1. Record Nr. UNISA996201053203316

Titolo	Reviews in computational chemistry . Volume 18 [[electronic resource] /] / edited by Kenny B. Lipkowitz and Donald B. Boyd
Pubbl/distr/stampa	New York, N.Y., : Wile-VCH, c2002
ISBN	1-280-36682-6 9786610366828 0-470-34940-9 0-471-46142-3 0-471-43351-9
Edizione	[1st ed.]
Descrizione fisica	1 online resource (384 p.)
Collana	Reviews in computational chemistry ; ; v. 18
Altri autori (Persone)	BoydDonald B LipkowitzKenny B
Disciplina	542.85 542/.8
Soggetti	Chemistry - Data processing 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	Reviews in Computational Chemistry Volume 18; Preface; Epilogue and Dedication; Contents; Contributors; Contributors to Previous Volumes*; Topics Covered in Volumes 1-18*; 1. Clustering Methods and Their Uses in Computational Chemistry; 2. The Use of Scoring Functions in Drug Discovery Applications; 3. Potentials and Algorithms for Incorporating Polarizability in Computer Simulations; 4. New Developments in the Theoretical Description of Charge-Transfer Reactions in Condensed Phases; 5. Linear Free Energy Relationships Using Quantum Mechanical Descriptors 6. The Development of Computational Chemistry in GermanyAppendix. Examination of the Employment Environment for Computational Chemistry; Author Index; Subject Index
Sommario/riassunto	This volume, like those prior to it, features chapters by experts in various fields of computational chemistry. Topics covered in Volume 18 include molecular modeling, computer-assisted molecular design (camd), quantum chemistry, molecular mechanics and dynamics, and

quantitative structure-activity relationships (qsar).