1. Record Nr. UNINA9910824359903321

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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.