

IUL Biotechnology Series

Pharmacophore Perception, Development, and Use in Drug Design



edited by

OSMAN F. GÜNER

Pharmacophore Perception Development And Use In Drug Design Iul Biotechnology Series

**Richard B. Silverman, Mark W.
Holladay**



Pharmacophore Perception Development And Use In Drug Design Iul Biotechnology Series:

Pharmacophore Perception, Development, and Use in Drug Design Osman F. Güner, 2000 In the early 1900s Paul Ehrlich first defined pharmacophores as molecule frameworks that carry the essential features responsible for a drug's biological activity and the modern definition is little changed The 27 studies here begin by tracing the evolution of the concept in pharmaceutical research then cover analog based and receptor based varieties new algorithms and the future of research Among the specific topics pharmacophores based on multiple common feature alignments modeling programs including HypoGen DISCO Catalyst HipHop GASP Chem X Apex 3D CoMFA pharmacophore based molecular docking a technique for developing a pharmacophore model that accommodates inherent protein flexibility and the effect of variable weights and tolerances on predictive model generation Books in Print lists only one other book on the topic of pharmacophores Annotation copyrighted by Book News Inc Portland OR *Pharmacological Aspects of Molecular Recognition* F. S. Dukhovich, 2005 In the monograph recognition of the receptors by drugs is described as a complex phenomenon that has not been yet entirely understood The description of molecular structure information necessary to achieve specific receptors without getting lost among huge amounts of non specific acceptors is present Various examples of receptor binding features for narcotic analgetics neuroleptics tranquilisators ligands of acetylcholine receptors are also included The three stages of drug interaction with acceptors are considered namely distant stage stage of orientation of the molecule on the acceptor stage of molecule fixation Kinetics and thermodynamics of these stages as well as factors preventing drug binding to non specific acceptors are described Some considerations concerning methods of changing activity and selectivity of drugs are given Literature information needed for analysis of molecular mechanisms of interactions between drugs and receptors is present *The Organic Chemistry of Drug Design and Drug Action* Richard B. Silverman, Mark W. Holladay, 2014-03-29 The Organic Chemistry of Drug Design and Drug Action Third Edition represents a unique approach to medicinal chemistry based on physical organic chemical principles and reaction mechanisms that rationalize drug action which allows reader to extrapolate those core principles and mechanisms to many related classes of drug molecules This new edition includes updates to all chapters including new examples and references It reflects significant changes in the process of drug design over the last decade and preserves the successful approach of the previous editions while including significant changes in format and coverage This text is designed for undergraduate and graduate students in chemistry studying medicinal chemistry or pharmaceutical chemistry research chemists and biochemists working in pharmaceutical and biotechnology industries Updates to all chapters including new examples and references Chapter 1 Introduction Completely rewritten and expanded as an overview of topics discussed in detail throughout the book Chapter 2 Lead Discovery and Lead Modification Sections on sources of compounds for screening including library collections virtual screening and computational methods as well as hit to lead and scaffold hopping expanded sections on sources of lead compounds fragment based lead discovery and

molecular graphics and deemphasized solid phase synthesis and combinatorial chemistry Chapter 3 Receptors Drug receptor interactions cation p and halogen bonding atropisomers case history of the insomnia drug suvorexant Chapter 4 Enzymes Expanded sections on enzyme catalysis in drug discovery and enzyme synthesis Chapter 5 Enzyme Inhibition and Inactivation New case histories for competitive inhibition the epidermal growth factor receptor tyrosine kinase inhibitor erlotinib and Abelson kinase inhibitor imatinib for transition state analogue inhibition the purine nucleoside phosphorylase inhibitors forodesine and DADMe ImmH as well as the mechanism of the multisubstrate analog inhibitor isoniazid for slow tight binding inhibition the dipeptidyl peptidase 4 inhibitor saxagliptin Chapter 7 Drug Resistance and Drug Synergism This new chapter includes topics taken from two chapters in the previous edition with many new examples Chapter 8 Drug Metabolism Discussions of toxicophores and reactive metabolites Chapter 9 Prodrugs and Drug Delivery Systems Discussion of antibody drug conjugates *Molecular Modelling Untersuchungen am Dopamin D3 Rezeptor und seinen Liganden* Robin

Ghosh,2002-01-01 **Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment** Kunal Roy,Supratik Kar,Rudra Narayan Das,2015-03-03 Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment describes the historical evolution of quantitative structure activity relationship QSAR approaches and their fundamental principles This book includes clear introductory coverage of the statistical methods applied in QSAR and new QSAR techniques such as HQSAR and G QSAR Containing real world examples that illustrate important methodologies this book identifies QSAR as a valuable tool for many different applications including drug discovery predictive toxicology and risk assessment Written in a straightforward and engaging manner this is the ideal resource for all those looking for general and practical knowledge of QSAR methods Includes numerous practical examples related to QSAR methods and applications Follows the Organization for Economic Co operation and Development principles for QSAR model development Discusses related techniques such as structure based design and the combination of structure and ligand based design tools **AIChE Symposium Series** American Institute of Chemical Engineers,2001

Foundations of Molecular Modeling and Simulation Peter T. Cummings,Phillip Ray Westmoreland,Brice Carnahan,2001

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