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Constraints Derived?; Molecular Interactions; Characterizing a Receptor When No Receptor Structure Is AvailableScalar Constraints; Accuracy and Appropriateness of Constraints; What Chemical Diversity Is Available?; Fragment Library Issues; Building Strategies; How Is Molecular Flexibility Handled?; Ligand Flexibility; Receptor Flexibility; Future Directions for Flexibility; How Useful Are Current Scoring Functions?; Why Are Scoring Functions Needed?; What Is Available?; Critique of Current Scoring Methods Used in De Novo Design; Future Directions for Scoring Methods; How Are Large Numbers of Generated Structures Handled?; Currently Available Tools and Protocols DiscussionHow Are the Best Designs Verified?; Molecular Dynamics; Molecular Docking; Free Energy Calculations; What About the Interface?; Interface with the User; Interface to Other Design Tools; When Are De Novo Design Techniques Applicable?; Published Test Cases; Validated Examples; Discussion; Practical Advice on the Application of De Novo Design Methods; Conclusions; Acknowledgments; References; Theoretical and Practical Aspects of Three-Dimensional Quantitative Structure-Activity Relationships; An Introduction to the QSAR Problem; Chemical Space and the Linear Free Energy Formalism
Hansch Analysis and Classical QSARThree-Dimensional QSAR: An Overview; Assumptions in 3D-QSAR; Current 3D-QSAR Methods; CoMFA Application Notes; Training Set Composition; Alignment Rules; Electrostadc Descriptors and Choice of Partial Atomic Charges; CoMFA Region Description; CoMFA Standard Fields; Additional CoMFA Fields; PCA/PLS: A Brief Overview; Cross-Validation Techniques; Frequently Used Statistical Indices in 3D-QSAR; Interpretation of CoMFA Results; Model Predictivity; Explanatory Power; Model Simplicity; Variable Selection; Lateral Validation; Basic Qualities of a Good QSAR Model Final Remarks

Sommario/riassunto

Volume 11 Reviews in Computational Chemistry Kenny B. Lipkowitz and Donald B. Boyd The Theme of this Eleventh Volume is Computer-Aided Ligand Design and Modeling of Biomolecules. A Stellar Group of Scientists from Around the World Join in this Volume to Provide Tutorials for Beginners and Experts. Chapters 1 and 2 Take A Detailed Look at De Novo Design Methodologies for Discovering New Ligands which May Become Pharmaceuticals. Chapters 3 and 4 Cover the Methods and Applications of Three-Dimensional Quantitative Structure-Activity Relationships (3D-QSAR) Currently Used in Drug Discovery. Ways t