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## Drug Discovery Today

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Review

### Pharmaceutical profiling in drug discovery

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#### Abstract

Drug discovery research organizations are building capability for measuring an ensemble of crucial “drug-like” properties. These structure–property relationship (SPR) data complement current SAR information. This pharmaceutical profiling strategy enables research teams to better plan and interpret discovery experiments, be alerted to potential “show stoppers”, improve property liabilities, and select the best candidates for advancement. High throughput property assays for physicochemical properties – solubility, permeability, lipophilicity, stability, and  $pK_a$  – *in vitro* ADME – metabolism, transporters, protein binding and CYP inhibition – and *in vivo* PK/exposure provide a wealth of data for teams to make informed decisions.



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Keywords

Drug Discovery; Molecular Medicine; Pharmaceutical Science; Structural Biology

## Keywords

pharmaceutical profiling; drug discovery; structure-activity relationships; structure-property relationships; druglike properties

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