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Nota di contenuto	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 2.2.1 Drug Discovery2.2.2 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

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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