screening and Its Tools -- 2.6 Chemoinformatic -- 2.6.1 Exploratory Data Analysis -- 2.6.2 Example Discovery -- 2.6.3 Pattern Explanation -- 2.6.4 New Technologies -- 2.7 Concluding Remarks and Future Prospects -- References -- 3 Role of Bioinformatics in Early Drug Discovery: An

Overview and Perspective -- 3.1 Introduction -- 3.2 Bioinformatics and Drug Discovery -- 3.2.1 Structure-Based Drug Design (SBDD) -- 3.2.2 Ligand-Based Drug Design (LBDD) -- 3.3 Bioinformatics Tools in Early Drug Discovery -- 3.3.1 Possible Biological Activity Prediction Tools -- 3.3.2 Possible Physicochemical and Drug-Likeness Properties Verification Tools -- 3.3.3 Possible Toxicity and ADME/T Profile Prediction Tools -- 3.4 Future Directions With Bioinformatics Tool. 3.5 Conclusion -- Acknowledgements -- References -- 4 Role of Data Mining in Bioinformatics -- 4.1 Introduction -- 4.2 Data Mining Methods/Techniques -- 4.2.1 Classification -- 4.2.1.1 Statistical Techniques -- 4.2.1.2 Clustering Technique -- 4.2.1.3 Visualization -- 4.2.1.4 Induction Decision Tree Technique -- 4.2.1.5 Neural Network -- 4.2.1.6 Association Rule Technique -- 4.2.1.7 Classification -- 4.3 DNA Data Analysis -- 4.4 RNA Data Analysis -- 4.5 Protein Data Analysis -- 4.6 Biomedical Data Analysis -- 4.7 Conclusion and Future Prospects -- References -- 5 In Silico Protein Design and Virtual Screening -- 5.1 Introduction -- 5.2 Virtual Screening Process -- 5.2.1 Before Virtual Screening -- 5.2.2 General Process of Virtual Screening -- 5.2.2.1 Step 1 (The Establishment of the Receptor Model) -- 5.2.2.2 Step 2 (The Generation of Small-Molecule Libraries) -- 5.2.2.3 Step 3 (Molecular Docking) -- 5.2.2.4 Step 4 (Selection of Lead Protein Compounds) -- 5.3 Machine Learning and Scoring Functions -- 5.4 Conclusion and Future Prospects -- References -- 6 New Bioinformatics Platform-Based Approach for Drug Design -- 6.1 Introduction -- 6.2 Platform-Based Approach and Regulatory Perspective -- 6.3 Bioinformatics Tools and Computer-Aided Drug Design -- 6.4 Target Identification -- 6.5 Target Validation -- 6.6 Lead Identification and Optimization -- 6.7 High-Throughput Methods (HTM) -- 6.8 Conclusion and Future Prospects -- References -- 7 Bioinformatics and Its Application Areas -- 7.1 Introduction -- 7.2 Review of Bioinformatics -- 7.3 Bioinformatics Applications in Different Areas -- 7.3.1 Microbial Genome Application -- 7.3.2 Molecular Medicine -- 7.3.3 Agriculture -- 7.4 Conclusion -- References -- 8 DNA Microarray Analysis: From Affymetrix CEL Files to Comparative Gene Expression -- 8.1 Introduction -- 8.2 Data Processing. 8.2.1 Installation of Workflow -- 8.2.2 Importing the Raw Data for Processing -- 8.2.3 Retrieving Sample Annotation of the Data -- 8.2.4 Quality Control -- 8.3 Normalization of Microarray Data Using the RMA Method -- 8.3.1 Background Correction -- 8.3.2 Normalization -- 8.3.3 Summarization -- 8.4 Statistical Analysis for Differential Gene Expression -- 8.5 Conclusion -- References -- 9 Machine Learning in Bioinformatics -- 9.1 Introduction and Background -- 9.1.1 Bioinformatics -- 9.1.2 Text Mining -- 9.1.3 IoT Devices -- 9.2 Machine Learning Applications in Bioinformatics -- 9.3 Machine Learning Approaches -- 9.4 Conclusion and Closing Remarks -- References -- 10 DNA-RNA Barcoding and Gene Sequencing -- 10.1 Introduction -- 10.2 RNA -- 10.3 DNA Barcoding -- 10.3.1 Introduction -- 10.3.2 DNA Barcoding and Molecular Phylogeny -- 10.3.3 Ribosomal DNA (rDNA) of the Nuclear Genome (nuDNA)-ITS -- 10.3.4 Chloroplast DNA -- 10.3.5 Mitochondrial DNA -- 10.3.6 Molecular Phylogenetic Analysis -- 10.3.7 Metabarcoding -- 10.3.8 Materials for DNA Barcoding -- 10.4 Main Reasons of DNA Barcoding -- 10.5 Limitations/Restrictions of DNA Barcoding -- 10.6 RNA Barcoding -- 10.6.1 Overview of the Method -- 10.7 Methodology -- 10.7.1 Materials Required -- 10.7.2 Barcoded RNA Sequencing High-Level Mapping of Single-Neuron Projections -- 10.7.3 Using RNA to Trace Neurons -- 10.7.4 A Life Conservation Barcoder -- 10.7.5 Gene Sequencing -- 10.7.5.1 DNA Sequencing Methods -- 10.7.5.2 First-