Impact of Drug-Like Properties on Hit Selection and Optimization for Quality Clinical Candidates

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Drug-like properties are a necessary characteristic of orally active clinical candidates. Drug discovery organizations have integrated the evaluation and optimization of drug-like properties into the workflow in parallel with activity evaluation and optimization. Properties result from the structure of the compound, thus, medicinal chemists can modify structures to improve properties. Key properties for discovery are solubility, permeability and metabolic stability. A recent advance was the recognition that properties also affect biological assay data and assays must be optimized to deal with compounds over a wide property range.