1.	Record Nr.	UNINA9910456114303321
	Titolo	Frontiers in polar biology in the genomic era [[electronic resource] /] / Committee on Frontiers in Polar Biology, Polar Research Board, National Research Council of the National Academies
	Pubbl/distr/stampa	Washington, D.C., : National Academies Press, 2003
	ISBN	1-280-18014-5
		9786610180141
		0-309-51229-8
	Descrizione fisica	1 online resource (185 p.)
	Disciplina	577.5/86
	Soggetti	Marine biology - Polar Regions
		Marine biology - Arctic regions
		Biology - Polar Regions
		Biology - Arctic regions
		Genomes
		Electronic books.
	Lingua di pubblicazione	Inglese
	Formato	Materiale a stampa
	Livello bibliografico	Monografia
	Note generali	Issued in conjunction with the Workshop on Frontiers in Polar Biology, held Sept. 9-10, 2002, in Tahoe City, Calif.
	Nota di bibliografia	Includes bibliographical references.

2. **Record Nr.** UNISALENTO991002604589707536

Titolo Finzioni. - 1979-(??)

Pubbl/distr/stampa Genova, 1979- (??)

Lingua di pubblicazione Italiano

Formato Materiale a stampa

Livello bibliografico Periodico

3. **Record Nr.** UNINA9910824359903321

Autore Kerber Adalbert

Titolo Mathematical chemistry and chemoinformatics : structure generation, elucidation, and quantitative structure-property relationships / / Adalbert Kerber [and four others]

Pubbl/distr/stampa Berlin : , : Walter de Gruyter GmbH & Co., KG, , [2014]
©2014

Descrizione fisica 1 online resource (521 p.)

Classificazione VE 5300

Disciplina 542/.85

Soggetti Cheminformatics
Chemistry - Mathematics

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 matter -- Preface -- Contents -- List of figures -- List of figures -- List of symbols -- Introduction and outline -- 1. Basics of graphs and molecular graphs -- 2. Advanced properties of molecular graphs -- 3. Chirality -- 4. Stereoisomers -- 5. Molecular structure generation -- 6. Supervised statistical learning -- 7. Quantitative structure-property relationships -- 8. Molecular structure elucidation -- 9. Case studies of CASE -- A. Lists of molecular descriptors -- B. Substructures for MS classifiers -- C. Molecular formulas by mass and ion type -- D. Isomers by mass and molecular formula -- Bibliography -- Index

Sommario/riassunto More than 20 years of experience in molecular structure generation,

from conceptualization through to applications Innovative, interdisciplinary text demonstrating example queries with software packages such as MOLGEN-online Detailed explanations on establishing QSPRs and QSARs as well as structure elucidation using mass spectrometry and structure generation. Aims and Scope This work provides an introduction to mathematical modeling of molecules and the resulting applications (structure generation, structure elucidation, QSAR/QSPR etc.). Most chemists have experimented with some software that represents molecules in an electronic form, and such models and applications are of increasing interest in diverse and growing fields such as drug discovery, environmental science and metabolomics. Furthermore, structure generation remains the only way to systematically create molecules that are not (yet) present in a database. This book starts with the mathematical theory behind representing molecules, explaining chemical concepts in mathematical terms and providing exercises that can be completed online. The later chapters cover applications of the theory, with detailed explanations on QSPR and QSAR investigations and finally structure elucidation combining mass spectrometry and structure generation. This book is aimed in particular at the users of structure generation methods and corresponding techniques, but also for those interested in teaching and learning mathematical chemistry, and for software designers in chemoinformatics.