Hit and Lead Profiling: Identification and Optimization of Drug-like Molecules
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Hardcover  ISBN: 978-3-527-32331-9  September 2009  $271.50

DESCRIPTION

The only reference on current methods to generate pharmacokinetic and safety profiles of drug candidates, as well as how they must be balanced against one other for the best selection of candidates for further development.

Following a brief introduction to the necessities of filtering and risk assessment of potential new drug molecules before actual drug development, the two equally important aspects of pharmacological (ADME) and safety (toxicity) profiling are covered in separate parts.

The ADME section covers the profiling of basic physicochemical parameters, such as solubility and permeability, as well as more complex traits, such as the likelihood of drug-drug interactions, metabolic clearance and protein binding properties.

The toxicology part addresses, among others, recent advances in early genetic toxicity testing, bioactivation screening, organ-specific toxicity assays for liver, heart, kidney and blood, as well as profiling for autoimmune reactions.

By addressing both drug efficiency and drug safety, this modern practical reference shows readers how each individual aspect figures in shaping the key decisions on which the entire drug development process hinges. In short, this is a complete toolbox for assessing the risk/benefit ratio for any novel compound during the early drug development stages, using both in vitro and in silico methods.

Both editors are based at one of the leading research-driven pharmaceutical companies, and the authors have been recruited from numerous other global players in the field.

Invaluable know-how for every medicinal chemist and drug developer.
Laszlo Urban is global head of Preclinical Safety Profiling at the Novartis Institutes for Biomedical Research (NIBR), Cambridge, MA, and previously was the Deputy Head of the Novartis Institute for Medical Sciences in London, UK. He received his MD and PhD in neurophysiology/neuropharmacology in Hungary, and was visiting professor at Duke University between 1987-1989. He joined the Sandoz Institute for Medical Research, London, in 1990, where he was head of pharmacology. Dr. Urban has published over 130 scientific articles, book chapters and patents and has served on the editorial board of several journals, while also serving as President of the European Neuropeptide Club, between 1999 and 2001.

Bernard Faller is currently director in the Metabolism and Pharmacokinetics department at NIBR, Basel, Switzerland. He graduated as a biochemist from the University of Strasbourg, France, where he obtained his PhD in 1991. He then started at Ciba-Geigy as a post-doctoral fellow, becoming head of laboratory in 1995. In 1999 he moved to central technologies and established the foundations of the Novartis biopharmaceutical profiling group that addresses early ADME properties in drug discovery, and two years later became technology program head for physicochemical profiling in the Preclinical Compound Profiling Unit. In 2007 Dr. Faller was named "Hero of Chemistry" by the ACS for the discovery of Exjade®, the first orally-active iron chelator for the treatment of transfusional iron overload.