SCS
Swiss Chemical Society

SCS Spring School on Digital Chemistry

Collaborative Project

Input SMILES

COC(=O)c1ccc(CBr)cc1

Minimum similarity %: 50

SEARCH

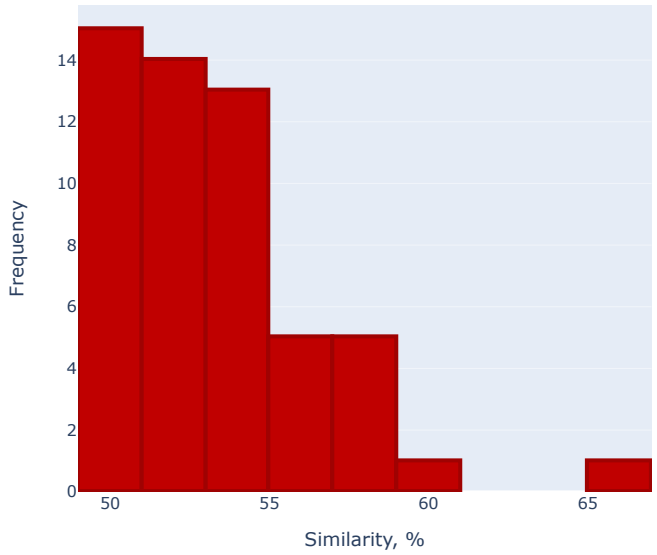
Results Summary

Found 54 molecules

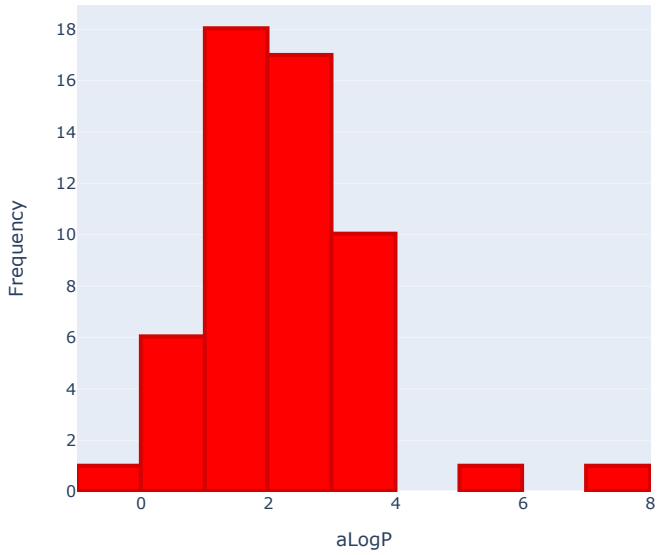
property_name	average	std	maximum	minimum
Similarity	53.085	3.056	65.517	50
aLogP	2.236	1.302	7.4	-0.14
Molecule weight	262.307	90.606	651.8	137.14
Number of aromatic rings	1.556	0.629	4	1
H-bond acceptors	3.815	1.402	9	1
H-bond donors	1.367	0.605	3	1
Number of 'rule of five' violations	1.5	0.5	2	1
Polar surface area	57.456	21.716	114.99	26.3

