

## MuSSEL Prediction IC<sub>50</sub>:

1 rank

Acetylcholinesterase : Electrophorus electricus

score: 6.335 on ChEMBL4078 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL470867		0.727273	330.00	*
MFP1	ChEMBL470867		0.575758	330.00	*
RDKit7	ChEMBL258893		0.596059	3780.00	
Pattern	ChEMBL258893		0.893987	3780.00	*
AP_bits	ChEMBL1270850		0.610592	1800.00	*
TT_bits	ChEMBL258893		0.590909	3780.00	*
FP2	ChEMBL258893		0.640449	3780.00	*
hybridization	ChEMBL258893		0.661157	3780.00	*
substructure	ChEMBL3793762		0.842105	465.96	
graph	ChEMBL3819248		0.814159	131.00	*
pubchem	ChEMBL374981		0.819512	2.73	
cdk_maccs	ChEMBL1271342		0.820896	1740.00	*
klekota_roth	ChEMBL1271342		0.563380	1740.00	

\*\*\* ic50 ACTIVITY \*\*\* value prediction

based on 9 locally validated fgps ---> 2034.977

["TT\_bits", "Pattern", "AP\_bits", "MFP1", "graph", "FP2", "FeatMFP1", "cdk\_maccs", "hybridization"]

2 rank

Acetylcholinesterase : Homo sapiens

score: 5.542 on ChEMBL220 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL470867		0.727273	540.00	*
MFP1	ChEMBL507903		0.588235	7.70	*
RDKit7	ChEMBL258893		0.596059	1540.00	
Pattern	ChEMBL258893		0.893987	1540.00	*
AP_bits	ChEMBL12089		0.603226	40.00	*
TT_bits	ChEMBL258893		0.590909	1540.00	*
FP2	ChEMBL258893		0.640449	1540.00	*
hybridization	ChEMBL258893		0.661157	1540.00	*
substructure	ChEMBL3335056		0.842105	6700.00	
graph	ChEMBL3233992		0.836364	61400.00	*
pubchem	ChEMBL374981		0.819512	5.08	
cdk_maccs	ChEMBL3407582		0.780822	8400.00	
klekota_roth	ChEMBL491526		0.560000	2370.00	

\*\*\* ic50 ACTIVITY \*\*\* value prediction

based on 8 locally validated fgps ---> 8912.199

["TT\_bits", "Pattern", "AP\_bits", "MFP1", "graph", "FP2", "FeatMFP1", "hybridization"]

3 rank

Reverse transcriptase : Human immunodeficiency virus 1

score: 4.855 on ChEMBL2366516 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL485509		0.482759	4677.35	
MFP1	ChEMBL292540		0.529412	5500.00	*
RDKit7	ChEMBL8443		0.650138	49.00	
Pattern	ChEMBL8443		0.887122	49.00	*
AP_bits	ChEMBL8443		0.596215	49.00	*
TT_bits	ChEMBL8443		0.645161	49.00	*
FP2	ChEMBL8443		0.678571	49.00	*
hybridization	ChEMBL8443		0.709821	49.00	*
substructure	ChEMBL292540		0.684211	5500.00	
graph	ChEMBL8443		0.809091	49.00	*
pubchem	ChEMBL2407273		0.737374	3850.00	
cdk_maccs	ChEMBL3338519		0.698630	25770.00	

klekota\_roth CHEMBL3338519 0.412500 25770.00  
 \*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 7 locally validated fgps ---> 1454.398  
 ["TT\_bits", "Pattern", "AP\_bits", "MFP1", "graph", "FP2",  
 "hybridization"]

4 rank

Cholinesterase : Equus caballus

score: 4.739 on CHEMBL5763 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3323054		0.666667	5220.0	
MFP1	CHEMBL1186488		0.531250	19340.0	*
RDKit7	CHEMBL258893		0.596059	6330.0	
Pattern	CHEMBL258893		0.893987	6330.0	*
AP_bits	CHEMBL12089		0.603226	18200.0	*
TT_bits	CHEMBL258893		0.590909	6330.0	*
FP2	CHEMBL258893		0.640449	6330.0	*
hybridization	CHEMBL258893		0.661157	6330.0	*
substructure	CHEMBL2323351		0.833333	71700.0	
graph	CHEMBL3819247		0.818182	9820.0	*
pubchem	CHEMBL3819248		0.819095	4249.0	
cdk_maccs	CHEMBL1164080		0.782609	1310.0	
klekota_roth	CHEMBL1186488		0.565217	19340.0	

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 7 locally validated fgps ---> 10339.888  
 ["TT\_bits", "Pattern", "AP\_bits", "MFP1", "graph", "FP2",  
 "hybridization"]

5 rank

Butyrylcholinesterase : Homo sapiens

score: 4.674 on CHEMBL1914 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3335057		0.695652	33200.00	*
MFP1	CHEMBL507903		0.588235	3000.00	*
RDKit7	CHEMBL258893		0.596059	10340.00	
Pattern	CHEMBL258893		0.893987	10340.00	*
AP_bits	CHEMBL12089		0.603226	18970.00	*
TT_bits	CHEMBL258893		0.590909	10340.00	*
FP2	CHEMBL258893		0.640449	10340.00	*
hybridization	CHEMBL258893		0.661157	10340.00	*
substructure	CHEMBL3335056		0.842105	14100.00	
graph	CHEMBL12089		0.747899	18970.00	
pubchem	CHEMBL374981		0.819512	1.38	
cdk_maccs	CHEMBL3407582		0.780822	5900.00	
klekota_roth	CHEMBL491526		0.560000	88800.00	

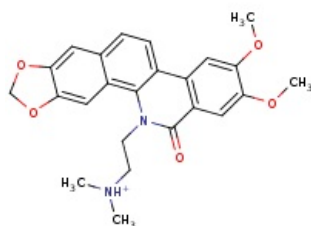
\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 7 locally validated fgps ---> 10781.231  
 ["TT\_bits", "Pattern", "AP\_bits", "MFP1", "FP2", "FeatMFP1",  
 "hybridization"]

# SwissTargetPrediction report:

## Reference:

Gfeller D., Michielin O. & Zoete V.  
 Shaping the interaction landscape of  
 bioactive molecules, *Bioinformatics*  
 (2013) 29:3073-3079.

