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
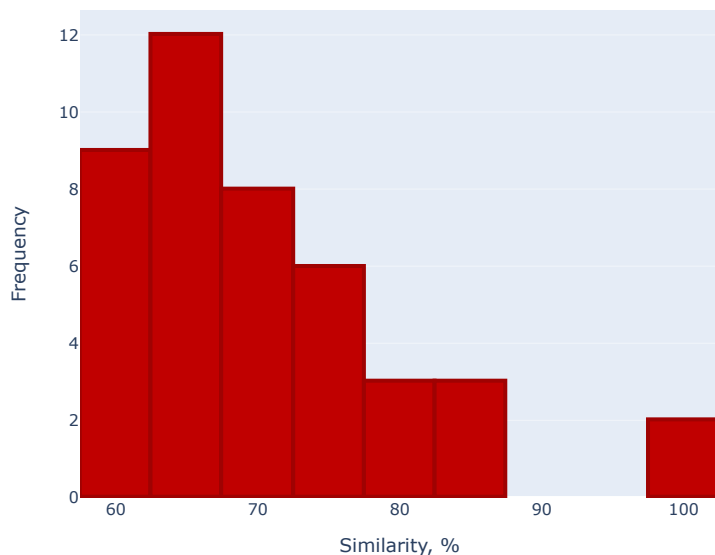
Similarity % `60`

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