

1. Record Nr.	UNINA9910146237303321
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 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 Structures; 2.4.5 Standard
Structure Exchange Formats; 2.4.6 Tutorial: Molfiles and SDFfiles;
2.4.6.1 Structure of a Molfile; 2.4.6.2 Structure of an SDFfile; 2.4.6.3
Libraries and Toolkits
2.5 Processing Constitutional Information 2.5.1 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 Aromaticity 2.6.2.4 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

2. Record Nr.	UNINA9910793736403321
Titolo	Education for employability . Volume 2 Learning for future possibilities // edited by Joy Higgs, Geoffrey Crisp and Will Letts [[electronic resource]]
Pubbl/distr/stampa	Leiden, The Netherlands ; ; Boston : , : Brill Sense, , 2019 2019
ISBN	9789004418707 (electronic book)
Descrizione fisica	1 online resource (ix, 277 pages.) : illustrations
Collana	Practice futures ; ; 4
Soggetti	Education, Higher - Aims and objectives College graduates - Employment Employability
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references.
Sommario/riassunto	We often look back at changing trends in higher education and call them "bandwagons" (temporary fads that everyone rushes to be part of and "jump on"). While much of the hype and jargon of "The Employability Agenda" may fade from the tip of our tongues (or perhaps be subsumed into the norm) in the mid future, there are two fundamental changes that will not: the digital revolution embedded in changing work and economic practices and the "re-globalisation" of the world that this and other politico-economic changes have brought about. These will continue to be part of how we live and work, so tertiary education will need to take its part in supporting employ-ability far beyond either the timing or scope of preparation for initial employment. Employability is important to local, national and international labour market contexts, parameters and policies. As well as impacting workforces, employability is an essential characteristic of workers. It is very important that employability is understood and enacted as personal employability not just employment of individuals. We have found that employability is defined as much, if not more, by mindset rather than skillset. Part of this mindset involves recognising

the unknowns of future work and an even bigger part is recognising our responsibilities as workers and educators lies in shaping our own employability and that of the novice learners and workers in our spaces of influence and communities of practice. In Education for Employability (Volume 2): Learning for Future Possibilities we continue on from the big agenda discussions of Education for Employability (Volume 1): The Employability Agenda to explore education for employability in a variety of spaces: in the context of higher education as an entrance into the workforce, in joining communities of practice and in the lifelong pursuit of employability – preparing people for a portfolio of careers rather than a job-for-life. These two books show how educational leaders, educators, industry partners and thought leaders are imagining and addressing the challenges posed by the current and future changes facing our work, practices and workplaces.--

3. Record Nr.	UNINA9910974100303321
Titolo	Economist with a public purpose : essays in honour of John Kenneth Galbraith // edited by Michael Keaney
Pubbl/distr/stampa	London ; ; New York, : Routledge, 2001
ISBN	1-134-61456-X 1-134-61457-8 0-429-23241-1 1-280-31761-2 0-203-46116-9 0-203-25331-0
Edizione	[1st ed.]
Descrizione fisica	1 online resource (287 p.)
Collana	Routledge frontiers of political economy ; ; 32
Altri autori (Persone)	GalbraithJohn Kenneth <1908-2006.> KeaneyMichael <1968->
Disciplina	330/.092
Soggetti	Economists - United States Economics
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

Book Cover; Title; Contents; List of contributors; Acknowledgements; John Kenneth Galbraith: economist with a public purpose; The useful economist; The making of a heterodox economist: the impact of Henry S. Dennison on the economic thought of John Kenneth Galbraith; Social capital and political economy: Galbraith on states and groups; The role of the state in the good society; From Veblen to Galbraith: what is the essence of institutional economics?; The virtues of their defects and the defects of their virtues: reflections on John Kenneth Galbraith and Thorstein Veblen
The economist and business Galbraith, uncertainty and the modern corporation; Progress denied: the unraveling of the New Industrial State; Galbraith, globalism and the good life: making the best of the capitalist predicament; The New Deal and 'domesticated Keynesianism' in America; Adam Smith on the mercantile system: the unnecessary loss of America?; Index

Sommario/riassunto

This text discusses the continuing relevance of one of the most prominent economists of the twentieth century. The contributors explore the continuing relevance of Galbraith's arguments to current controversies and problems.