## Query Molecule



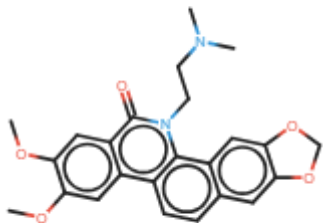
## Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
DNA topoisomerase 1	P11387	TOP1	CHEMBL1781	<div><div></div></div>	21 / 15	Enzyme
DNA topoisomerase I, mitochondrial (by homology)	Q969P6	TOP1MT		<div><div></div></div>	21 / 15	Enzyme
Cyclin-dependent kinase 1	P06493	CDK1	CHEMBL308	<div><div></div></div>	226 / 5	Ser_Thr Kinase
Cyclin-dependent kinase 4	P11802	CDK4	CHEMBL331	<div><div></div></div>	221 / 5	Ser_Thr Kinase
Cyclin-dependent kinase 2	P24941	CDK2	CHEMBL301	<div><div></div></div>	226 / 5	Ser_Thr Kinase
Cyclin-dependent kinase 3 (by homology)	Q00526	CDK3	CHEMBL4442	<div><div></div></div>	226 / 5	Ser_Thr Kinase
Cyclin-dependent kinase 6 (by homology)	Q00534	CDK6	CHEMBL2508	<div><div></div></div>	221 / 5	Ser_Thr Kinase
Aurora kinase A	O14965	AURKA	CHEMBL4722	<div><div></div></div>	201 / 2	Ser_Thr Kinase
Aurora kinase B (by homology)	Q96GD4	AURKB	CHEMBL2185	<div><div></div></div>	201 / 2	Ser_Thr Kinase
Aurora kinase C (by homology)	Q9UQB9	AURKC	CHEMBL3935	<div><div></div></div>	201 / 2	Ser_Thr Kinase
Cholinesterase	P06276	BCHE	CHEMBL1914	<div><div></div></div>	124 / 7	Enzyme
Acetylcholinesterase	P22303	ACHE	CHEMBL220	<div><div></div></div>	124 / 7	Enzyme
Cytochrome P450 19A1	P11511	CYP19A1	CHEMBL1978	<div><div></div></div>	31 / 10	Enzyme
Adenosine receptor A1 (by homology)	P30542	ADORA1	CHEMBL226	<div><div></div></div>	170 / 1	Membrane receptor
Protein kinase C eta type	P24723	PRKCH	CHEMBL3616	<div><div></div></div>	60 / 2	Ser_Thr Kinase

# Polypharmacology Browser 2 Prediction:

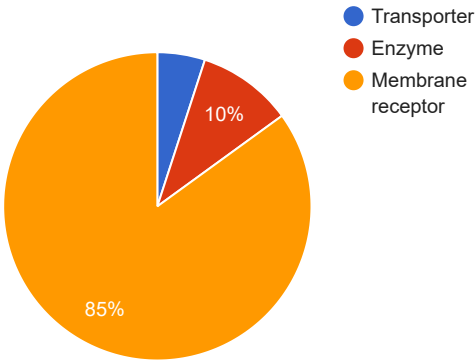
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL214 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL214">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL214</a> )	Serotonin 1a (5-HT1a) receptor	Show NN
2	CHEMBL273 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL273">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL273</a> )	Serotonin 1a (5-HT1a) receptor	Show NN
3	CHEMBL339 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL339">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL339</a> )	Dopamine D2 receptor	Show NN
4	CHEMBL217 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL217">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL217</a> )	Dopamine D2 receptor	Show NN
5	CHEMBL1827 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1827">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1827</a> )	Phosphodiesterase 5A	Show NN
6	CHEMBL253 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL253">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL253</a> )	Cannabinoid CB2 receptor	Show NN
7	CHEMBL319 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL319">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL319</a> )	Alpha-1a adrenergic receptor	Show NN
8	CHEMBL326 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL326">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL326</a> )	Alpha-1d adrenergic receptor	Show NN
9	CHEMBL225 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL225">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL225</a> )	Serotonin 2c (5-HT2c) receptor	Show NN
10	CHEMBL224 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL224">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL224</a> )	Serotonin 2a (5-HT2a) receptor	Show NN
11	CHEMBL220 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL220">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL220</a> )	Acetylcholinesterase	Show NN
12	CHEMBL2056 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2056">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2056</a> )	Dopamine D1 receptor	Show NN
13	CHEMBL4302 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4302">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4302</a> )	P-glycoprotein 1	Show NN
14	CHEMBL234 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL234">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL234</a> )	Dopamine D3 receptor	Show NN
15	CHEMBL3155 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3155">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3155</a> )	Serotonin 7 (5-HT7) receptor	Show NN
16	CHEMBL232 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL232">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL232</a> )	Alpha-1b adrenergic receptor	Show NN
17	CHEMBL229 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL229">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL229</a> )	Alpha-1a adrenergic receptor	Show NN
18	CHEMBL3371 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3371">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3371</a> )	Serotonin 6 (5-HT6) receptor	Show NN

19	CHEMBL287 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL287">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL287</a> )	Sigma opioid receptor	Show NN
20	CHEMBL223 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL223">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL223</a> )	Alpha-1d adrenergic receptor	Show NN