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PHARMACOKINETIC PROFILING IN DRUG RESEARCH (HARDBACK)



Helvitica Chimica Acta Verlag, Switzerland, Switzerland, 2006. Hardback. Condition: New. 1. Auflage. Language: English . Brand New Book. Informatics and robotics are the workhorses of a technological revolution in drug research. On them are based combinatorial chemistry, which yields compounds by the many thousands, and high-throughput bioassays, which screen them for activity. The results are avalanches of hits, which invade the databases like swarms of locusts. But far from being a plague, these innumerable compounds become a blessing if properly screened for drugability, i.e., for drug-like properties such as good pharmacokinetic (PK) behavior. Pharmacokinetic profiling of bioactive compounds has, thus, become a sine qua non condition for cherry-picking the most promising hits. Just as important, but less visible, are the structure-property and structure-ADME relations, which emerge from PK profiling and provide useful feedback when designing new synthetic series. As a result, the screening, design, and optimization of pharmacokinetic properties has become the bottleneck and a major challenge in drug research. To shorten the time-consuming development and high rate of attrition of active compounds ultimately doomed by hidden pharmacokinetic defects, powerful biological, physicochemical, and computational approaches are being developed, whose objectives are to increase the clinical relevance of drug design and to eliminate as soon as possible compounds with unfavorable physicochemical properties and pharmacokinetic profiles. The profiling of ADME properties (absorption, distribution, metabolism, and excretion) is the topic of this book. Following the extraordinary success of the previous work (Pharmacokinetic Optimization in Drug Research: Biological, Physicochemical, and Computational Strategies, Eds. B. Testa, H. van de Waterbeemd, G. Volkers, R. Guy, Verlag Helvetica Chimica Acta, Zurich, 2001, 655 pages), there was a need for an essentially new edition focusing on the latest theoretical and technological breakthroughs. In this unique work, international authorities and practicing experts from academia and industry...

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