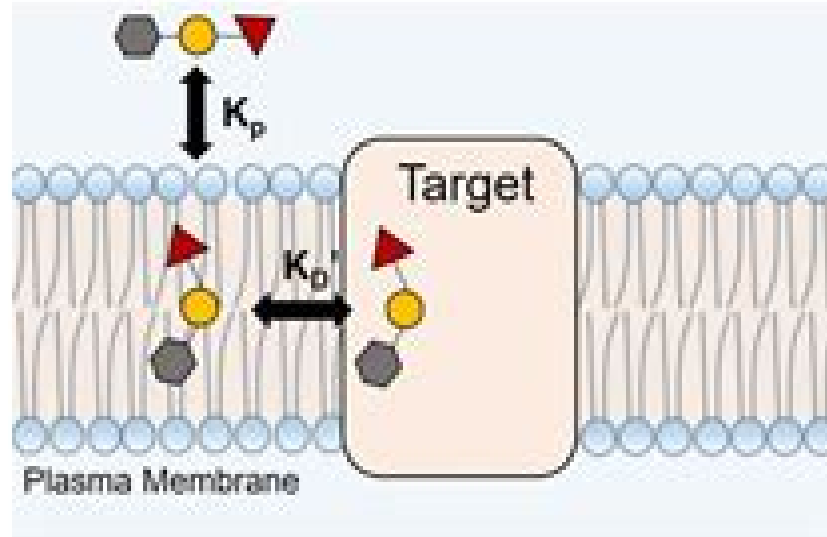
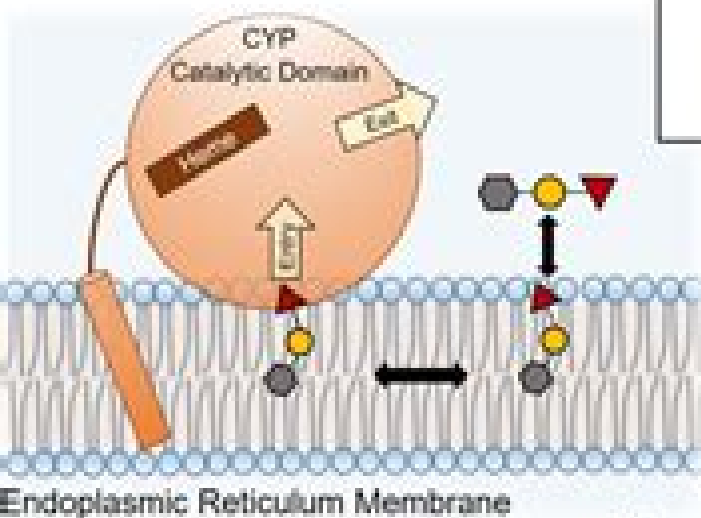


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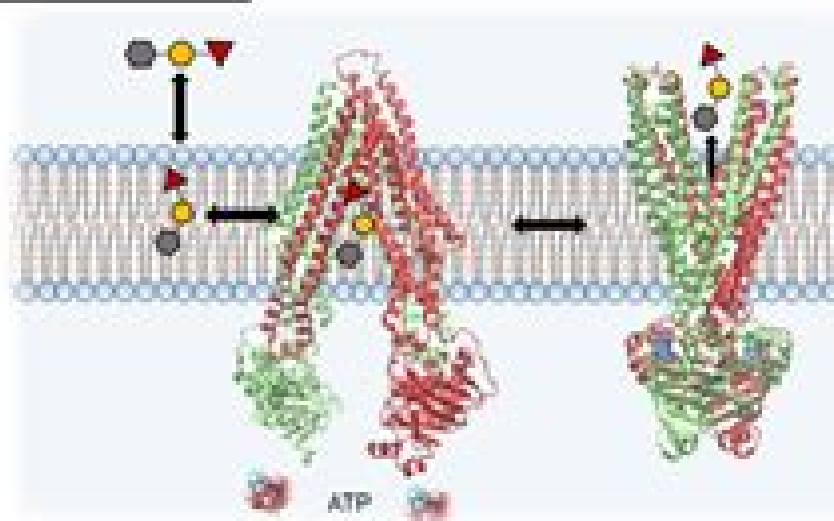


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Proteinligand Interactions From Molecular Recognition To Drug Design

Hans-Joachim Böhm, Gisbert Schneider



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Chemistry fills a gap in the list of available medicinal chemistry literature It is a single volume source on the practical aspects of medicinal chemistry Considered the Bible by medicinal chemists the book emphasizes the methods that chemists use to conduct their research and design new drug entities It serves as a practical handbook about the drug discovery process from conception of the molecules to drug production The first part of the book covers the background of the subject matter which includes the definition and history of medicinal chemistry the measurement of biological activities and the main phases of drug activity The second part of the book presents the road to discovering a new lead compound and creating a working hypothesis The main parts of the book discuss the optimization of the lead compound in terms of potency selectivity and safety The Practice of Medicinal Chemistry can be considered a first read or bedside book for readers who are embarking on a career in medicinal chemistry NEW TO THIS EDITION Focus on chemoinformatics and drug discovery Enhanced pedagogical features New chapters including Drug absorption and transport Multi target drugs Updates on hot new areas NEW Drug discovery and the latest techniques NEW How potential drugs can move through the drug discovery development phases more quickly NEW Chemoinformatics New Developments in Medicinal Chemistry: Volume 1 Carlton Anthony

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Molecular Recognition Stanley M. Roberts,1989 This book consists of articles which describe work involved in determining small molecule large molecule interactions It highlights the interactions of an enzyme with a substrate and gives a detailed understanding of this recognition More specifically it covers the importance of understanding the energetics of intra and inter molecular interactions using molecular mechanics calculations plus the importance in the understanding of the mechanism of action and improvement of heterogenous catalysts No index Annotation copyrighted by Book News Inc Portland OR **Computational Techniques for Modeling Protein-ligand Interactions and Their Application to Serine Proteases and Asparaginyl-tRNA Synthetase** Paul C. Sanschagrin,2001 *Computational Approaches to Biochemical Reactivity* Gábor Náray-Szabó,Arieh Warshel,1997-04-30 This book summarises recent results in the rapidly developing discipline of the computational aspects of biochemical reactivity It presents a comprehensive and critical treatise on the subject with numerous references covering practically all relevant and recent work The chapters written by eminent experts in the field deal with quantum mechanical models for reactions in solution ab initio molecular orbital studies on enzymatic reactions combined quantum classical models for proteins force field approaches for modelling enzymes electrostatic effects in proteins electrostatic basis of enzyme catalysis the mechanism of proteases modelling of proton transfer reactions in enzymes and protein ligand interactions Audience This volume will be of interest to graduate students and researchers working in molecular biophysics structural biology or structure based molecular design Molecular Interactions Steve Scheiner,1997-05-05 Complete coverage of the many types of forces from the weakest to the strongest that are involved in the interaction between molecules including the underlying theory experimental methods and examples

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