1. Record Nr. UNINA9910144317103321

Titolo	Reviews in computational chemistry . Volume 16 [[electronic resource] /] / edited by Kenny B. Lipkowitz and Donald B. Boyd
Pubbl/distr/stampa	New York, : Wiley-VCH, 2000
ISBN	1-282-30831-9 9786612308314 0-470-12593-4 0-470-12621-3
Descrizione fisica	1 online resource (370 p.)
Collana	Reviews in computational chemistry ; ; 16
Altri autori (Persone)	LipkowitzKenny B BoydDonald 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 indexes.
Nota di contenuto	Reviews in Computational Chemistry Volume 16; Contents; Computer-Aided Molecular Diversity Analysis and Combinatorial Library Design; Introduction; Molecular Recognition: Similarity and Diversity; Describing Diversity Space; Types of Descriptor; Choosing Appropriate Descriptors; Validation of Descriptors; Applications; Diversity Analysis; Combinatorial Library Design; Diversity Is Not the Be-All and End-All!; Current Issues and Future Directions; Diversity Descriptors; Library Design; Speed Requirement; "Quick and Dirty" QSAR; Integration with Other Modeling Tools; Persuading the Customers ConclusionsAcknowledgments; References; Artificial Neural Networks and Their Use in Chemistry; Introduction; Overview and Goals; What Are Artificial Neural Networks?; Analogy with the Brain; Artificial Neural Networks; Summary of Neural Network Operation; Brief History of Neural Networks; What Can Neural Networks Be Used for and When Should You Use Them?; Classification; Modeling; Mapping and Associations; General Comments on ANNs, Statistics, and Artificial Intelligence; Processing Elements; Summation Functions; Transfer

Functions; Output Functions; Error Functions; Learning Rules
Collections of Processing ElementsDifferent Types of Artificial Neural Network; Adaptive Resonance Theory (ART) Networks; Backpropagation (BP) and Related Networks; Biassociative Memory (BAM) Networks; Counterpropagation Networks; Generalized Regression Networks (GRN); Hopfield Networks; Kohonen Self-organizing Map (SOM) Networks; Perceptron Networks; Radial Basis Function (RBF) Networks; Recirculation Networks; Miscellaneous Networks; Practical Considerations in Solving Problems with Neural Networks; What Type of Network?; Data Preprocessing
Variable Selection, Reduction, and OrthogonalizationTraining and Testing Sets; Training the Network; Learning Versus Generalization; Performance Metrics; Classification Problems; Nonclassification, Supervised Learning Problems; Miscellaneous Remarks; Analysis of Neural Networks; Concluding Remarks; Appendix: Neural Network Software; References; Use of Force Fields in Materials Modeling; Introduction; The Force Field Approach to Describing Structures of Materials; What Are Force Fields?; Ion Pair and Shell Model Potentials; Molecular Mechanics Force Fields
Comparison of Ion Pair and Molecular Mechanics Force FieldsForce Field Parameterization; Ab Initio Based Force Fields; Empirical Force Fields; Transferability; Rule-Based Force Fields; Application of Force Fields in Materials Science; Metal Oxides and Ceramics; Superconductors; Zeolites and Related Microporous Materials; Glasses; Polymers; Conclusions; Acknowledgments; References; Free Energy Calculations: Use and Limitations in Predicting Ligand Binding Affinities; Introduction; Theory; Methodology Overview; Computational Details; Molecular Mechanics Force Fields
Treatment of Long-Range Forces

Sommario/riassunto

Volume 16Reviews In Computational ChemistryKenny B. Lipkowitz and Donald B. BoydThe focus of this book is on methods useful in molecular design. Tutorials and reviews span (1) methods for designing compound libraries for combinatorial chemistry and high throughput screening, (2) the workings of artificial neural networks and their use in chemistry, (3) force field methods for modeling materials and designing new substances, and (4) free energy perturbation methods of practical usefulness in ligand design.From Reviews of the Series""This series spans all