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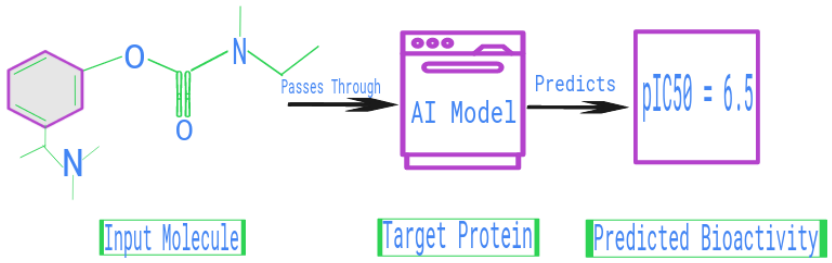
Drug Discovery Using AI for Breast Cancer



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aromatase_exp.txt 283.0B

Example input file

Predict

Input Data with Dataframe

	0	1
0	CCOc1nn(-c2cccc(OCc3ccccc3)c2)c(=O)o1	CHEMBL133897
1	O=C(N1CCCCC1)n1nc(-c2ccc(Cl)cc2)nc1SCC1CC1	CHEMBL336398
2	CN(C(=O)n1nc(-c2ccc(Cl)cc2)nc1SCC(F)(F)F)c1ccccc1	CHEMBL131588
3	O=C(N1CCCCC1)n1nc(-c2ccc(Cl)cc2)nc1SCC(F)(F)F	CHEMBL130628
4	CSc1nc(-c2ccc(OC(F)(F)F)cc2)nn1C(=O)N(C)C	CHEMBL130478

Calculated Molecular Descriptors

	Name	PubchemFP0	PubchemFP1	PubchemFP2	PubchemFP3	PubchemFP4	PubchemFI
0	CHEMBL130478	1	1	0	0	0	
1	CHEMBL130628	1	1	1	0	0	
2	CHEMBL133897	1	1	1	0	0	
3	CHEMBL131588	1	1	0	0	0	
4	CHEMBL336398	1	1	1	0	0	

(5, 882)

Subset of Descriptors from the Models

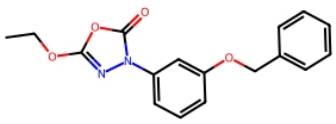
	PubchemFP2	PubchemFP12	PubchemFP14	PubchemFP15	PubchemFP16	PubchemFP18	Pubche
0	0	0	1	1	1	1	
1	1	1	1	1	1	1	
2	1	1	1	1	0	1	
3	0	1	1	1	1	1	
4	1	1	1	1	1	1	

(5, 250)

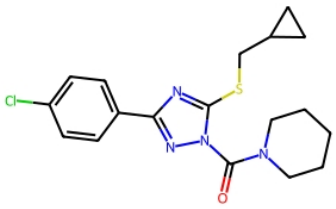
Prediction Output

	molecule_name	pIC50	smiles
0	CHEMBL133897	5.5947	CCOc1nn(-c2cccc(OCc3ccccc3)c2)c(=O)o1
1	CHEMBL336398	5.5157	O=C(N1CCCCC1)n1nc(-c2ccc(Cl)cc2)nc1SCC1CC1
2	CHEMBL131588	5.3468	CN(C(=O)n1nc(-c2ccc(Cl)cc2)nc1SCC(F)(F)F)c1ccccc1
3	CHEMBL130628	6.1526	O=C(N1CCCCC1)n1nc(-c2ccc(Cl)cc2)nc1SCC(F)(F)F
4	CHEMBL130478	5.6736	CSc1nc(-c2ccc(OC(F)(F)F)cc2)nn1C(=O)N(C)C

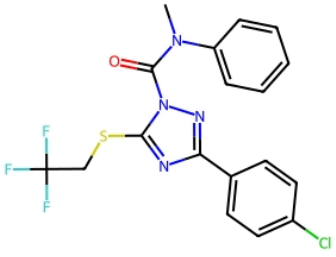
Chemical: CHEMBL133897



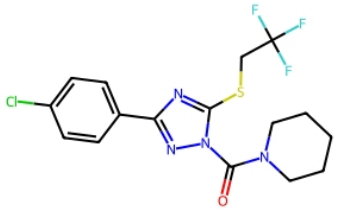
Chemical: CHEMBL336398



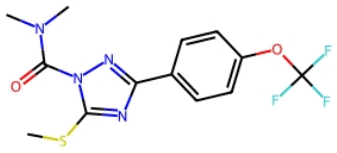
Chemical: CHEMBL131588



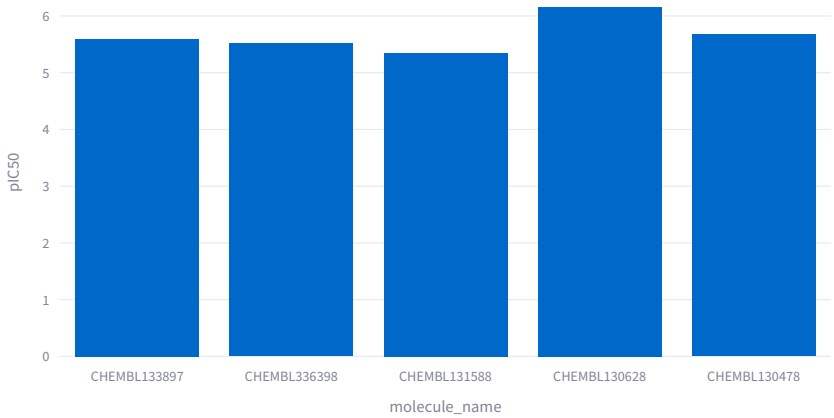
Chemical: CHEMBL130628



Chemical: CHEMBL130478



Graphical Prediction Output



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