Introduction to Biological and Small Molecule Drug Research and Development: Chapter 3. The small molecule drug discovery process - from target selection to candidate selection

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Drug discovery of small molecules from target selection through to clinical evaluation is a very complex, challenging but rewarding area of drug discovery. There are many obstacles along the journey from initial hit-finding activities, through optimization of compounds and eventually to delivery of robust candidate drugs (CDs) for clinical evaluation. This chapter presents key issues and literature solutions with respect to the optimization of hits into CDs. Details of the key hit-finding activities namely high-throughput screening, virtual screening, natural products, fragment-based drug discovery and fast-follower approaches are discussed. Key aspects of compound quality such as lipophilicity, solubility, drug metabolism and pharmacokinetic, plasma protein binding and cytochrome P450 inhibition/induction are discussed as well as potential safety liabilities such as human ether-a-go-go related gene, genotoxicity and phospholipidosis, Finally successful hit-to-lead and lead optimization case studies are presented to illustrate and highlight the key principles.

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