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Database Searching and the Drug Design Process; Advances in 3D Search Methodology; 3D Database and Pharmacophore Query Construction
Structure GenerationAtom Typing on Compound Registration; Search-Time-Defined Atom Environment; Dealing with Conformational Flexibility; Explicit Conformation Storage; 3D Screens Incorporating Conformational Flexibility; Torsional Fitting; Choice of Technique; Pharmacophore Generation and Validation; Molecular Graphics; Automating the Search for Pharmacophores; Molecular Similarity Calculations; Pharmacophore Validation; Pharmacophore Search Successes; Receptor-Constrained 3D Screening; Shape-Constrained 3D Database Searches; Vector-Constrained 3D Searches; De Novo Design; Conclusions
AcknowledgmentsReferences; Methods and Applications of Combined Quantum Mechanical and Molecular Mechanical Potentials; Introduction; Incorporation of Explicit Solvent Effects in Quantum Mechanical Calculations; Combined Quantum Mechanical and Molecular Mechanical Potentials; Boundary Conditions; Dividing Covalent Bonds across the QM and MM Regions; Solvent Polarization Effects; Simulation of Excited States and Solvatochromic Spectral Shifts; The QM Method; Implementations; A Critical Evaluation of the Combined Semiempirical AMl/MM Model; Bimolecular Hydrogen-Bonding Interactions
Free Energies of Solvation of Organic CompoundsElectronic Polarization; Conformational Equilibria in Aqueous and Organic Solutions; Relative Free Energies of Tautomeric Equilibria in Pyridone; Solvent Effects on Chemical Reactions; The Claisen Rearrangement of Allyl Vinyl Ether; Simulations of Nucleophilic Substitution Reactions; The Decarboxylation Reaction of 3-Carboxybenzisoxagole; Potential Surface for the Proton Transfer in [H3N-H-NH3]; Solvatochromic Shifts of Acetone in Aqueous and Organic Solutions; Enzymatic Reaction and Chemisorption on Surfaces; Conclusions; Acknowledgments References

Sommario/riassunto

This is the seventh volume in the successful series designed to help the chemistry community keep current with the many new developments in computational techniques. The writing style is refreshingly pedagogical and non-mathematical, allowing students and researchers access to computational methods outside their immediate area of expertise. Each invited author approaches a topic with the aim of helping the reader understand the material, solve problems, and locate key references quickly.