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Titolo	Sustainable Technologies for Transforming Businesses and Societies : The Keynote Lectures of the 6th International Conference on Entrepreneurship, Innovation and Leadership (ICEIL 2024) / / edited by Balvinder Shukla, K. M. Soni, Nitasha Hasteer
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Collana	Transactions on Computer Systems and Networks, , 2730-7492
Disciplina	006.3
Soggetti	Computational intelligence Artificial intelligence Quantitative research Computational Intelligence Artificial Intelligence Data Analysis and Big Data
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Dyadic Human-Robot Interaction: Emerging Technologies, Challenges, and Opportunities -- A Short Bibliometric Review of Metaheuristics -- Queuing for Civility: Regulating Emotions and Reducing Toxicity in Digital Discourse -- Effect of Multiwalled carbon nanotubes on the compressive strength and microstructural property of rubberized concrete using RSM modelling -- Complex Fermatean fuzzy graph and its application in networking problems.-South African Perceptions on Artificial Intelligence in the Context of Morality and Sentience.-Etc.
Sommario/riassunto	This edited volume is a compilation of peer-reviewed papers from the plenary lectures, keynote speeches, special presentations, and young researchers' lectures delivered at the 6th International Conference on Innovation, Entrepreneurship, and Leadership (ICEIL-2024). The book focuses on sustainability and the promotion of new ideas and innovations in areas such as generative artificial intelligence, the metaverse, blockchain, and the Internet of Things. It highlights the global impact of these advancements on businesses and societies.

	Presenting the latest research, information, technological advancements, practical challenges encountered, and solutions adopted in the field of innovation for sustainable technologies, this volume will be of interest to both academics and industry professionals. Readers will gain a comprehensive perspective on technological advancements that support indigenous innovations and their practical applications.

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Titolo	Protein-protein complexes : analysis, modeling and drug design / / edited by Martin Zacharias
Pubbl/distr/stampa	London, : Imperial College Press, 2010
ISBN	9786612759840 9781282759848 1282759841 9781848163409 1848163401
Edizione	[1st ed.]
Descrizione fisica	1 online resource (400 p.)
Altri autori (Persone)	ZachariasMartin
Disciplina	572.6 572.64
Soggetti	Protein-protein interactions Protein-protein interactions - Computer simulation Protein-protein interactions - Mathematical models Proteins - Structure Drugs - Design
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
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Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
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Evolutionary Important Residues -- 5.5 Molecular Determinants of GPCR Signal Transduction -- 5.6 Protein Function Prediction -- References -- 6. Protein-Protein Docking Adrien Saladin and Chantal Prevost -- 6.1 Introduction -- 6.2 Definition and Goals of Macromolecular Docking -- 6.2.1 Protein-Protein Docking Terminology -- 6.2.2 Goals and Strategies -- 6.3 Protein-Protein Docking Methods -- 6.3.1 Systematic Search Methods -- 6.3.1.1 Discrete Sampling: The Correlation Methods -- 6.3.1.2 Geometric Surface Matching -- 6.3.2 Guided Search Methods -- 6.3.2.1 Example of a Guided Search Programme: ICM-DISCO -- 6.3.2.2 Speeding up the Calculation -- 6.3.2.3 Data-driven Methods -- 6.3.3 Refinement -- 6.3.3.1 Increasing the Resolution -- 6.3.3.2 Accounting for Side Chain Conformational Change -- 6.3.3.3 Explicit Solvation -- 6.3.3.4 Hierarchical Approaches -- 6.3.4 Scoring the Predictions -- 6.4 Evaluation of the Docking Methods -- 6.4.1 The CAPRI Experience -- 6.4.2 Docking Benchmarks -- 6.4.3 Challenges -- 6.5 Conclusions and Outlook -- Acknowledgements -- References -- 7. Data-driven Docking: Using External Information to Spark the Biomolecular Rendez-vous Adrien S.J. Melquiond and Alexandre M.J.J. Bonvin -- 7.1 Introduction -- 7.2 Stoichiometry and Composition -- 7.3 Shape of a Biomolecular Complex -- 7.4 Nature of the Interface: Which Residues are Engaged in a Date? -- 7.5 Orientation and Symmetry Problems.
7.6 Flexibility: How to Cope with Conformational Changes Occurring upon Complex Formation? -- 7.7 How to Implement Data-driven Docking, the HADDOCK Example -- 7.8 Conclusions and Outlook -- Acknowledgements -- References -- 8. High-resolution Protein-Protein Docking Nir London and Ora Schueler-Furman -- 8.1 Introduction -- 8.1.1 From Molecules to Networks: Making Sense of Large-scale Data, Starting from the Atomic Details of Protein-Protein Interactions -- 8.1.2 Docking - The Creation of Protein Complex Structures Starting from the Monomers -- 8.1.3 Explicit Modelling of the Atomic Details of the Protein-Protein Interface Allows Distinguishing the Correct from Alternative Conformations -- 8.1.4 The Scope of this Chapter -- 8.2 High-resolution Docking, as Defined by CAPRI -- 8.3 Accounting for Conformational Changes of Monomers is Crucial to High-resolution Modelling -- 8.3.1 Modelling Side Chain Flexibility -- 8.3.2 Taking it to the Next Step: Modelling Backbone Flexibility -- 8.3.2.1 Ensemble Docking -- 8.3.2.2 Refinement and Minimization -- 8.3.2.3 Modelling Hinge Motion -- 8.4 The High-resolution RosettaDock Protocol - Explicit Modelling of Full Side Chain Flexibility (and Beyond) Allows Accurate Modelling of Protein Complexes -- 8.4.1 Adding Backbone Conformational Flexibility to the RosettaDock Protocol -- 8.4.2 Ensemble Docking with RosettaDock -- 8.5 Additional High-resolution Docking Approaches -- 8.5.1 High-accuracy Modelling with Rigid Body Docking -- 8.5.2 A New Generation of Docking Protocols: Combining Successful Approaches of Low-resolution and High-resolution Searches -- 8.6 The Contribution of High-resolution Docking to the Understanding of Interactions of Biological Interest -- 8.6.1 Entry Mechanism of Anthrax Toxin -- 8.6.2 Antitumor Monoclonal Antibody 806 (mAb806) and the Epidermal Growth Factor Receptor (EGFR).
8.6.3 High-resolution Docking in the Service of Biochemistry -- 8.6.4 Applications of High-resolution Docking: Structure-based Prediction of Binding Specificity -- 8.7 Conclusions and Outlook -- 8.7.1 Impact of Docking on the Modelling Field -- Acknowledgements -- References -- 9. Scoring and Refinement of Predicted Protein-Protein Complexes Martin Zacharias -- 9.1 Introduction -- 9.2 Generation of Protein-Protein Complexes by Docking Methods -- 9.3 Protein-Protein

