



SCS  
Swiss Chemical  
Society

# SCS Spring School on Digital Chemistry

## Collaborative Project

### Input SMILES

CN1C(=O)C=C(c2cccc(Cl)c2)c3cc(ccc13)[C@@](N)(c4ccc(Cl)cc4)c5cncn5C

Similarity  
%

50

SEARCH

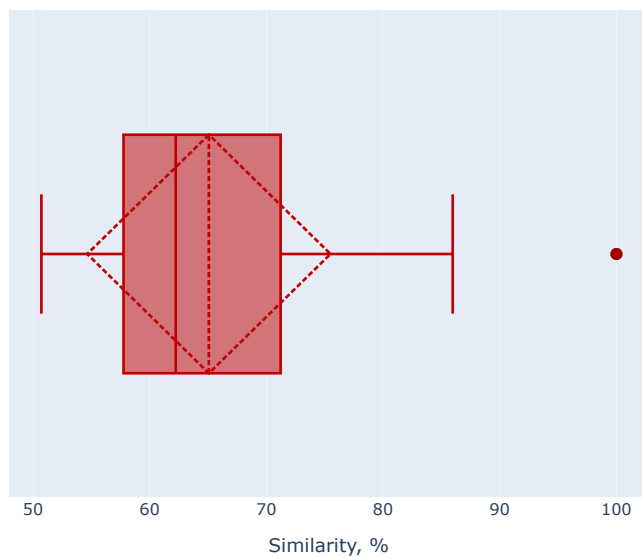
### Results Summary

Found 70 molecules

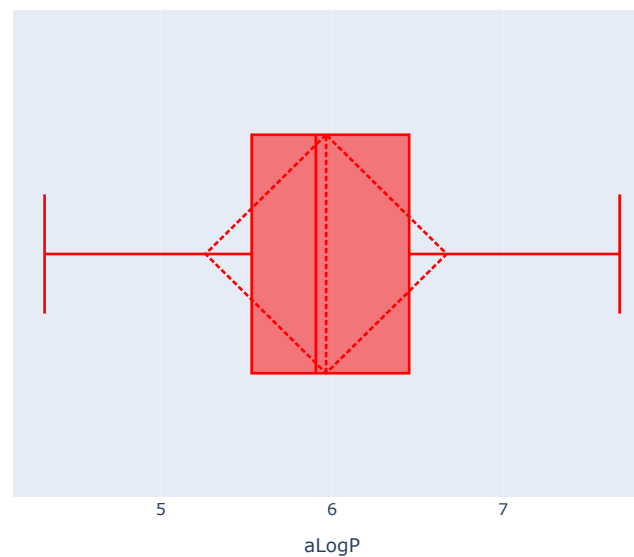
property_name	average	median	std	maximum	minimum	IRQ	quartiles
Similarity	65.062	62.22	10.428	100	50.704	13.375	57.837, 62.22, 71.212
aLogP	5.965	5.905	0.705	7.68	4.32	0.915	5.53, 5.905, 6.445
Molecule weight	504.453	501.91	23.189	575.5	454.96	27.762	489.41, 501.91, 517.172
Number of aromatic rings	5.2	5	0.466	7	4	0	5.0, 5.0, 5.0
H-bond acceptors	5.243	5	0.664	8	4	0	5.0, 5.0, 5.0
H-bond donors	1.053	1	0.223	2	1	0	1.0, 1.0, 1.0
Number of 'rule of five' violations	1.578	2	0.494	2	1	1	1.0, 2.0, 2.0
Polar surface area	59.958	60.05	12.933	99.81	39.82	19.37	49.05, 60.05, 68.42

