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   Nota di bibliografia Includes bibliographical references and index.

   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

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