Record Nr. UNINA9910141254203321 ADME-enabling technologies for drug design and development **Titolo** [[electronic resource] /] / edited by Donglu Zhang, Sekhar Surapaneni Pubbl/distr/stampa Hoboken, N.J., : Wiley, c2012 **ISBN** 1-280-59257-5 9786613622402 1-118-18076-3 1-118-18077-1 1-118-18074-7 Descrizione fisica 1 online resource (623 p.) Altri autori (Persone) ZhangDonglu SurapaneniSekhar Disciplina 615.1/9 Soggetti Drugs - Design Drug development Drugs - Metabolism Pharmaceutical chemistry **Pharmacokinetics** Pharmaceutical technology Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Note generali Description based upon print version of record. Nota di bibliografia Includes bibliographical references and index. Nota di contenuto ADME-Enabling Technologies in Drug Design and Development; CONTENTS: FOREWORD: PREFACE: CONTRIBUTORS: PART A: ADME: OVERVIEW AND CURRENT TOPICS; 1: REGULATORY DRUG DISPOSITION AND NDA PACKAGE INCLUDING MIST; 1.1 INTRODUCTION; 1.2 NONCLINICAL OVERVIEW; 1.3 PK; 1.4 ABSORPTION; 1.5 DISTRIBUTION; 1.5.1 Plasma Protein Binding; 1.5.2 Tissue Distribution; 1.5.3 Lacteal and Placental Distribution Studies; 1.6 METABOLISM; 1.6.1 In vitro Metabolism Studies; 1.6.2 Drug-Drug Interaction Studies; 1.6.3 In vivo Metabolism (ADME) Studies; 1.7 EXCRETION; 1.8 IMPACT OF METABOLISM INFORMATION ON LABELING

1.9 CONCLUSIONSREFERENCES: 2: OPTIMAL ADME PROPERTIES FOR

CLINICAL CANDIDATE AND INVESTIGATIONAL NEW DRUG (IND)

PACKAGE: 2.1 INTRODUCTION: 2.2 NCE AND INVESTIGATIONAL NEW DRUG (IND) PACKAGE; 2.3 ADME OPTIMIZATION; 2.3.1 Absorption; 2.3.2 Metabolism; 2.3.3 PK; 2.4 ADME OPTIMIZATION FOR CNS DRUGS; 2.5 SUMMARY; REFERENCES; 3: DRUG TRANSPORTERS IN DRUG INTERACTIONS AND DISPOSITION; 3.1 INTRODUCTION; 3.2 ABC TRANSPORTERS; 3.2.1 Pgp (MDR1, ABCB1); 3.2.2 BCRP (ABCG2); 3.2.3 MRP2 (ABCC2); 3.3 SLC TRANSPORTERS; 3.3.1 OCT1 (SLC22A1) and OCT2 (SLC22A2); 3.3.2 MATE1 (SLC47A1) and MATE2K (SLC47A2) 3.3.3 OAT1 (SLC22A6) and OAT3 (SLC22A8)3.3.4 OATP1B1 (SLCO1B1, SLC21A6), OATP1B3 (SLCO1B3, SLC21A8), and OATP2B1 (SLCO2B1, SLC21A9); 3.4 IN VITRO ASSAYS IN DRUG DEVELOPMENT; 3.4.1 Considerations for Assessing Candidate Drugs as Inhibitors; 3.4.2 Considerations for Assessing Candidate Drugs as Substrates; 3.4.3 Assay Systems; 3.5 CONCLUSIONS AND PERSPECTIVES; REFERENCES; 4: PHARMACOLOGICAL AND TOXICOLOGICAL ACTIVITY OF DRUG METABOLITES; 4.1 INTRODUCTION; 4.2 ASSESSMENT OF POTENTIAL FOR ACTIVE METABOLITES; 4.2.1 Detection of Active Metabolites during Drug Discovery 4.2.2 Methods for Assessing and Evaluating the Biological Activity of Metabolite Mixtures 4.2.3 Methods for Generation of Metabolites; 4.3 ASSESSMENT OF THE POTENTIAL TOXICOLOGY OF METABOLITES; 4.3.1 Methods to Study the Formation of Reactive Metabolites; 4.3.2 Reactive Metabolite Studies: In vitro; 4.3.3 Reactive Metabolite Studies: In vivo; 4.3.4 Reactive Metabolite Data Interpretation: 4.3.5 Metabolite Contribution to Off-Target Toxicities: 4.4 SAFETY TESTING OF DRUG METABOLITES: 4.5 SUMMARY: REFERENCES 5: IMPROVING THE PHARMACEUTICAL PROPERTIES OF BIOLOGICS IN DRUG DISCOVERY: UNIQUE CHALLENGES AND ENABLING SOLUTIONS5.1 INTRODUCTION; 5.2 PHARMACOKINETICS; 5.3 METABOLISM AND DISPOSITION; 5.4 IMMUNOGENICITY; 5.5 TOXICITY AND PRECLINICAL ASSESSMENT; 5.6 COMPARABILITY; 5.7 CONCLUSIONS; REFERENCES; 6: CLINICAL DOSE ESTIMATION USING

Sommario/riassunto

Modeling

A comprehensive guide to cutting-edge tools in ADME research The last decade has seen tremendous progress in the development of analytical techniques such as mass spectrometry and molecular biology tools, resulting in important advances in drug discovery, particularly in the area of absorption, distribution, metabolism, and excretion (ADME). ADME-Enabling Technologies in Drug Design and Development focuses on the current state of the art in the field, presenting a comprehensive review of the latest tools for generating ADME data in drug discovery. It examines the broadest possible rang

PD; 6.2.3 Biomarkers; 6.3 MODEL-BASED CLINICAL DRUG

6.3.4 Quantitative Pharmacology (QP) and Pharmacometrics

DEVELOPMENT; 6.3.1 Modeling; 6.3.2 Simulation; 6.3.3 Population

PHARMACOKINETIC/PHARMACODYNAMIC MODELING AND SIMULATION; 6.1 INTRODUCTION; 6.2 BIOMARKERS IN PK AND PD; 6.2.1 PK; 6.2.2