



Lead Generation Approaches in Drug Discovery

Zoran Rankovic, Richard Morphy

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Lead Generation Approaches in Drug Discovery Zoran Rankovic, Richard Morphy An integrated overview of modern approaches to lead discovery

Lead generation is increasingly seen as a distinct and success-determining phase of the drug discovery process. Over recent years, there have been major advances in the understanding of what constitutes a good lead compound and how to improve the chances of finding such a compound. Written by leading scientists and established opinion leaders from industry and academia, this book provides an authoritative overview of the field, as well as the theory, practice, and scope, of the principal *Lead Generation Approaches in Drug Discovery*, including:

- The evolution of the lead discovery process, key concepts, current challenges, and future directions
- Strategies and technologies driving the high-throughput screening (HTS) approach to lead discovery, including the shifting paradigms in the design of compound collections and best practice in the hit confirmation process
- Knowledge-based in silico or "virtual" screening
- Theory and practice of the fragment-based approach to lead discovery
- The opportunities and challenges presented by multi-target drug discovery (MTDD)
- De novo design of lead compounds and new approaches to estimating the synthetic accessibility of de novo–designed molecules
- The impact of natural products on drug discovery, and potential of natural product–like compounds for exploring regions of biologically relevant chemical space
- Using early screening of hits and leads for metabolic, pharmacokinetic, and toxicological liabilities to reduce attrition during the later phases of drug discovery
- The utility of parallel synthesis and purification in lead discovery

With each topic supported by numerous case studies, this is indispensable reading for researchers in industry and academia who wish to keep up to date with the latest strategies and approaches in drug discovery.

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