Chemoinformatics: A Textbook

By -

Wiley-VCH, 2003. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service! Summary: Foreword.Preface.Addresses of the Authors.1. Introduction.1.1. The Domain of Chemistry.1.2. A Chemists 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. 101.6.2. 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 Compounds.2.1. 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 Coding.2.3.3.1. 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

Reviews

An exceptional pdf and the typeface utilized was fascinating to read through. It can be writter in straightforward words and phrases instead of confusing. I am just quickly could possibly get a delight of looking at a written ebook.
-- Prof. Arlie Bogan

It in a single of the best book. This is for those who statte there had not been a well worth reading through. Once you begin to read the book, it is extremely difficult to leave it before concluding.
-- Dr. Barney Robel Jr.