

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

1 rank

HERG : Homo sapiens

score: 5.867 on ChEMBL240 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	ChEMBL549438	0.740741	50118.72	*
MFP1	ChEMBL2069398	0.564103	6000.00	*
RDKit7	ChEMBL2041188	0.511613	23000.00	
Pattern	ChEMBL258176	0.877510	25118.86	*
AP_bits	ChEMBL2043004	0.512195	220.00	*
TT_bits	ChEMBL575475	0.363636	2658.23	
FP2	ChEMBL2041188	0.537736	23000.00	
hybridization	ChEMBL100566	0.471223	8200.00	
substructure	ChEMBL214983	0.875000	4000.00	*
graph	ChEMBL485161	0.672515	50000.00	
pubchem	ChEMBL2325987	0.846995	26957.00	*
cdk_maccs	ChEMBL214983	0.842105	4000.00	*
klekota_roth	ChEMBL552023	0.608696	3100.00	*

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

based on 8 locally validated fgps ---> 14170.092

["substructure", "Pattern", "MFP1", "pubchem", "AP\_bits", "FeatMFP1",  
"klekota\_roth", "cdk\_maccs"]

## MuSSEL Prediction k<sub>i</sub>:

1 rank

Orexin receptor 2 : Homo sapiens

score: 3.177 on ChEMBL4792 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL3646199		0.730769	716.00	
MFP1	ChEMBL3646199		0.564103	716.00	
RDKit7	ChEMBL3670574		0.494475	72.00	
Pattern	ChEMBL3099889		0.874747	4.80	*
AP_bits	ChEMBL3669443		0.567929	35.00	*
TT_bits	ChEMBL3670618		0.316327	28.00	
FP2	ChEMBL3670574		0.571429	72.00	
hybridization	ChEMBL3670574		0.522772	72.00	
substructure	ChEMBL2435413		0.800000	12.88	
graph	ChEMBL3663562		0.660606	934.00	
pubchem	ChEMBL2435401		0.897727	20.89	*
cdk_maccs	ChEMBL3646199		0.836364	716.00	*
klekota_roth	ChEMBL1083358		0.500000	0.17	

\*\*\* ki ACTIVITY \*\*\* value prediction

based on 4 locally validated fgps ---> 219.194

["Pattern", "cdk\_maccs", "pubchem", "AP\_bits"]

2 rank

Orexin receptor 1 : Homo sapiens

score: 3.177 on ChEMBL5113 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL3646199		0.730769	10000.00	
MFP1	ChEMBL3646199		0.564103	10000.00	
RDKit7	ChEMBL3670574		0.494475	3841.00	
Pattern	ChEMBL3099889		0.874747	833.00	*
AP_bits	ChEMBL3669443		0.567929	365.00	*
TT_bits	ChEMBL3670618		0.316327	143.00	
FP2	ChEMBL3670574		0.571429	3841.00	
hybridization	ChEMBL3670574		0.522772	3841.00	
substructure	ChEMBL2435413		0.800000	58.88	
graph	ChEMBL3663562		0.660606	77.00	
pubchem	ChEMBL2435401		0.897727	1445.44	*
cdk_maccs	ChEMBL3646199		0.836364	10000.00	*
klekota_roth	ChEMBL1083358		0.500000	1.80	

\*\*\* ki ACTIVITY \*\*\* value prediction

based on 4 locally validated fgps ---> 3000.118

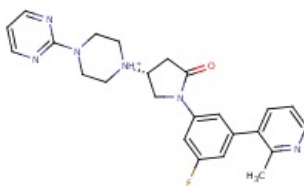
["Pattern", "cdk\_maccs", "pubchem", "AP\_bits"]

