



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
%

60

SEARCH

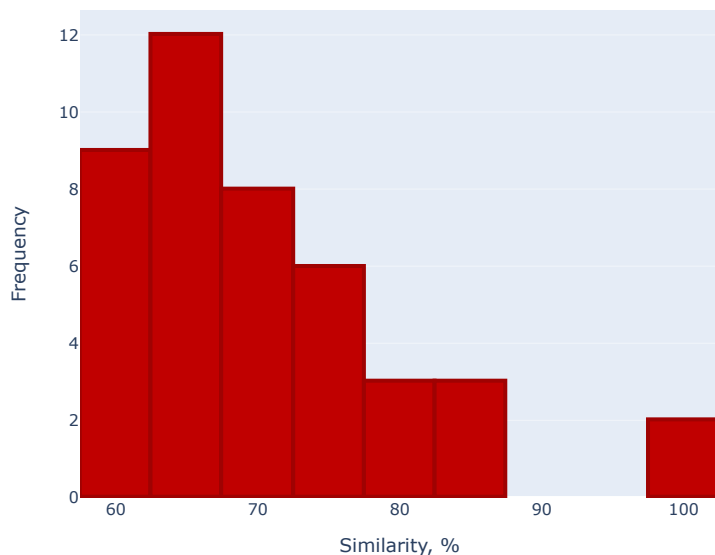
Results Summary

Total 43 molecules

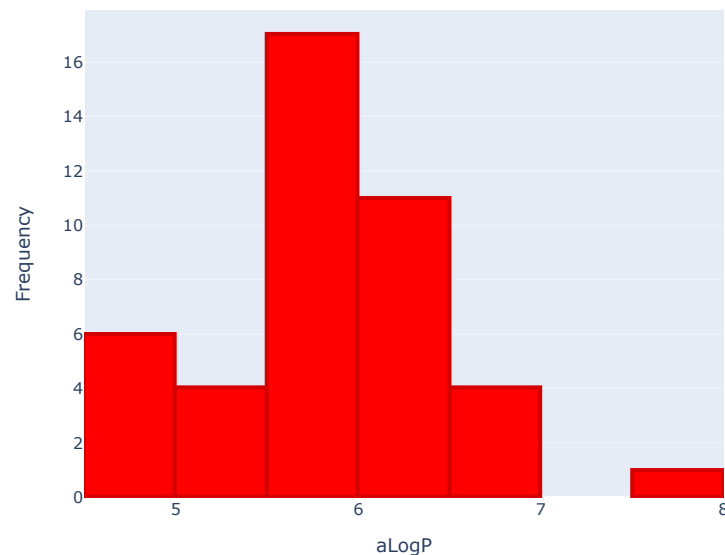
property_name	average	median	std	maximum	minimum	IRQ	quartiles
Similarity	70.609	67.647	9.655	100	60.294	11.118	64.087, 67.647, 75.205
aLogP	5.802	5.84	0.585	7.51	4.63	0.65	5.5, 5.84, 6.15
Molecule weight	498.855	499.41	19.328	575.5	454.96	15.01	489.41, 499.41, 504.42
Number of aromatic rings	5.302	5	0.507	7	5	1	5.0, 5.0, 6.0
H-bond acceptors	5.326	5	0.738	8	4	1	5.0, 5.0, 6.0
H-bond donors	1.033	1	0.18	2	1	0	1.0, 1.0, 1.0
Number of 'rule of five' violations	1.526	2	0.499	2	1	1	1.0, 2.0, 2.0
Polar surface area	63.407	65.84	13.13	99.81	39.82	24.98	49.05, 65.84, 74.03

