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Autore	Di Napoli, Francesco
Titolo	Foresta ed energia: valutazione tecnico economica per la sostenibilità della produzione [Tesi di dottorato] / Dottorando: Francesco Di Napoli ; Coordinatore: Severino Romano ; Tutor: Severino Romano ; Co-tutor: Mario Cozzi
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Autore	Kerns Edward Harvel
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Nota di bibliografia	Includes bibliographical references (p. 492) and index.
Nota di contenuto	Front Cover; Drug-like Properties: Concepts, Structure Design and Methods: from ADME to Toxicity Optimization; Copyright Page; Table of Contents; Preface; Dedication; Part 1 Introductory Concepts; Chapter 1 Introduction; Problems; References; Chapter 2 Advantages of Good Drug-like Properties; 2.1 Drug-like Properties Are an Integral Part of Drug Discovery; 2.1.1 Many Properties Are of Interest in Discovery; 2.1.2 Introduction to the Drug Discovery and Development Process; 2.1.3 Development Attrition is Reduced by Improving Drug Properties 2.1.4 Poor Drug Properties Also Cause Discovery Inefficiencies2.1.5 Marginal Drug Properties Cause Inefficiencies During Development; 2.1.6 Poor Properties Can Cause Poor Discovery Research; 2.2 Changing Emphasis on Properties in Discovery; 2.3 Property Profiling in Discovery; 2.4 Drug-like Property Optimization in Discovery; Problems; References; Chapter 3 Barriers to Drug Exposure in Living Systems; 3.1 Introduction to Barriers; 3.2 Drug Dosing; 3.3 Barriers in the Mouth and Stomach; 3.4 Gastrointestinal Tract Barriers; 3.4.1 Permeation of the Gastrointestinal Cellular Membrane 3.4.2 Passive Diffusion at the Molecular Level3.4.3 Metabolism in the Intestine; 3.4.4 Enzymatic Hydrolysis in the Intestine; 3.4.5 Absorption Enhancement in the Intestine; 3.5 Barriers in the Bloodstream; 3.5.1 Plasma Enzyme Hydrolysis; 3.5.2 Plasma Protein Binding; 3.5.3 Red Blood Cell Binding; 3.6 Barriers in the Liver; 3.6.1 Metabolism; 3.6.2 Biliary Excretion; 3.7 Barriers in the Kidney; 3.8 Blood-Tissue Barriers; 3.9 Tissue Distribution; 3.10 Consequences of Chirality on Barriers and Properties; 3.11 Overview of In Vivo Barriers; Problems; References; Part 2 Physicochemical Properties Chapter 4 Rules for Rapid Property Profiling from Structure4.1 Lipinski Rules; 4.2 Veber Rules; 4.3 Other Rules; 4.4 Application of Rules for Compound Assessment; Problems; References; Chapter 5 Lipophilicity; 5.1 Lipophilicity Fundamentals; 5.2 Lipophilicity Effects; 5.3 Lipophilicity Case Studies and Structure Modification; Problems; References; Chapter 6 pKa; 6.1 pKa Fundamentals; 6.2 pKa Effects; 6.3 pKa Case Studies; 6.4 Structure Modification Strategies for pKa; Problems; References; Chapter 7 Solubility; 7.1 Solubility Fundamentals 7.1.1 Solubility Varies with Structure and Physical Conditions7.1.2 Dissolution Rate; 7.1.3 Structural Properties Affect Solubility; 7.1.4 Kinetic and Thermodynamic Solubility; 7.2 Effects of Solubility; 7.2.1 Low Solubility Limits Absorption and Causes Low Oral Bioavailability; 7.2.2 Good Solubility is Essential for IV Formulation; 7.2.3 Acceptance Criteria and Classifications for Solubility; 7.2.4 Molecular Properties for Solubility and Permeability Often are Opposed; 7.3 Effects of Physiology on Solubility and Absorption; 7.3.1 Physiology of the Gastrointestinal Tract 7.3.2 Species Differences in Gastrointestinal Tract
Sommario/riassunto	Of the thousands of novel compounds that a drug discovery project team invents and that bind to the therapeutic target, typically only a fraction of these have sufficient ADME/Tox properties to become a drug product. Understanding ADME/Tox is critical for all drug researchers, owing to its increasing importance in advancing high quality candidates to clinical studies and the processes of drug discovery. If the properties are weak, the candidate will have a high risk of failure or be less desirable as a drug product. This book is a tool and resource for scientists engaged in, or preparing for,