



Pharmacophores and Pharmacophore Searches (Methods and Principles in Medicinal Chemistry, Vol. 32)

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This handbook is the first to address the practical aspects of this novel method. It provides a complete overview of the field and progresses from general considerations to real life scenarios in drug discovery research. Starting with an introductory historical overview, the authors move on to discuss ligand-based approaches, including 3D pharmacophores and 4D QSAR, as well as the concept and application of pseudoreceptors. The next section on structure-based approaches includes pharmacophores from ligand-protein complexes, FLIP and 3D protein-ligand binding interactions. The whole is rounded off with a complete section devoted to applications and examples, including modeling of ADME properties. With its critical evaluation of pharmacophore-based strategies, this book represents a valuable aid for project leaders and decision-makers in the pharmaceutical industry, as well as pharmacologists, and medicinal and chemists.

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Editorial Review

Review

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(*Anticancer Research*, 2007)

From the Back Cover

In their search for new drugs, medicinal chemists are trying to pinpoint and optimize only the active part of a pharmaceutical substance, without interference from other parts of the molecule. The "pharmacophore" is a virtual representation of the active part of a drug that enables them to do just that. Once identified, pharmacophores can then be used for the screening of drug libraries and drug targets to find novel active substances that can be developed into drugs.

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About the Author

Thierry Langer (b. 1962) is heading the Computer Aided Molecular Design Group at the University of Innsbruck (Tyrol, Austria). After his pharmacy M.S. degree (1987) he obtained a Ph.D. degree in organic chemistry at the University of Vienna (Austria) in 1991. He then spent one year as a post-doc fellow at the Université de Louis Pasteur (Strasbourg, France) with C. G. Wermuth. In 1992 he moved to the University of Innsbruck, where he established the molecular modeling group. Since 1997 he is associate professor for pharmaceutical chemistry.

In addition to his academic appointments, he is also the founder and CEO of the Inteligand, a company specialized in providing computational services for the pharmaceutical industry.

Professor Langer's main research interests are focused on theoretical pharmaceutical chemistry, drug design, and pharmacophore modeling using molecular modeling techniques as well as QSAR and 3D-QSAR.

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