

Protein-ligand interactions from molecular recognition to drug design

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Abstrak

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 contribution to the constant search for, e. g., improved enzyme inhibitors, and new concepts such as that of pharmacophores are being developed.