Empowering medicinal chemists to move quickly and confidently from concept to candidate

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Learn more

Real-time collaboration enables teams to select superior compounds faster

Design better compounds: Leverage all past knowledge to build on successes and avoid repeating failures.

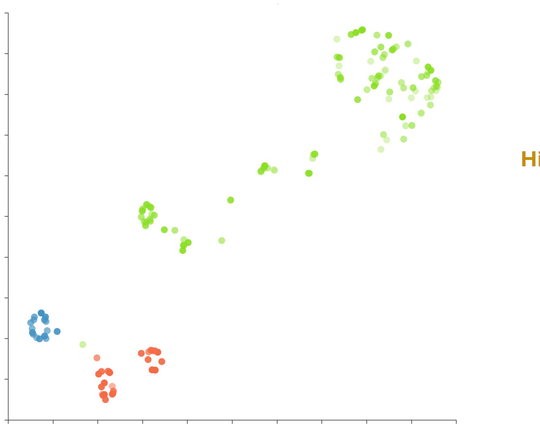
Progress faster together: Automatically keep teams in sync on the latest data and decisions, even across different time zones.

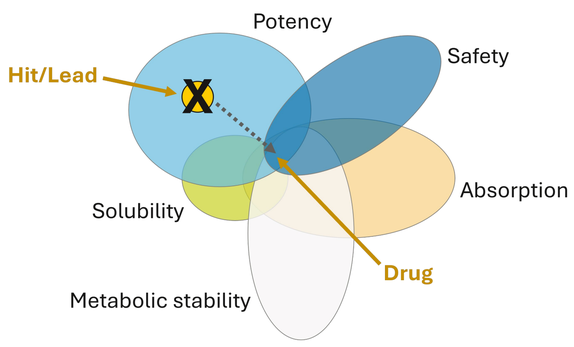
Maximise experimental impact: Focus synthesis and testing where the likelihood of success is highest, with alignment on compounds and priorities.

Solve problems faster: Uncover and combine diverse insights with parallel exploration of shared data.

Hit to lead → Lead Optimisation → Pre-clinical

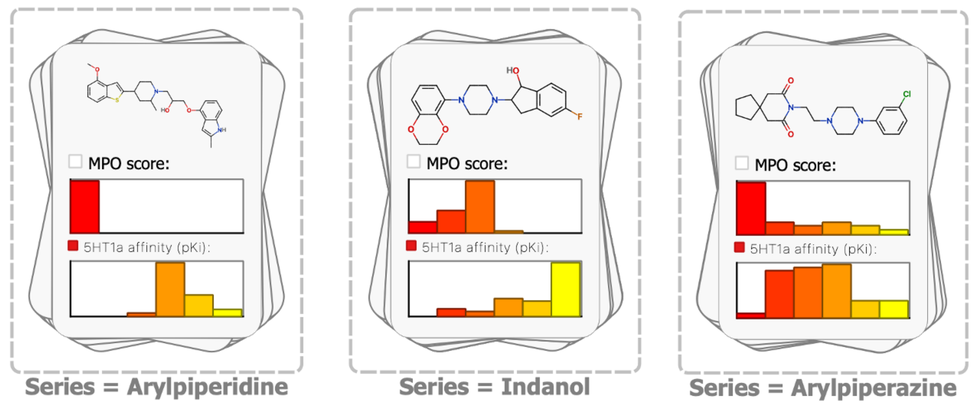
1 Quickly identify lead compounds balancing multiple parameters

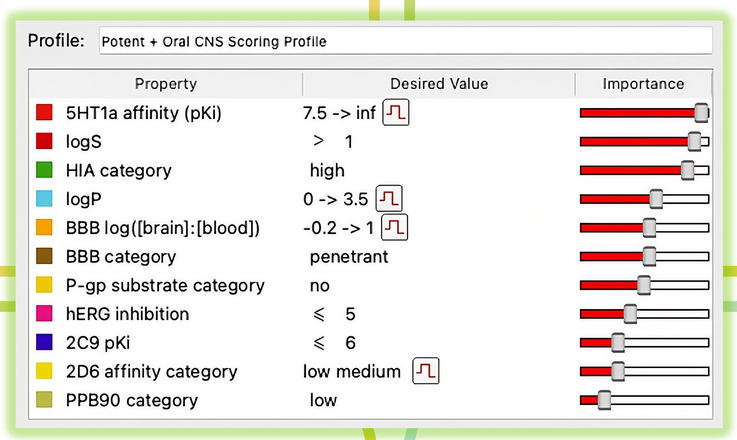




There are potent compounds in multiple chemical series, but the most potent compounds are not necessarily the best starting point for lead optimisation. It's more efficient to consider multiple key properties at once.