Molecules Properties

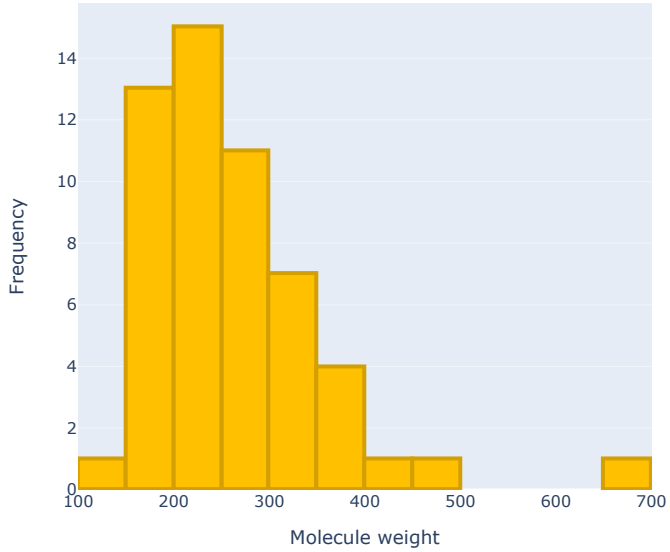
Similarity



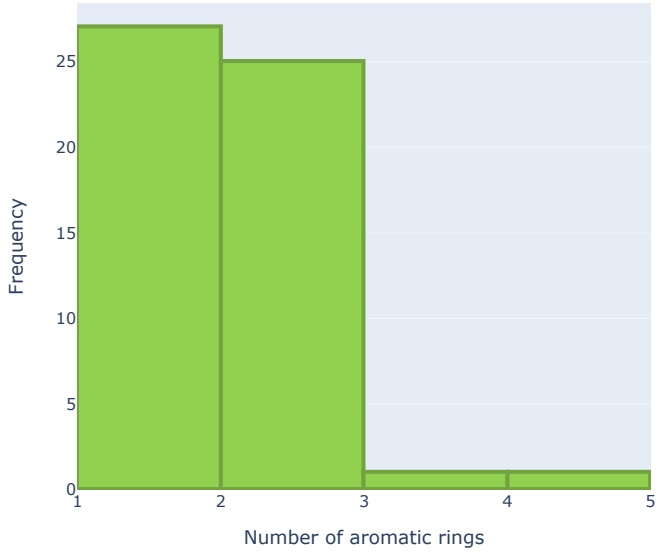
aLogP



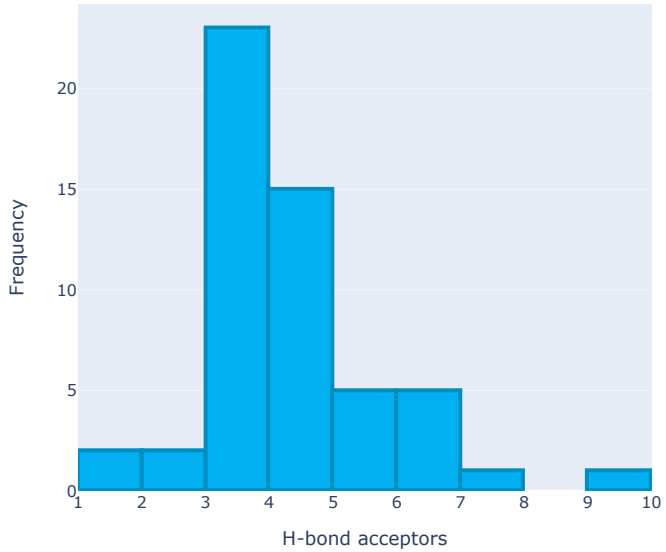
Molecule weight



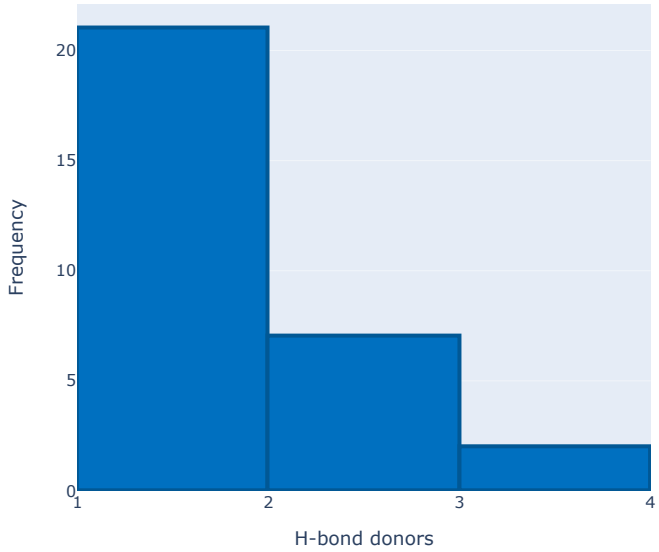
Number of aromatic rings



Number of H-bond acceptors

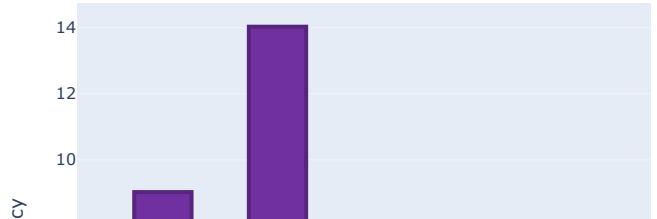


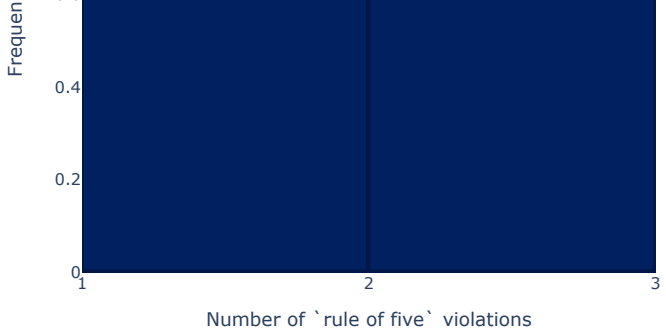
Number of H-bond donors

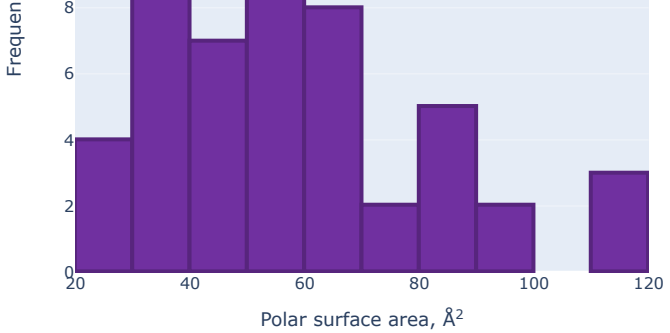


'Rule of five' violations

Polar surface area

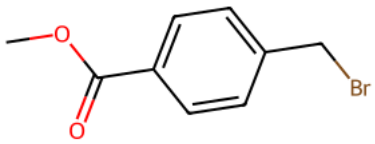






Examples of molecules

Input molecule

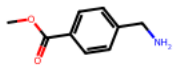
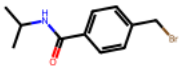
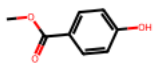
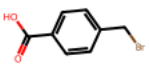
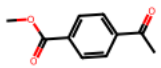
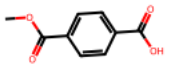
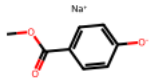
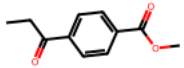
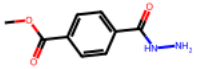
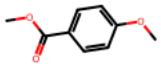
