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Chelate Effect; 2.3 Geometric Fitting: The Hole-size Concept; 2.4 Di- and Polytopic Interactions: Change of Binding Mechanism with Different Fit; 2.5 Deviations from the Lock-and-Key Principle
2.5.1 Strain in Host-Guest Complexes2.5.2 Solvent Effects; 2.5.3 Enthalpy/Entropy Variations; 2.5.4 Loose Fit in Hydrophobically Driven Complex Formation; 2.6 Conformational Pre-organization: Flexible vs. Rigid Hosts; 2.7 Selectivity and Stability in Supramolecular Complexes; 2.8 Induced Fit, Cooperativity, and Allosteric Effects; 2.9 Quantification of Non-covalent Forces; 2.9.1 Ion Pairs and Electrostatic Donor-Acceptor Interactions; 2.9.2 Hydrogen Bonds; 2.9.3 Weak Hydrogen Bonds: The Use of Intramolecular ""Balances"; 2.9.4 Polarization Effects; 2.9.5 Dispersive Interactions
2.10 Conclusions2.11 References; 3 Experimental Approaches to Determine the Thermodynamics of Protein-Ligand Interactions; 3.1 Introduction; 3.2 Basic Thermodynamics of Protein-Ligand Interactions; 3.3 Measurement of Thermodynamic Parameters; 3.3.1 Calorimetric Determination of Thermodynamic Parameters; 3.3.2 van't Hoff Determination of Thermodynamic Parameters; 3.3.2.1 Relationship to Equilibrium Constant; 3.3.2.2 Obtaining the Equilibrium Constant; 3.4 Applications; 3.4.1 Calorimetric Determination of Thermodynamic Parameters; 3.4.2 van't Hoff Determination of Thermodynamic Parameters
3.5 Caveats3.6 Summary; 3.7 References; 4 The Biophore Concept; 4.1 Introduction; 4.2 Methodology for Pharmacophore Detection and Searching; 4.2.1 Definition of Pharmacophoric Groups; 4.2.2 Ligand-based Methods for Pharmacophore Perception; 4.2.3 Protein Structure-based Pharmacophore Perception; 4.2.4 Methods for Pharmacophore Searching; 4.3 Pharmacophore Fingerprints; 4.4 Applications of the Biophore Concept; 4.4.1 Lead Generation; 4.4.2 Multi-pharmacophore Descriptors in Diversity Analysis and Library Design; 4.4.3 Structure-based Design; 4.5 The Biophore Concept in ADME Prediction
4.6 Summary

Sommario/riassunto

The lock-and-key principle formulated by Emil Fischer as early as the end of the 19th century has still not lost any of its significance for the life sciences. The basic aspects of ligand-protein interaction may be summarized under the term 'molecular recognition' and concern the specificity as well as stability of ligand binding. Molecular recognition is thus a central topic in the development of active substances, since stability and specificity determine whether a substance can be used as a drug. Nowadays, computer-aided prediction and intelligent molecular design make a large contributio

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