1. Record Nr. UNINA9910830816903321

Titolo	Chemoinformatics : a textbook / / Johann Gasteiger and Thomas Engel (editors)
Pubbl/distr/stampa	Weinheim : , : Wiley-VCH GmbH & Co. KGaA, , [2003] ©2003
ISBN	1-280-55862-8 9786610558629 3-527-60650-5 3-527-60164-3
Descrizione fisica	1 online resource (682 p.)
Disciplina	542.85
Soggetti	Cheminformatics Structure-activity relationships (Biochemistry) Chemical reactions
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes index.
Nota di contenuto	Chemoinformatics; Foreword; Contents; Preface; Addresses of the Authors; 1 Introduction; 1.1 The Domain of Chemistry; 1.2 A Chemist's Fundamental Questions; 1.3 The Scope of Chemoinformatics; 1.4 Learning in Chemoinformatics; 1.5 Major Tasks; 1.5.1 Representation of the Objects; 1.5.2 Data; 1.5.3 Learning; 1.6 History of Chemoinformatics; 1.6.1 Structure Databases; 1.6.2 Quantitative Structure-Activity Relationships; 1.6.3 Molecular Modeling; 1.6.4 Structure Elucidation; 1.6.5 Chemical Reactions and Synthesis Design; 1.7 The Scope of this Book; 1.8 Teaching Chemoinformatics 2 Representation of Chemical Compounds2.1 Introduction; 2.2 Chemical Nomenclature; 2.2.1 Development of Chemical Nomenclature; 2.2.2 Representation of Chemical Elements; 2.2.2.1 Characterization of Elements; 2.2.3 Representation of the Empirical Formulas of (Inorganic) Compounds; 2.2.3.1 Present-Day Representation; 2.2.4 Representation of the Empirical Formulas of Organic Compounds; 2.2.4.1 Present-Day Representation; 2.2.5 Systematic Nomenclature of Inorganic and Organic Compounds; 2.3 Line Notations; 2.3.1 Wiswesser Line

Notation; 2.3.1.1 Applications; 2.3.2 ROSDAL; 2.3.2.1 Applications
2.3.3 The SMILES Coding2.3.3.1 Applications; 2.3.4 Sybyl Line Notation; 2.3.4.1 Applications; 2.4 Coding the Constitution; 2.4.1 Graph Theory; 2.4.1.1 Basics of Graph Theory; 2.4.2 Matrix Representations; 2.4.2.1 Adjacency Matrix; 2.4.2.2 Distance Matrix; 2.4.2.3 Atom Connectivity Matrix; 2.4.2.4 Incidence Matrix; 2.4.2.5 Bond Matrix; 2.4.3 Connection Table; 2.4.4 Input and Output of Chemical Structures; 2.4.5 Standard Structure Exchange Formats; 2.4.6 Tutorial: Molfiles and SDfiles; 2.4.6.1 Structure of a Molfile; 2.4.6.2 Structure of an SDfile; 2.4.6.3 Libraries and Toolkits
2.5 Processing Constitutional Information2.5.1 Ring Perception; 2.5.1.1 Minimum Number of Cycles; 2.5.1.2 All Cycles; 2.5.1.3 Smallest Fundamental Basis; 2.5.2 Unambiguous and Unique Representations; 2.5.2.1 Structure Isomers and Isomorphism; 2.5.2.2 Canonicalization; 2.5.3 The Morgan Algorithm; 2.5.3.1 Tutorial: Morgan Algorithm; 2.6 Beyond a Connection Table; 2.6.1 Deficiencies in Representing Molecular Structures by a Connection Table; 2.6.2 Representation of Molecular Structures by Electron Systems; 2.6.2.1 General Concepts; 2.6.2.2 Simple Single and Double Bonds
2.6.2.3 Conjugation and Aromaticity2.6.2.4 Orthogonality of -Systems; 2.6.2.5 Non-bonding Orbitals; 2.6.2.6 Charged Species and Radicals; 2.6.2.7 Ionized States; 2.6.2.8 Electron-Deficient Compounds; 2.6.2.9 Organometallic Compounds; 2.6.3 Generation of RAMSES from a VB Representation; 2.7 Special Notations of Chemical Structures; 2.7.1 Markush Structures; 2.7.2 Fragment Coding; 2.7.2.1 Applications; 2.7.3 Fingerprints; 2.7.3.1 ""Hashed Fingerprints""; 2.7.4 Hash Codes; 2.7.4.1 Applications; 2.8 Representation of Stereochemistry; 2.8.1 General Concepts
2.8.2 Representation of Configuration Isomers and Molecular Chirality

Sommario/riassunto

This first work to be devoted entirely to this increasingly important field, the ""Textbook"" provides both an in-depth and comprehensive overview of this exciting new area.Edited by Johann Gasteiger and Thomas Engel, the book provides an introduction to the representation of molecular structures and reactions, data types and databases/data sources, search methods, methods for data analysis as well as such applications as structure elucidation, reaction simulation, synthesis planning and drug design. A ""hands-on"" approach with step-by-step tutorials and detailed descriptions of software