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Nota di contenuto	Cover; Title Page; Copyright; Preface; Chapter 1: The Drug Discovery Process; Summary; Question for Review; References; Chapter 2: Drug-Likeness and Physicochemical Property Space of known Drugs; Summary; Questions for Review; References; Chapter 3: Basic Pharmacokinetic Properties; Absorption; Plasma Protein Binding; Distribution; Volume of Distribution; Unbound Volume of Distribution; Half-Life; Metabolism and Clearance; Free Drug Hypothesis; Summary; Questions for Review; References; Chapter 4: Principles and Methods of Chromatography for the Application of Property Measurements Theoretical Background of Chromatography; Retention Factor and its Relation to the Distribution Constant Between the Mobile and the Stationary Phases; Measure of Separation Efficiency; Resolution and Separation Time; Gradient Elution; Applicability of Chromatography for Measurements of Molecular Properties; Summary; Questions for Review; References; Chapter 5: Molecular Physicochemical Properties that Influence Absorption and Distribution-Lipophilicity; Partition

Coefficient; Lipophilicity Measurements by Reversed Phase Chromatography with Isocratic Elution
Lipophilicity Measurements by Reversed Phase Chromatography with Gradient ElutionLipophilicity of Charged Molecules-pH Dependence of Lipophilicity; Biomimetic Lipophilicity Measurements by Chromatography; Comparing Various Lipophilicity Measures by the Solvation Equation Model; Summary; Questions for Review; References; Chapter 6: Molecular Physicochemical Properties that Influence Absorption and Distribution-Solubility; Definition of Solubility; Molecular Interactions with Water; Various Solubility Measurements that can be Applied During the Drug Discovery Process
Conditions that Affect SolubilitySolubility-pH Profile; Solubility and Dissolution in Biorelevant Media; Composition of Fasted State Simulated Intestinal Fluid (FaSSIF); Preparation of FaSSIF Solution; Composition of Fed State Simulated Intestinal Fluid (FeSSIF); Preparation of FeSSIF Solution; Summary; Questions for Review; References; Chapter 7: Molecular Physicochemical Properties that Influence Absorption and Distribution-Permeability; Biological Membranes; Artificial Membranes; Physicochemical Principles of Permeability; Experimental Methods to Measure Artificial Membrane Permeability
Relationships Between Permeability, Lipophilicity, and SolubilityChromatography as a Potential Tool for Measuring the Rate of Permeation; Summary; Questions for Review; References; Chapter 8: Molecular Physicochemical Properties that Influence Absorption and Distribution-Acid Dissociation Constant-pKa; Definition of pKa; Methods for Determining pKa; Spectrophotometric Determination of pKa; Determination of pKa by Capillary Electrophoresis; Chromatographic Approaches for the Determination of pKa; Summary; Questions for Review; References
Chapter 9: Models with Measured Physicochemical and Biomimetic Chromatographic Descriptors-Absorption

Sommario/riassunto

Demonstrating how and why to measure physicochemical and biomimetic properties in early stages of drug discovery for lead optimization, Physicochemical and Biomimetic Properties in Drug Discovery encourages readers to discover relationships between various measurements and develop a sense of interdisciplinary thinking that will add to new research in drug discovery. This practical guide includes detailed descriptions of state-of-the-art chromatographic techniques and uses real-life examples and models to help medicinal chemists and scientists and advanced graduate students apply measure