Complexes Based on Homology to Known Complexes -- 9.4 Structural Refinement of Modelled Protein-Protein Complexes -- 9.4.1 Force Field Description of Proteins and Protein Complexes -- 9.4.2 Optimization Based on Energy Minimization -- 9.4.3 Accounting for Global Conformational Changes -- 9.4.4 Molecular Dynamics Simulation of Protein-Protein Complexes -- 9.4.5 Refinement of Docked Complexes by Molecular Dynamics Simulation -- 9.4.6 Monte Carlo and Brownian Dynamics Refinement of Docked Complexes -- 9.5 Scoring of Modelled Protein-Protein Complexes -- 9.5.1 Driving Forces for Molecular Association and the Scoring Problem -- 9.5.2 Scoring Based on Physical Force Fields -- 9.5.2.1 Scoring Based on Ensembles of Structures -- 9.5.3 Knowledge-based Scoring of Docked Complexes -- 9.5.3.1 Principles of Statistical Potentials to Score Predicted Complexes -- 9.5.3.2 Application of Statistical Potentials to Score Predicted Complexes -- 9.6 Conclusions and Outlook -- Acknowledgements -- References -- 10. Motif-mediated Protein Interactions and their Role in Disease Holger Dinkel and Heinrich Sticht -- 10.1 Introduction -- 10.2 Protein Interaction Domains -- 10.2.1 SH3 Domains -- 10.2.2 SH2 Domains -- 10.2.3 Signalling Adaptors: Proteins Containing Multiple Interaction Domains -- 10.3 Properties and Regulation of Motif-mediated Interactions -- 10.3.1 Inducible Interactions -- 10.3.2 Cooperative Effects.
10.3.3 Mutually Exclusive Interactions.

Sommario/riassunto

Given the immense progress achieved in elucidating protein-protein complex structures and in the field of protein interaction modeling, there is great demand for a book that gives interested researchers/students a comprehensive overview of the field. This book does just that. It focuses on what can be learned about protein-protein interactions from the analysis of protein-protein complex structures and interfaces. What are the driving forces for protein-protein association? How can we extract the mechanism of specific recognition from studying protein-protein interfaces? How can this knowledge be used to predict and design protein-protein interactions (interaction regions and complex structures)? What methods are currently employed to design protein-protein interactions, and how can we influence protein-protein interactions by mutagenesis and small-molecule drugs or peptide mimetics?The book consists of about 15 review chapters, written by experts, on the characterization of protein-protein interfaces, structure determination of protein complexes (by NMR and X-ray), theory of protein-protein binding, dynamics of protein interfaces, bioinformatics methods to predict interaction regions, and prediction of protein-protein complex structures (docking and homology modeling of complexes, etc.) and design of protein-protein interactions. It serves as a bridge between studying/analyzing protein-protein complex structures (interfaces), predicting interactions, and influencing/designing interactions.