Drug-like Properties: Concepts, Structure Design and Methods

from ADME to Toxicity Optimization

A successful drug is a combination of both biological activity and drug-like properties. This book explains the drug discovery process and how property-based design can increase the success rate of bringing compounds to market. Written from the perspective of a drug discovery scientist it is a practical guide for medicinal and pharmaceutical chemists, ADME scientists (who study the *absorption, distribution, metabolism,* and *excretion* of pharmaceuticals) and advanced students in these fields.

Drug-like properties, such as solubility, permeability, and metabolism, are examined as the fundamental determinants of how drugs behave *in vivo*. The concepts of pharmacokinetics are discussed with a minimum of mathematical equations, placing emphasis on their practical applications to drug discovery projects. Separate chapters discuss each important property, covering the (1) fundamentals, (2) applications, and (3) case studies on modifying chemical structures for improved properties. This enables the reader to understand the property and learn about useful ways to apply the information. Further chapters describe methods for measuring properties using high throughput, diagnostic, and in-depth methods. Finally, strategies are provided for integrating drug-like properties into a successful drug discovery program.

Each chapter outlines key learning goals and provides questions and answers to test that the area has been clearly understood. For those wanting more information an extensive list of further reading is provided. This book will serve as learning material for scientists interested in drug discovery and also as a reference for regular use.