Molecules Properties

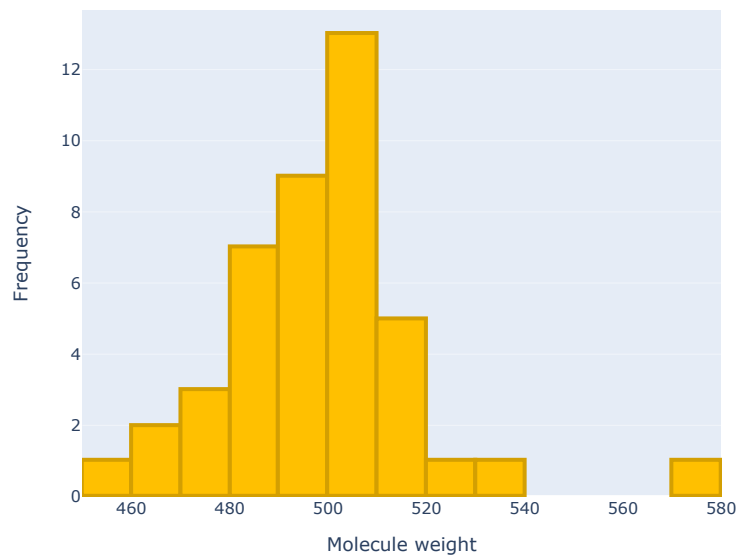
Similarity



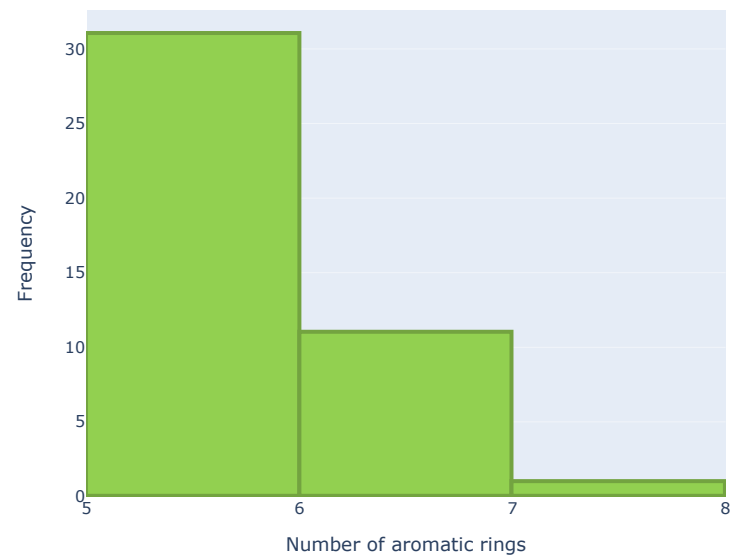
aLogP



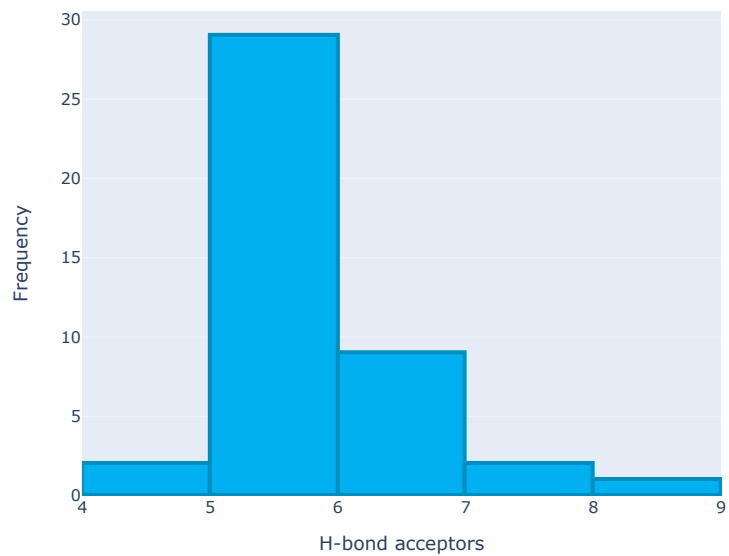
Molecule weight



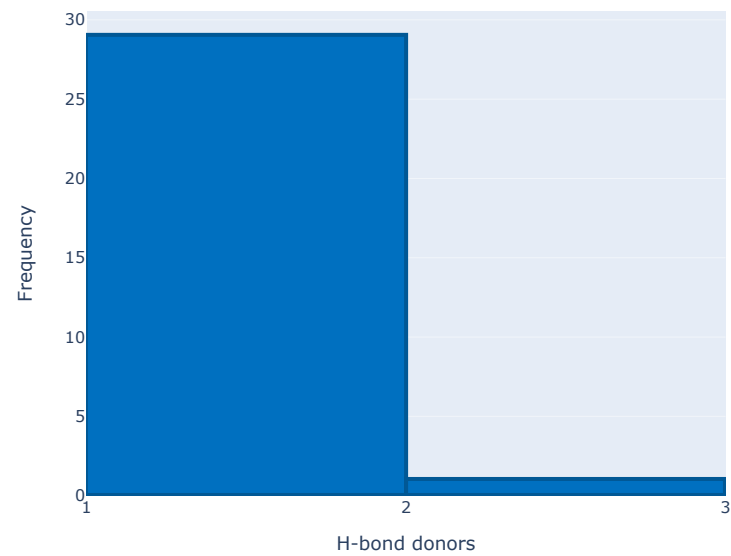
Number of aromatic rings



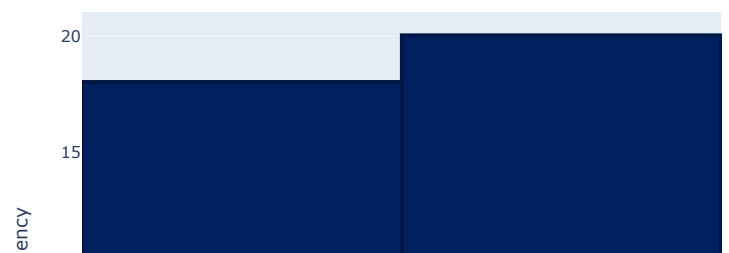
Number of H-bond acceptors