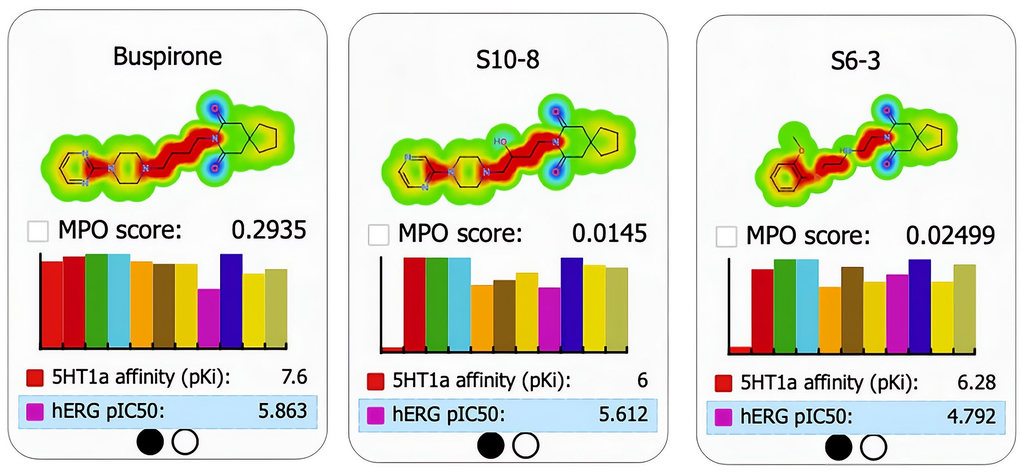
2 Navigate trade-offs between activity and ADME properties





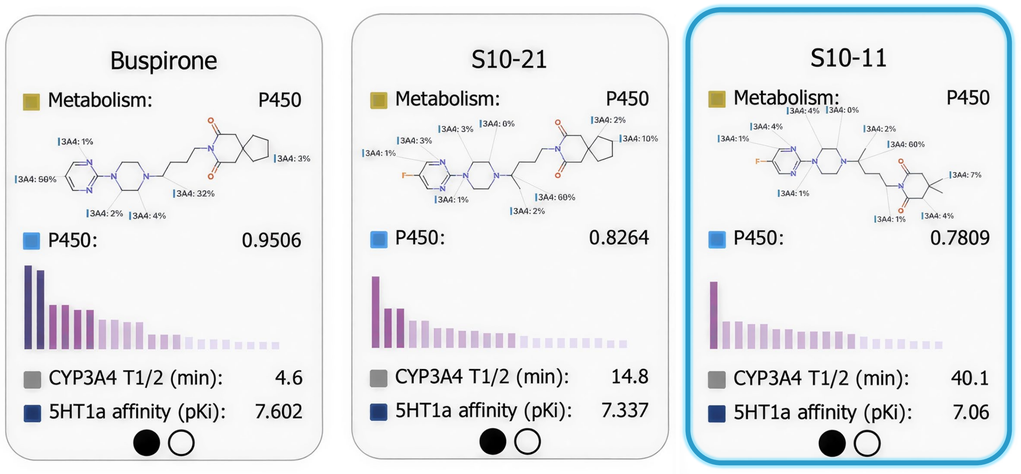
Multi-parameter optimisation (MPO) scoring[1,2] shows that some potent series likely have ADME liabilities. Card View™[3] intuitively visualises relationships in the data to quickly identify the series with the best chance of success.

3 Interactively design around ADME liabilities



The Glowing Molecule™[4] highlights regions in the compound where changes are most likely to impact specific properties, guiding interactive design to explore trade-offs between potency and hERG liability, enabling rapid optimisation before synthesis.

4 Optimise for metabolic stability



Addressing metabolic liabilities is critical for *in vivo* success. Predicted metabolically labile sites[5,6] guide targeted modifications to optimise for stability. The selected pre-clinical candidate balances potency with a reduced risk of rapid clearance.

References

[1] M. Segall (2012) Curr. Pharm. Des. 18(9) pp. 1292-1310
[2] US patent Nos. 9,224,098 and 9,367,812
[3] M. Segall *et al.* (2015) Drug Discov. Today 20(9) pp. 1093-1103
[4] M. Segall *et al.* (2009) Chem. & Biodiv. 6(11) p. 2144-2151
[5] J Tyzack et al. (2017) J. Chem. Inf. Model. 56(1) pp. 2180-2193
[6] M. Öeren et al. (2022) J. Med. Chem. 65(20) pp. 14066-14081