# SwissTargetPrediction report:

## Reference:

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

## Query Molecule



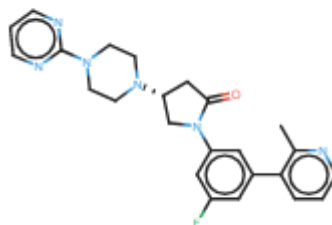
## Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
cGMP-specific 3',5'-cyclic phosphodiesterase	O76074	PDE5A	CHEMBL1827	<div><div></div></div>	143 / 2	Enzyme
Dual 3',5'-cyclic-AMP and -GMP phosphodiesterase 11A	Q9HCR9	PDE11A	CHEMBL2717	<div><div></div></div>	125 / 2	Enzyme
D(2) dopamine receptor	P14416	DRD2	CHEMBL217	<div><div></div></div>	2174 / 33	Membrane receptor
Dipeptidyl peptidase 4 membrane form	P27487	DPP4	CHEMBL284	<div><div></div></div>	592 / 22	Serine Protease
Seprase ( <i>by homology</i> )	Q12884	FAP	CHEMBL4683	<div><div></div></div>	592 / 22	Serine Protease
D(4) dopamine receptor	P21917	DRD4	CHEMBL219	<div><div></div></div>	685 / 11	Membrane receptor
D(3) dopamine receptor	P35462	DRD3	CHEMBL234	<div><div></div></div>	1132 / 15	Membrane receptor
Alpha-1D adrenergic receptor	P25100	ADRA1D	CHEMBL223	<div><div></div></div>	426 / 7	Membrane receptor
Alpha-1A adrenergic receptor	P35348	ADRA1A	CHEMBL229	<div><div></div></div>	487 / 16	Membrane receptor
Alpha-1B adrenergic receptor	P35368	ADRA1B	CHEMBL232	<div><div></div></div>	426 / 7	Membrane receptor
Neuronal acetylcholine receptor subunit alpha-7 ( <i>by homology</i> )	P36544	CHRNA7	CHEMBL2492	<div><div></div></div>	141 / 24	Ion channel
CHRNA7-FAM7A fusion protein ( <i>by homology</i> )	Q494W8	CHRFAM7A		<div><div></div></div>	141 / 24	Ion channel
Egl nine homolog 2	Q96KS0	EGLN2	CHEMBL3028	<div><div></div></div>	10 / 35	Enzyme
Egl nine homolog 1	Q9GZT9	EGLN1	CHEMBL5697	<div><div></div></div>	10 / 35	Enzyme
Potassium voltage-gated channel subfamily H member 2	Q12809	KCNH2	CHEMBL240	<div><div></div></div>	518 / 34	Ion channel

## Polypharmacology Browser 2 Prediction:

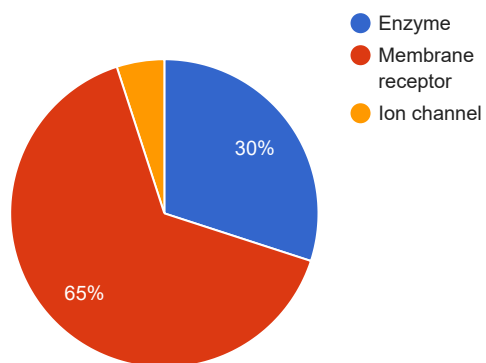
## Targets predicted using NN(ECfp4) + NB(ECfp4).

### Save Table



Query molecule

## Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL284">CHEMBL284</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL284)	Dipeptidyl peptidase IV	Show NN
2	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3227">CHEMBL3227</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3227)	Metabotropic glutamate receptor 5	Show NN
3	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4005">CHEMBL4005</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4005)	PI3-kinase p110-alpha subunit	Show NN
4	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL217">CHEMBL217</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL217)	Dopamine D2 receptor	Show NN
5	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL234">CHEMBL234</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL234)	Dopamine D3 receptor	Show NN
6	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2842">CHEMBL2842</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2842)	Serine/threonine-protein kinase mTOR	Show NN
7	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL240">CHEMBL240</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL240)	HERG	Show NN
8	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL224">CHEMBL224</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL224)	Serotonin 2a (5-HT2a) receptor	Show NN
9	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4409">CHEMBL4409</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4409)	Phosphodiesterase 10A	Show NN
10	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL214">CHEMBL214</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL214)	Serotonin 1a (5-HT1a) receptor	Show NN
11	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3371">CHEMBL3371</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3371)	Serotonin 6 (5-HT6) receptor	Show NN
12	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL339">CHEMBL339</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL339)	Dopamine D2 receptor	Show NN
13	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL219">CHEMBL219</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL219)	Dopamine D4 receptor	Show NN
14	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL225">CHEMBL225</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL225)	Serotonin 2c (5-HT2c) receptor	Show NN
15	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL279">CHEMBL279</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL279)	Vascular endothelial growth factor receptor 2	Show NN
16	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL273">CHEMBL273</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL273)	Serotonin 1a (5-HT1a) receptor	Show NN
17	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4657">CHEMBL4657</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4657)	Dipeptidyl peptidase VIII	Show NN
18	<a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL5652">CHEMBL5652</a> (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL5652)	Glucose-dependent insulintropic receptor	Show NN

19	CHEMBL2564 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2564">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2564</a> )	Metabotropic glutamate receptor 5	Show NN
20	CHEMBL4616 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4616">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4616</a> )	Ghrelin receptor	Show NN