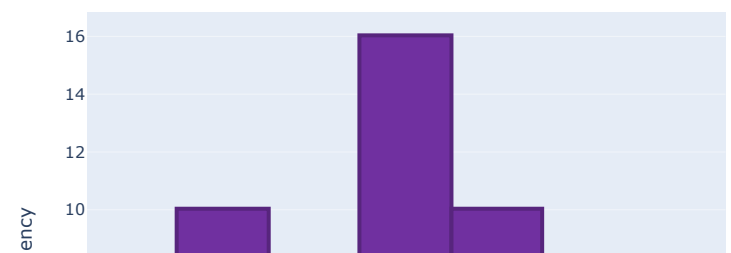
Number of H-bond donors

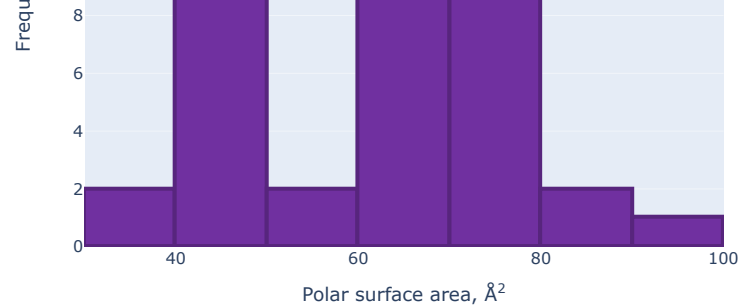
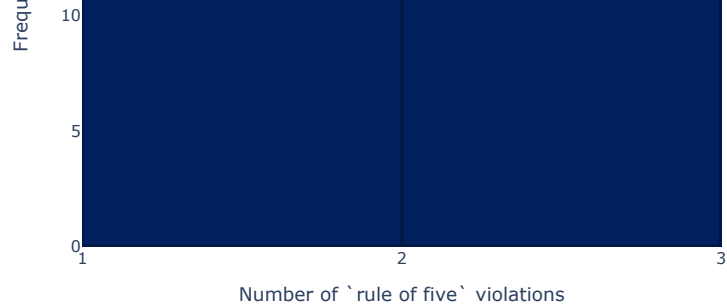


'Rule of five' violations



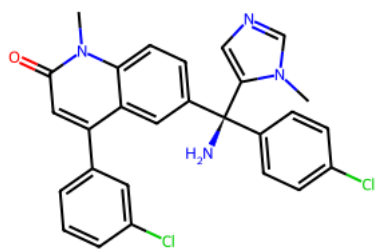
Polar surface area





Examples of molecules

Input molecule



Similarity



100

aLogP



Polar surface area



100

Found 43 molecules



