Record Nr. UNINA9910960327803321 Virtual ADMET assessment in target selection and maturation / / edited **Titolo** by B. Testa and L. Turski Pubbl/distr/stampa Amsterdam; ; Washington, DC, : IOS Press, c2006 **ISBN** 1-280-81056-4 9786610810567 1-4294-6772-X 1-60750-219-4 600-00-0604-7 1-4337-0155-3 Edizione [1st ed.] Descrizione fisica 1 online resource (268 p.) Collana Solvay Pharmaceuticals Conferences, , 1566-7685;; v. 6 Altri autori (Persone) **TestaBernard** TurskiLechoslaw Disciplina 615/.190285 Soggetti Drug development - Computer simulation Pharmacology Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Organized May 11-13th, 2005 in Lucerne, Switzerland. Note generali Nota di bibliografia Includes bibliographical references and index. Nota di contenuto Preface; List of Contributors; Contents; Conference Preface; The Risky Business of Developing Drugs; Benefits and Limits of in Silico Predictions: Musings on ADME Predictions and Molecular Structure: Lipophilicity: Its Calculation and Application in ADMET Predictions; Interpretation of the Role of the Electrotopological State and Molecular Connectivity Indices in the Prediction of Physical Properties and ADME-Tox Behavior - Case Study: Human Plasma Protein Binding: Molecular Descriptors for Predicting ADMET Properties; Molecular Fields to Assess Recognition Forces and Property Spaces Extracting Pharmacophores from Bio-Active Molecules In Silico Models for Human Bioavailability; In Silico Models to Predict Brain Uptake; Algorithms to Predict Affinity for Transporters; Predicting Affinity for and Metabolism by Cytochromes P450; Expert Systems to Predict Biotransformation; Expert Systems to Predict Toxicity; From in Vivo to in Vitro/in Silico ADME: Progress and Challenges; Author Index

Today, biologists and medicinal chemists realize that there is a strong

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relationship between pharmacodynamic (what the drug does to the organism) and pharmacokinetic (what the organism does to the drug) effects. A significant contributing factor to the evolution in drug discovery was the methodological and technological revolution with the advent of combinatorial chemistry, high-throughput screening and profiling, and in silico prediction of target-based activity and ADMET (absorption, distribution, metabolism, excretion and toxicity) properties. High-throughput screening and in silico methods