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

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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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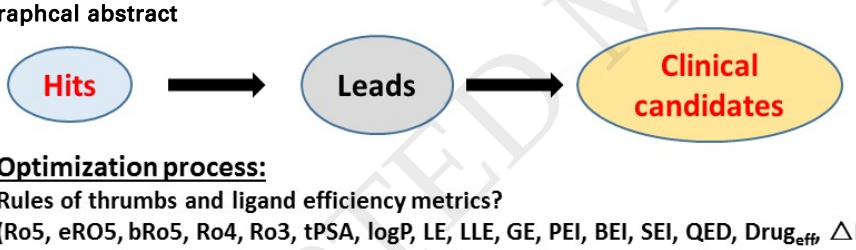
Graphcal abstract



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