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Nota di contenuto	<p>ADMET for Medicinal Chemists: A Practical Guide; CONTENTS; Preface; Contributors; 1 Introduction; 1.1 Introduction; 1.2 Voyage Through The Digestive System; 1.2.1 The Mouth; 1.2.2 The Stomach; 1.2.3 The Small Intestine: Duodenum; 1.2.4 The Small and Large Intestine: Jejunum, Ileum, Colon; 1.2.5 Hepatic-Portal Vein; 1.3 The Liver Metabolism; 1.3.1 CYP450 (CYPs); 1.4 The Kidneys; 1.4.1 Active Tubular Secretion; 1.4.2 Passive Tubular Reabsorption; 1.5 Conclusions; References; 2 In Silico ADME/Tox Predictions; 2.1 Introduction; 2.2 Key Computer Methods for ADME/Tox Predictions</p> <p>2.2.1 Drug Discovery 2.2.2 Applying or Not ADME/Tox Predictions, Divided Opinions; 2.2.3 In Silico ADME/Tox Methods and Modeling Approaches; 2.2.4 Physicochemistry, Pharmacokinetics, Drug-Like and Lead-Like Concepts; 2.2.5 Lipophilicity; 2.2.6 pKa; 2.2.7 Transport Proteins; 2.2.8 Plasma Protein Binding; 2.2.9 Metabolism; 2.2.10 Elimination; 2.2.11 Toxicity; 2.3 Preparation of Compound Collections and Computer Programs, Challenging ADME/Tox Predictions and Statistical Methods; 2.3.1 Preparation of Compound Collections and Computer Programs</p> <p>2.3.2 Preparing a Compound Collection: Materials and Methods 2.3.3 Cleaning and Designing the Compound Collection; 2.3.4 Searching for Similarity; 2.3.5 Generating 3D Structures; 2.4 ADME/Tox Predictions within Pharmaceutics Companies; 2.4.1 Actelion Pharmaceuticals Ltd.; 2.4.2 Bayer; 2.4.3 Bristol-Myers Squibb; 2.4.4 Hoffmann-La Roche Ltd.; 2.4.5 Neurogen Corporation; 2.4.6 Novartis; 2.4.7 Schering AG; 2.4.8 Vertex Pharmaceuticals; 2.5 Challenging ADME/Tox Predictions; 2.5.1 Tolcapone; 2.5.2 Factor V Inhibitors; 2.5.3 CRF-1 Receptor Antagonists; 2.6 Statistical Methods</p> <p>2.6.1 Principal Component Analysis 2.6.2 Partial Least Square; 2.6.3 Support Vector Machine; 2.6.4 Decision Trees; 2.6.5 Neural Networks; 2.7 Conclusions; References; 3 Absorption and Physicochemical Properties of the NCE; 3.1. Introduction; 3.2. Physicochemical Properties; 3.3. Stability; 3.4. Dissolution and Solubility; 3.4.1. Dissolution Rate, Particle Size, and Solubility; 3.4.2. pH and Salts; 3.4.3. In Vivo Solubilization; 3.5. Solid State; References; 4 ADME; 4.1 Introduction; 4.2 Absorption; 4.2.1 Route of Administration; 4.2.2 Factors Determining Oral Bioavailability; 4.3 Distribution</p> <p>4.3.1 Drug Distribution 4.3.2 Volume of Distribution; 4.3.3 Free Drug Concentration; 4.3.4 CNS Penetration; 4.4 Elimination; 4.4.1 Elimination Versus Clearance; 4.4.2 Metabolism Versus Excretion; 4.4.3 Drug-Free Fraction and Clearance; 4.4.4 Lipophilicity and Clearance; 4.4.5 Transporters and Clearance; 4.4.6 Metabolism; 4.4.7 Excretion; 4.5 Drug Interactions; 4.5.1 Absorption-Driven DDI; 4.5.2 Distribution-Driven DDI; 4.5.3 Excretion-Driven DDI; 4.5.4 Metabolism-Driven DDI; 4.5.5 Tools for Studying Drug Metabolism; 4.5.6 Applications of Drug Metabolism Tools</p>

4.5.7 Tools for Studying Drug Excretion

Sommario/riassunto

This book guides medicinal chemists in how to implement early ADMET testing in their workflow in order to improve both the speed and efficiency of their efforts. Although many pharmaceutical companies have dedicated groups directly interfacing with drug discovery, the scientific principles and strategies are practiced in a variety of different ways. This book answers the need to regularize the drug discovery interface; it defines and reviews the field of ADME for medicinal chemists. In addition, the scientific principles and the tools utilized by ADME scientists in a discovery setting, as appl