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# Present drug-likeness filters in medicinal chemistry during the hit and lead optimization process: how far can they be simplified?

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## Graphical abstract



## Optimization process:

Rules of thumbs and ligand efficiency metrics?

(Ro5, eRo5, bRo5, Ro4, Ro3, tPSA, logP, LE, LLE, GE, PEI, BEI, SEI, QED, Drug<sub>eff</sub>,  $\Delta H/\Delta S$ , K<sub>off</sub>/K<sub>on</sub> etc.)

## HIGHLIGHTS

Best descriptors to monitor molecular weight and lipophilicity for drugs optimization

How far can we simplify drug-likeness prediction tools?

Rules and ligand efficiency metrics in the drug discovery process: strategies

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