### Molecules Properties

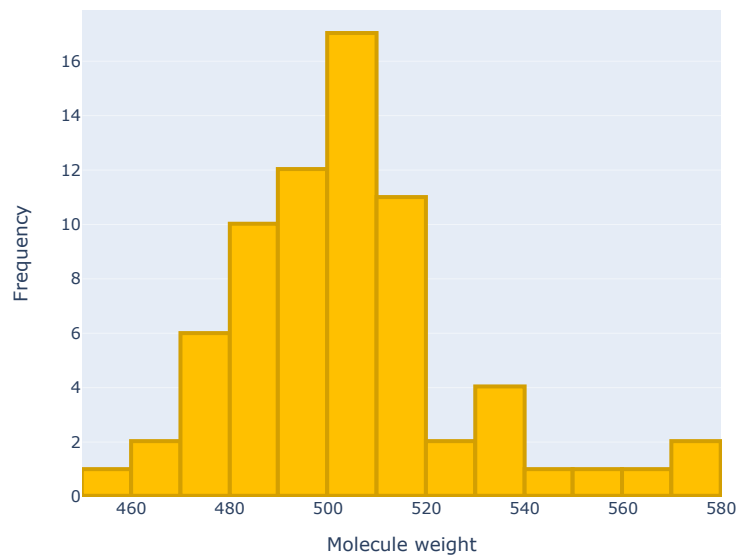
Similarity



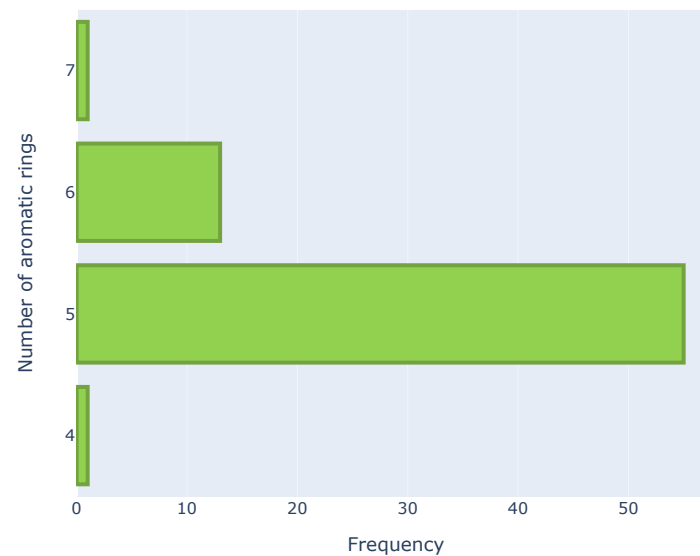
aLogP



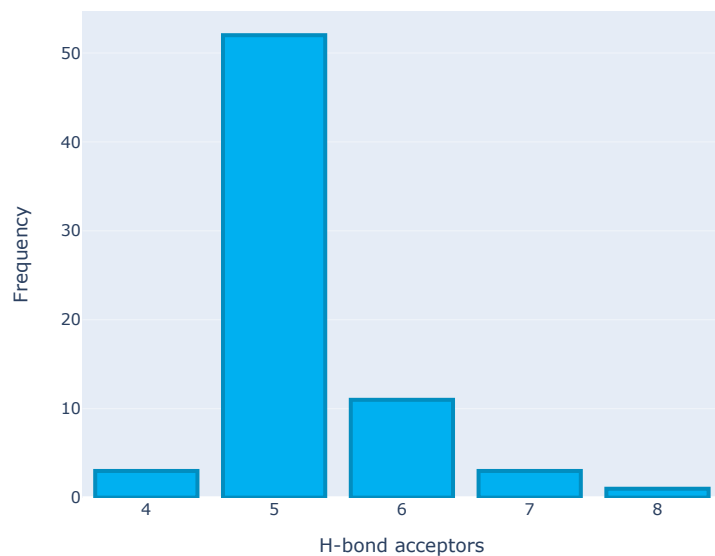
Molecule weight



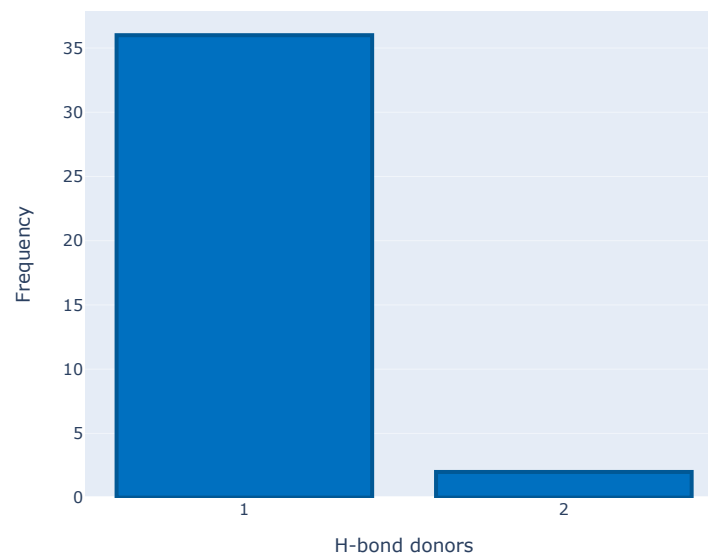
Number of aromatic rings



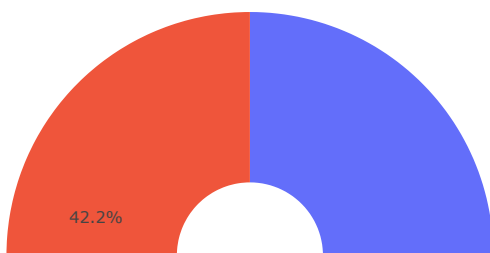
Number of H-bond acceptors



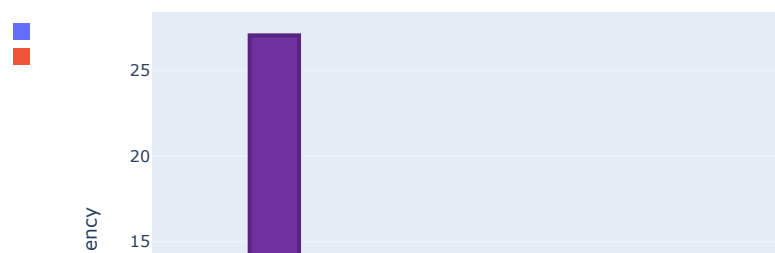
Number of H-bond donors

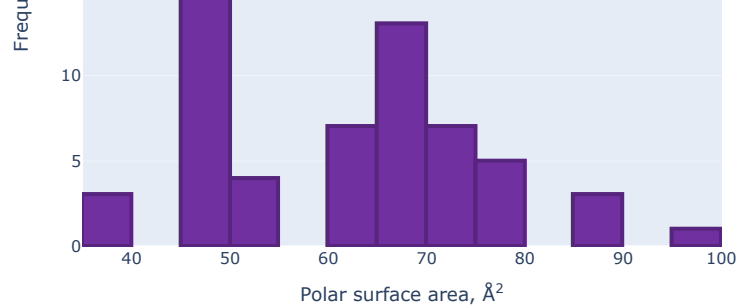


'Rule of five' violations



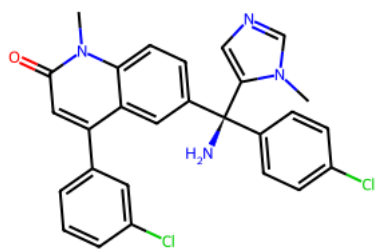
Polar surface area





## Examples of molecules

Input molecule



Similarity



100

aLogP



Polar surface area



100

Found 70 molecules





