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3.6.1 Potential of Redening BCS Solubility Class Boundary3.6.2 Biowaiver Extension Potential for Class II Drugs; 3.7 Conclusions; References; 4 In Silico Prediction of Solubility; 4.1 Introduction; 4.2 What Solubility Measures to Model?; 4.3 Is the Data Set Suitable for Modeling?; 4.4 Descriptors and Modeling Methods for Developing Solubility Models; 4.5 Comparing Literature Solubility Models; 4.6 What Is the Inuence of the Domain of Applicability?; 4.7 Can We Tell when Good Predictions Are Made?; 4.8 Conclusions; References
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5.6.1 Calculated Hydrogen-Bonding Descriptors

Sommario/riassunto

The gold standard for industrial research now completely revised in line with current trends in the field, with all contributions extensively updated or rewritten. In 21 chapters readers can benefit from the key working knowledge of today's leading pharmaceutical companies, including Pfizer, AstraZeneca, and Roche. Drug developers from industry and academia present all the factors governing drug bioavailability, complete with practical examples and real-life data. Part I focuses on in vitro and in vivo measurements of physicochemical properties, such as membrane permeability and ioniza