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Titolo	Handbook of chemoinformatics algorithms / / editors, Jean-Loup Faulon, Andreas Bender
Pubbl/distr/stampa	Boca Raton : , : Chapman & Hall/CRC, , 2010
ISBN	0-429-14091-6 1-4200-8299-X
Descrizione fisica	1 online resource (454 p.)
Collana	Chapman & Hall/CRC mathematical and computational biology series
Altri autori (Persone)	FaulonJean-Loup BenderAndreas <1976->
Disciplina	542/.85
Soggetti	Cheminformatics Algorithms Graph theory Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Front Cover; Contents; Preface; Acknowledgments; Contributors; Chapter 1: Representing Two-Dimensional (2D) Chemical Structureswith Molecular Graphs; Chapter 2: Algorithms to Store and Retrieve Two-Dimensional (2D) Chemical Structures; 3 Three-Dimensional (3D) MolecularRepresentations; Chapter 4: Molecular Descriptors; 5 Ligand- andStructure-Based VirtualScreening; Chapter 6: Predictive Quantitative Structure-Activity Relationships Modeling; Chapter 7: Predictive Quantitative Structure-Activity Relationships Modeling; Chapter 8: Structure Enumeration and Sampling Chapter 9: Computer-Aided Molecular DesignChapter 10: Computer-Aided Molecular Design; Chapter 11: Reaction Network Generation; Chapter 12: Open Source Chemoinformatics Software and DatabaseTechnologies; Chapter 13: Sequence Alignment Algorithms; Chapter 14: Machine Learning-Based Bioinformatics Algorithms; Chapter 15: Using Systems Biology Techniques to Determine Metabolic Fluxes and Metabolite Pool Sizes; Index; Back Cover
Sommario/riassunto	Describing the characteristics and limitations of key algorithms, this book covers various aspects of chemoinformatics, including structure

representation, molecular descriptors, similarity search, virtual screening, and structure-property model generation and validation.