

MuSSEL Prediction k_i:

1 rank

Dopamine D1 receptor : Homo sapiens

score: 8.188 on ChEMBL2056 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL3671282	0.782609	7.98	*
MFP1	CHEMBL3671282	0.741935	7.98	*
RDKit7	CHEMBL3671282	0.803384	7.98	*
Pattern	CHEMBL3671282	0.934236	7.98	*
AP_bits	CHEMBL3671282	0.865613	7.98	*
TT_bits	CHEMBL3671282	0.843750	7.98	*
FP2	CHEMBL3671282	0.732558	7.98	*
hybridization	CHEMBL3671282	0.797619	7.98	*
substructure	CHEMBL3671273	0.857143	34.80	
graph	CHEMBL3671282	0.800000	7.98	
pubchem	CHEMBL3671282	0.817073	7.98	
cdk_maccs	CHEMBL3671282	0.886364	7.98	*
klekota_roth	CHEMBL3671282	0.800000	7.98	*

*** ki ACTIVITY *** value prediction

based on 10 locally validated fgps ---> 32.870

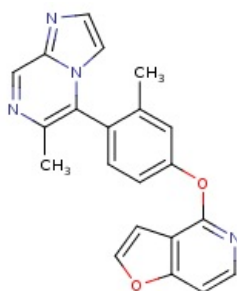
["TT_bits", "cdk_maccs", "Pattern", "FP2", "MFP1", "klekota_roth",
"AP_bits", "FeatMFP1", "RDKit7", "hybridization"]

SwissTargetPrediction report:

Reference:

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

Query Molecule



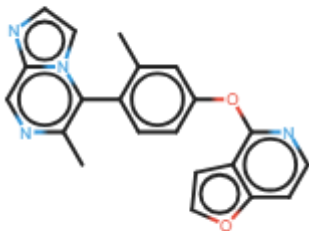
Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
Microtubule-associated protein tau	P10636	MAPT	CHEMBL1293224	<div><div></div></div>	386 / 13	Unclassified
Muscleblind-like protein 1	Q9NR56	MBNL1	CHEMBL1293317	<div><div></div></div>	185 / 3	Unclassified
Muscleblind-like protein 2 (by homology)	Q5VZF2	MBNL2		<div><div></div></div>	185 / 3	Unclassified
Muscleblind-like protein 3 (by homology)	Q9NUK0	MBNL3		<div><div></div></div>	185 / 3	Unclassified
Adenosine receptor A2a	P29274	ADORA2A	CHEMBL251	<div><div></div></div>	127 / 2	Membrane receptor
Adenosine receptor A1 (by homology)	P30542	ADORA1	CHEMBL226	<div><div></div></div>	127 / 2	Membrane receptor
cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A	Q9Y233	PDE10A	CHEMBL4409	<div><div></div></div>	27 / 12	Enzyme
cGMP-specific 3',5'-cyclic phosphodiesterase	O76074	PDE5A	CHEMBL1827	<div><div></div></div>	13 / 4	Enzyme
Dual 3',5'-cyclic-AMP and -GMP phosphodiesterase 11A	Q9HCR9	PDE11A	CHEMBL2717	<div><div></div></div>	10 / 4	Enzyme
Vascular endothelial growth factor receptor 1 (by homology)	P17948	FLT1	CHEMBL1868	<div><div></div></div>	107 / 4	Tyr Kinase
Vascular endothelial growth factor receptor 3 (by homology)	P35916	FLT4	CHEMBL1955	<div><div></div></div>	107 / 4	Tyr Kinase
Vascular endothelial growth factor receptor 2	P35968	KDR	CHEMBL279	<div><div></div></div>	107 / 4	Tyr Kinase
Glycogen synthase kinase-3 alpha (by homology)	P49840	GSK3A	CHEMBL2850	<div><div></div></div>	53 / 4	Ser_Thr Kinase
Glycogen synthase kinase-3 beta	P49841	GSK3B	CHEMBL262	<div><div></div></div>	53 / 4	Ser_Thr Kinase
Histamine H3 receptor	Q9Y5N1	HRH3	CHEMBL264	<div><div></div></div>	3 / 22	Membrane receptor

Polypharmacology Browser 2 Prediction:

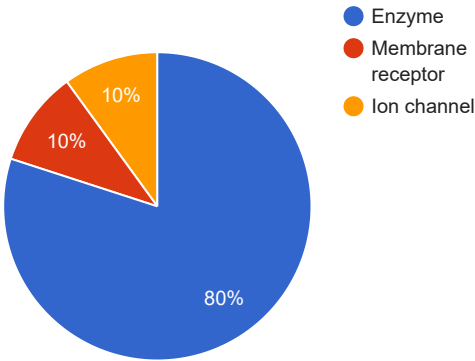
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL2056 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2056)	Dopamine D1 receptor	Show NN
2	CHEMBL279 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL279)	Vascular endothelial growth factor receptor 2	Show NN
3	CHEMBL262 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL262)	Glycogen synthase kinase-3 beta	Show NN
4	CHEMBL4409 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4409)	Phosphodiesterase 10A	Show NN
5	CHEMBL340 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL340)	Cytochrome P450 3A4	Show NN
6	CHEMBL6140 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL6140)	cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A	Show NN
7	CHEMBL1974 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1974)	Tyrosine-protein kinase receptor FLT3	Show NN
8	CHEMBL260 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL260)	MAP kinase p38 alpha	Show NN
9	CHEMBL1957 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1957)	Insulin-like growth factor I receptor	Show NN
10	CHEMBL4296 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4296)	Sodium channel protein type IX alpha subunit	Show NN
11	CHEMBL2185 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2185)	Serine/threonine-protein kinase Aurora-B	Show NN
12	CHEMBL1955 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1955)	Vascular endothelial growth factor receptor 3	Show NN
13	CHEMBL240 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL240)	HERG	Show NN

14	CHEMBL4005 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4005)	PI3-kinase p110-alpha subunit	Show NN
15	CHEMBL258 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL258)	Tyrosine-protein kinase LCK	Show NN
16	CHEMBL2276 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2276)	c-Jun N-terminal kinase 1	Show NN
17	CHEMBL4722 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4722)	Serine/threonine-protein kinase Aurora-A	Show NN
18	CHEMBL1951 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1951)	Monoamine oxidase A	Show NN
19	CHEMBL4439 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4439)	TGF-beta receptor type I	Show NN
20	CHEMBL226 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL226)	Adenosine A1 receptor	Show NN