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Stomach; 3.4 Gastrointestinal Tract Barriers; 3.4.1 Permeation of the Gastrointestinal Cellular Membrane
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 3.4.3 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 Structure
 4.1 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 Conditions
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 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,
