

Drug-like set creation (algorithm):

- 1) DLS does not include Advanced collection compounds (HTS compounds only)
- 2) Lypinskiy rule:
MW: 200...500
H-bond donors: 0...5
H-bond acceptors: 0...10
ClogP: -2 ... 5
- 3) Veber rule:
Rotatable bonds: 0...10
PSA: 0...140
- 4) LogS: -6...0.5
- 5) Toxic / reactive compounds: absence
- 6) The diversification of DLS by clusterization procedure using sphere exclusion method (similarity threshold = 0.8) with Chemaxon chemical hashed fingerprints.