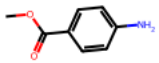
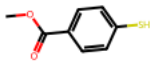
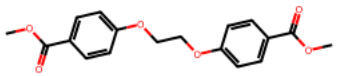
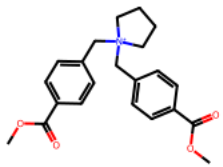
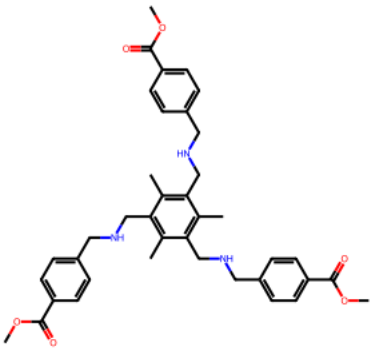
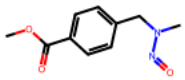
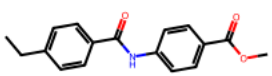
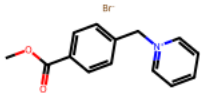
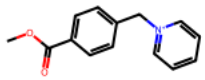
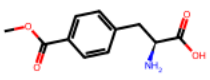
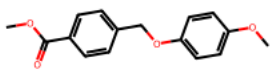
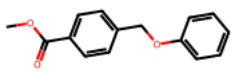
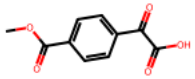
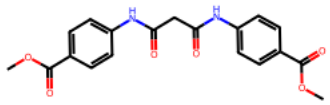
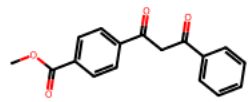
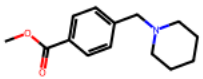
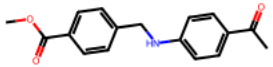
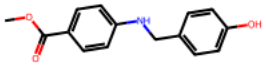
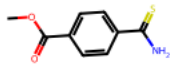
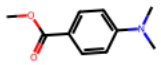


Similarity

aLogP

Polar surface area

Found 54 molecules






















Designed by O
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