



SCS
Swiss Chemical
Society

SCS Spring School on Digital Chemistry

Collaborative Project

Input SMILES

COC(=O)c1ccc(CBr)cc1

Minimum
similarity
%

50

SEARCH

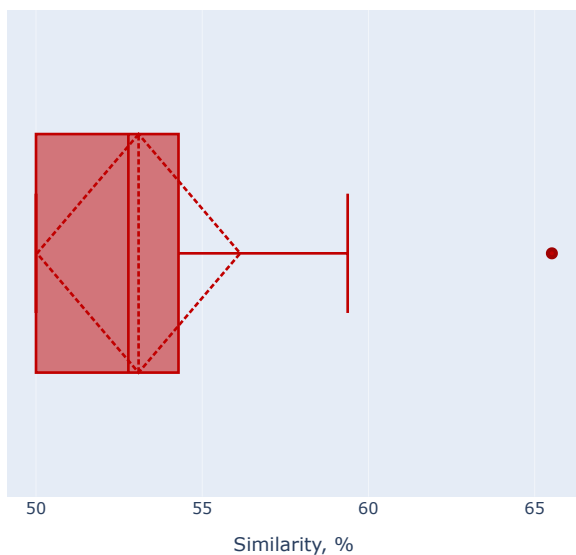
Results Summary

Found 54 molecules

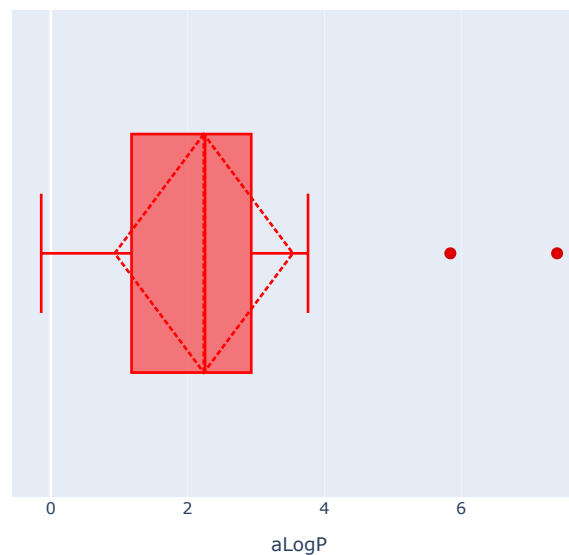
property_name	average	std	maximum	minimum
Similarity	53.085	3.056	65.517	50
aLogP	2.236	1.302	7.4	-0.14
Molecule weight	262.307	90.606	651.8	137.14
Number of aromatic rings	1.556	0.629	4	1
H-bond acceptors	3.815	1.402	9	1
H-bond donors	1.367	0.605	3	1
Number of 'rule of five' violations	1.5	0.5	2	1
Polar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

