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Nota di contenuto	Evolutionary Algorithms in Molecular Design; Contents; 1 Introduction to Evolutionary Algorithms; 1.1 History and Biological Motivation; 1.2 Descriptive Comparison of Algorithms; 1.2.1 Representation; 1.2.2 Evolotionary Operators; 1.2.3 Selection and the Next Generation; 1.2.4 Self-Adaptation and Learning-Rule Methods; 1.3 Implementation Issues and Representative Applications of EAs in Drug Design; 1.3.1 Problem-Adapted EA Features; 1.3.2 Problem Suitability for EA Implementation; 1.3.3 EA Combination Methods; 1.4 Conclusions; 2 Small-molecule Geometry Optimization and Conformational Search 2.1 Introduction2.2 Evolutionary Algorithms; 2.2.1 Diversity; 2.2.2 Creation of New Solutions; 2.2.3 Constraint Satisfaction; 2.3 Technical Aspects of Method Comparisons; 2.4 Traditional Methods for Structure Optimization; 2.5 Evolutionary Methods for Structure Optimization; 2.5.1 Satisfying Constraints from Experiments; 2.5.2 Energy Minimization; 2.6 Discussion; 2.7 Conclusions; 3 Protein-Ligand Docking; 3.1 Molecular Structure and Medicine; 3.2 Computational Protein-Ligand Docking; 3.2.1 Scoring Functions; 3.2.2 Level of

Allowed Molecular Flexibility

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5.2.1 Descriptor Tabulation5.2.2 Feature Selection; 5.2.3 Model Construction; 5.2.4 Model Validation; 5.3 Availability of GA Programs; 5.4 Applications of GAs in QSAR; 5.4.1 GA-MLR Approach; 5.4.2 GA-PLS; 5.4.3 GA-NN; 5.4.4 Chance Correlation; 5.5 Discussion; 6 Chemometrics; 6.1 Introduction; 6.2 Parameter Estimation; 6.2.1 Curve Fitting; 6.2.2 Nonlinear Modeling; 6.2.3 Neural Networks; 6.3 Subset Selection; 6.3.1 Feature Selection; 6.3.2 Object Selection; 6.4 Miscellaneous; 6.4.1 Clustering and Classification; 6.5 Discussion; 7 Chemical Structure Handling; 7.1 Introduction

7.2 Representation and Searching of Chemical Structures7.3 Processing of 2-D Chemical Graphs; 7.4 Processing of 3-D Chemical Graphs; 7.4.1 Flexible 3-D Substructure Searching; 7.4.2 Identification of Common Structural Features in Sets of Ligands; 7.5 Field-Based Similarity Searching; 7.6 Generation of Molecular Alignments; 7.7 Conclusions; 8 Molecular Diversity Analysis and Combmatorial Library Design; 8.1 Introduction; 8.2 The Diversity of Genotypes: The Space of Chemistry; 8.3 The Diversity of Phenotypes: The Property Space; 8.4 Diversity and Distance Calculation

8.5 Connecting the Structure and the Property Space: Evolutionary Algorithms

Sommario/riassunto

When trying to find new methods and problem-solving strategies for their research, scientists often turn to nature for inspiration. An excellent example of this is the application of Darwin's Theory of Evolution, particularly the notion of the 'survival of the fittest', in computer programs designed to search for optimal solutions to many kinds of problems. These 'evolutionary algorithms' start from a population of possible solutions to a given problem and, by applying evolutionary principles, evolve successive generations with improved characteristics until an optimal, or near-optimal, soluti