

MuSSEL Prediction IC₅₀:

1 rank

Tyrosine-protein kinase BTK : Homo sapiens

score: 8.563 on ChEMBL5251 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL3400977		0.675676	65.00	
MFP1	ChEMBL3674679		0.660000	16.00	*
RDKit7	ChEMBL3400973		0.743785	1568.00	*
Pattern	ChEMBL3402578		0.848787	1357.00	*
AP_bits	ChEMBL3402576		0.732558	21.30	*
TT_bits	ChEMBL3400973		0.619048	1568.00	*
FP2	ChEMBL3400973		0.670157	1568.00	*
hybridization	ChEMBL3402575		0.651261	38.80	*
substructure	ChEMBL3402576		0.916667	21.30	*
graph	ChEMBL3400973		0.754967	1568.00	
pubchem	ChEMBL3402576		0.913793	21.30	*
cdk_maccs	ChEMBL3402576		0.938462	21.30	*
klekota_roth	ChEMBL3649459		0.868852	39.35	*

*** ic50 ACTIVITY *** value prediction

based on 11 locally validated fgps ---> 308.391

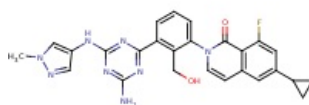
["TT_bits", "substructure", "cdk_maccs", "Pattern", "AP_bits", "MFP1",
"klekota_roth", "pubchem", "FP2", "RDKit7", "hybridization"]

SwissTargetPrediction report:

Reference:

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

Query Molecule



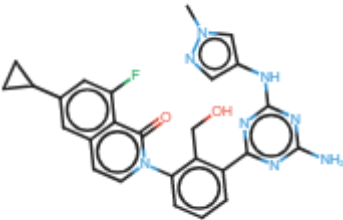
Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
Tyrosine-protein kinase TXK	P42681	TXK	CHEMBL4367	<div><div></div></div>	2 / 1	Tyr Kinase
Tyrosine-protein kinase BTK	Q06187	BTK	CHEMBL5251	<div><div></div></div>	2 / 1	Tyr Kinase
Tyrosine-protein kinase ITK/TSK	Q08881	ITK	CHEMBL2959	<div><div></div></div>	2 / 1	Tyr Kinase
Tyrosine-protein kinase Tec (<i>by homology</i>)	P42680	TEC	CHEMBL4246	<div><div></div></div>	2 / 1	Tyr Kinase
5-hydroxytryptamine receptor 1A	P08908	HTR1A	CHEMBL214	<div><div></div></div>	5 / 1	Membrane receptor
5-hydroxytryptamine receptor 1B	P28222	HTR1B	CHEMBL1898	<div><div></div></div>	5 / 1	Membrane receptor
Microtubule-associated protein tau	P10636	MAPT	CHEMBL1293224	<div><div></div></div>	18 / 1	Unclassified
Nitric oxide synthase, endothelial	P29474	NOS3	CHEMBL4803	<div><div></div></div>	1 / 1	Enzyme
Nitric oxide synthase, brain	P29475	NOS1	CHEMBL3568	<div><div></div></div>	1 / 1	Enzyme
Nitric oxide synthase, inducible	P35228	NOS2	CHEMBL4481	<div><div></div></div>	1 / 1	Enzyme
Muscarinic acetylcholine receptor M1	P11229	CHRM1	CHEMBL216	<div><div></div></div>	2 / 5	Membrane receptor
Muscarinic acetylcholine receptor M2 (<i>by homology</i>)	P08172	CHRM2	CHEMBL211	<div><div></div></div>	2 / 5	Membrane receptor
Muscarinic acetylcholine receptor M4 (<i>by homology</i>)	P08173	CHRM4	CHEMBL1821	<div><div></div></div>	2 / 5	Membrane receptor
Muscarinic acetylcholine receptor M3 (<i>by homology</i>)	P20309	CHRM3	CHEMBL245	<div><div></div></div>	1 / 5	Membrane receptor
D(2) dopamine receptor	P14416	DRD2	CHEMBL217	<div><div></div></div>	1 / 1	Membrane receptor

Polypharmacology Browser 2 Prediction:

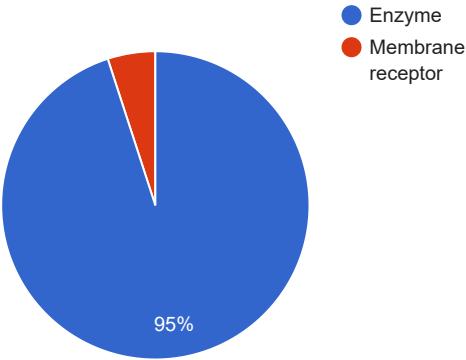
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL5251 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL5251)	Tyrosine-protein kinase BTK	Show NN
2	CHEMBL279 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL279)	Vascular endothelial growth factor receptor 2	Show NN
3	CHEMBL2971 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2971)	Tyrosine-protein kinase JAK2	Show NN
4	CHEMBL2842 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2842)	Serine/threonine-protein kinase mTOR	Show NN
5	CHEMBL2599 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2599)	Tyrosine-protein kinase SYK	Show NN
6	CHEMBL2276 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2276)	c-Jun N-terminal kinase 1	Show NN
7	CHEMBL4722 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4722)	Serine/threonine-protein kinase Aurora-A	Show NN
8	CHEMBL251 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL251)	Adenosine A2a receptor	Show NN
9	CHEMBL1974 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1974)	Tyrosine-protein kinase receptor FLT3	Show NN
10	CHEMBL1936 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1936)	Stem cell growth factor receptor	Show NN
11	CHEMBL258 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL258)	Tyrosine-protein kinase LCK	Show NN
12	CHEMBL4247 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4247)	ALK tyrosine kinase receptor	Show NN
13	CHEMBL2815 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2815)	Nerve growth factor receptor Trk-A	Show NN
14	CHEMBL2185 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2185)	Serine/threonine-protein kinase Aurora-B	Show NN
15	CHEMBL3717 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3717)	Hepatocyte growth factor receptor	Show NN
16	CHEMBL2534 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2534)	3-phosphoinositide dependent protein kinase-1	Show NN
17	CHEMBL4179 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4179)	c-Jun N-terminal kinase 2	Show NN
18	CHEMBL2147 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2147)	Serine/threonine-protein kinase PIM1	Show NN

19	CHEMBL2148 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2148)	Tyrosine-protein kinase JAK3	Show NN
20	CHEMBL301 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL301)	Cyclin-dependent kinase 2	Show NN