Molecules Properties

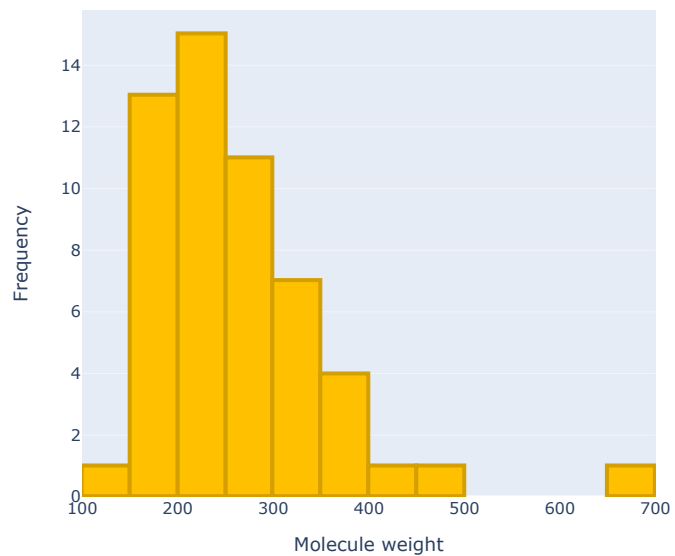
Similarity



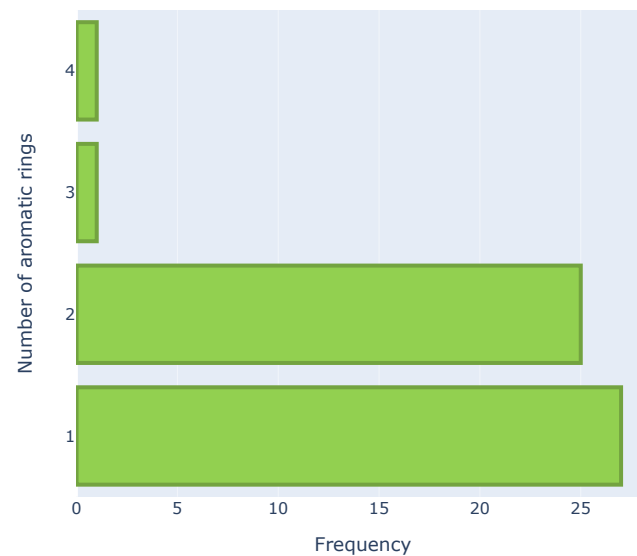
aLogP



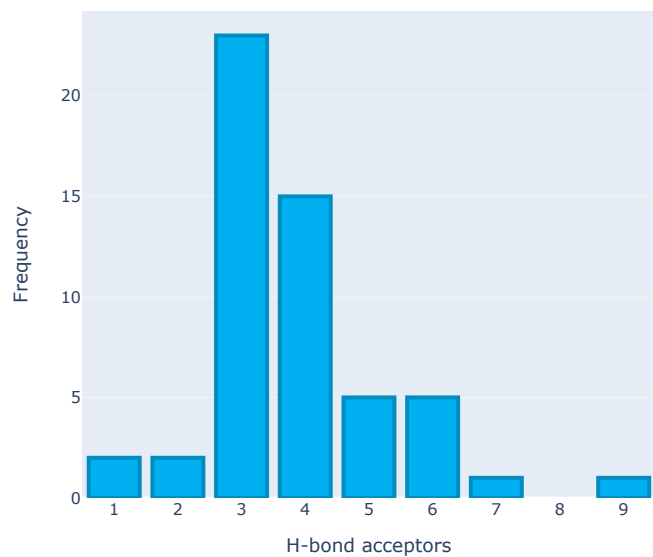
Molecule weight



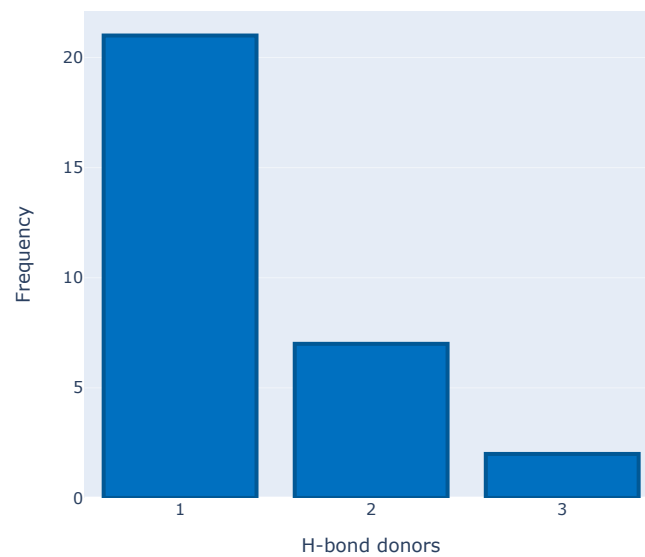
Number of aromatic rings



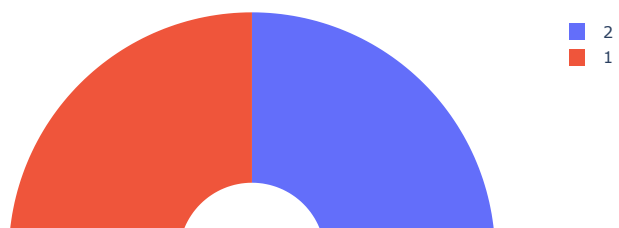
Number of H-bond acceptors



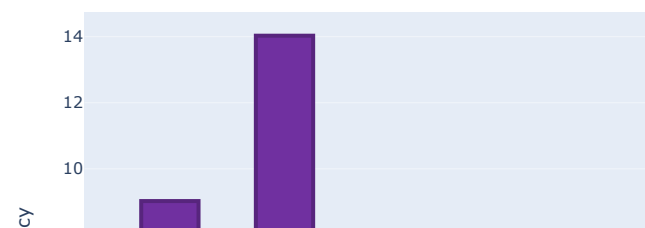
Number of H-bond donors

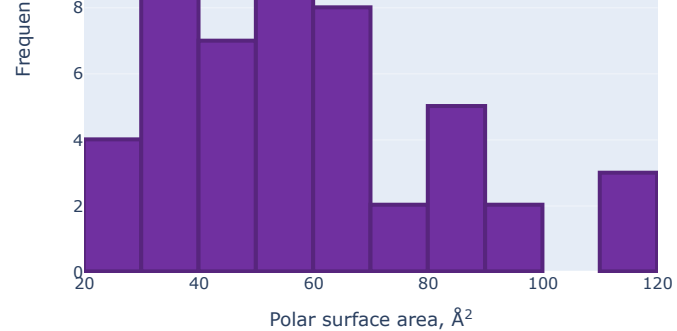


'Rule of five' violations



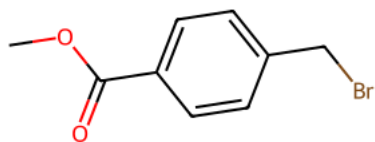
Polar surface area





Examples of molecules

Input molecule



Similarity



aLogP



Polar surface area



Found 54 molecules



