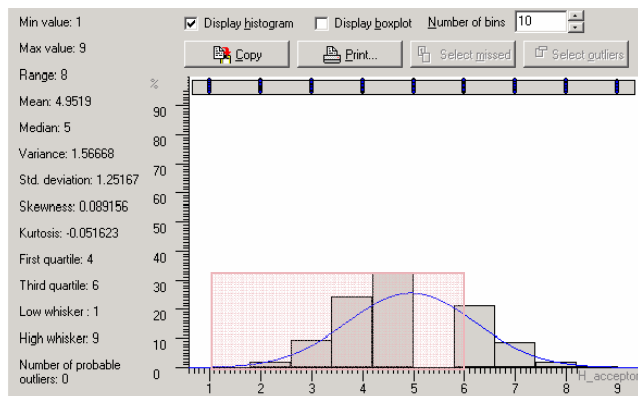
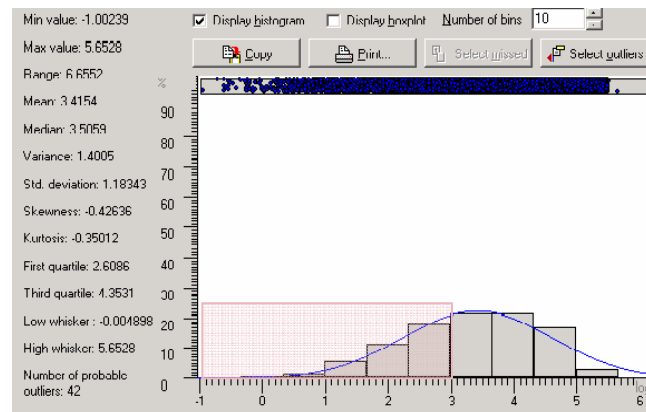


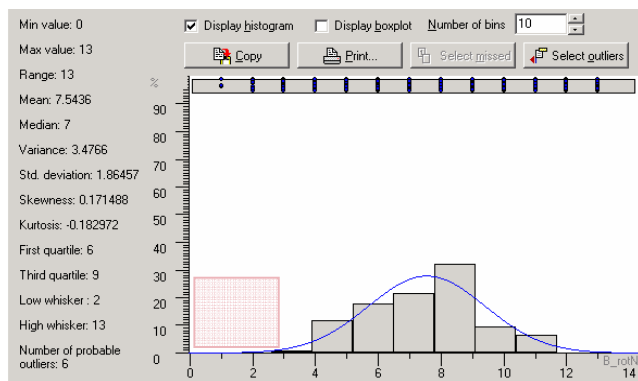
Fragment Properties curation I. Drug-like” vs. lead-like and more.



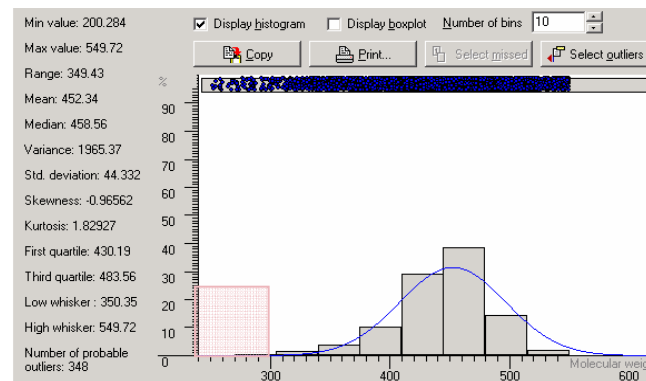
H-bond acceptors



clogP



Rotatable bonds

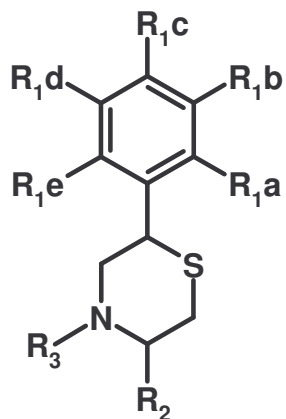


Molecular Weight

- mol Polar surface area ≤ 80
- Rings > 0
- $0 < \text{NRB} \leq 3c$

- $1 \leq \text{N} + \text{O} < 6$
- S atoms < 3 , Cl < 3 , Br < 2 ,
- $\text{F} + \text{Cl} + \text{Br} \leq 4$
- non-H atoms ≤ 20

Lead-like set of fragment: Example of Synthetic Strategy

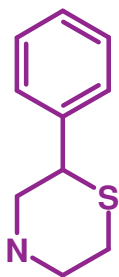


R1 = H, Me, Hal, OH, CF3, etc

R2 = H, COOMe;

R3 = H, Alkyl, Acyl, etc

Scaffold for 250-300
compounds



Selected Fragment
for 5-15 compounds
synthesis

R1	R2	R3	MW	ClogP	HBD	HBA	RTB	logSW	Score
H	H	H	179	2.22	1	1	1	-2.05	+++
H	COOMe	H	237	1.61	1	3	3	-2.0	+++
H	COOH	H	223	1.15	2	3	2	-1.9	+++
3-OMe	H	PhCO	313	3.92	0	3	4	-3.2	---
3-F	H	Et	225	3.0	0	1	2	-2.3	++-