

MuSSEL Prediction IC₅₀:

1 rank

Heat shock protein HSP 90-alpha : Homo sapiens

score: 4.912 on ChEMBL3880 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	ChEMBL3653872	0.730769	1490.0	*
MFP1	ChEMBL3656930	0.625000	340.0	*
RDKit7	ChEMBL3653943	0.532567	290.0	
Pattern	ChEMBL2237431	0.790155	17300.0	
AP_bits	ChEMBL3653862	0.448363	140.0	
TT_bits	ChEMBL3653862	0.561404	140.0	*
FP2	ChEMBL3653943	0.661157	290.0	*
hybridization	ChEMBL3653857	0.652582	270.0	*
substructure	ChEMBL3653882	0.818182	280.0	
graph	ChEMBL3653943	0.737500	290.0	
pubchem	ChEMBL3653857	0.752688	270.0	
cdk_maccs	ChEMBL3653855	0.836735	150.0	*
klekota_roth	ChEMBL3653883	0.844828	120.0	*

*** ic50 ACTIVITY *** value prediction

based on 7 locally validated fgps ---> 315.768

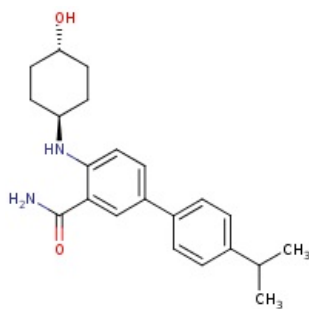
["TT_bits", "klekota_roth", "MFP1", "FP2", "FeatMFP1", "cdk_maccs",
"hybridization"]

SwissTargetPrediction report:

Reference:

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

Query Molecule



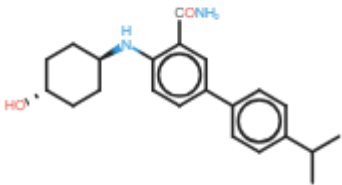
Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
Proteinase-activated receptor 1	P25116	F2R	CHEMBL3974	<div><div></div></div>	17 / 1	Membrane receptor
Mitogen-activated protein kinase 8 (by homology)	P45983	MAPK8	CHEMBL2276	<div><div></div></div>	232 / 42	Ser_Thr Kinase
Mitogen-activated protein kinase 9 (by homology)	P45984	MAPK9	CHEMBL4179	<div><div></div></div>	232 / 42	Ser_Thr Kinase
Mitogen-activated protein kinase 10 (by homology)	P53779	MAPK10	CHEMBL2637	<div><div></div></div>	232 / 42	Ser_Thr Kinase
Mitogen-activated protein kinase 11 (by homology)	Q15759	MAPK11	CHEMBL3961	<div><div></div></div>	240 / 42	Ser_Thr Kinase
Mitogen-activated protein kinase 14	Q16539	MAPK14	CHEMBL260	<div><div></div></div>	240 / 42	Ser_Thr Kinase
Cannabinoid receptor 1	P21554	CNR1	CHEMBL218	<div><div></div></div>	331 / 6	Membrane receptor
Cannabinoid receptor 2	P34972	CNR2	CHEMBL253	<div><div></div></div>	202 / 6	Membrane receptor
C-C chemokine receptor type 1	P32246	CCR1	CHEMBL2413	<div><div></div></div>	133 / 9	Membrane receptor
C-C chemokine receptor type 2	P41597	CCR2	CHEMBL4015	<div><div></div></div>	133 / 9	Membrane receptor
C-C chemokine receptor type 3 (by homology)	P51677	CCR3	CHEMBL3473	<div><div></div></div>	133 / 9	Membrane receptor
C-C chemokine receptor type 5 (by homology)	P51681	CCR5	CHEMBL274	<div><div></div></div>	133 / 9	Membrane receptor
Histamine H3 receptor	Q9Y5N1	HRH3	CHEMBL264	<div><div></div></div>	28 / 4	Membrane receptor
Mu-type opioid receptor	P35372	OPRM1	CHEMBL233	<div><div></div></div>	105 / 53	Membrane receptor
Delta-type opioid receptor	P41143	OPRD1	CHEMBL236	<div><div></div></div>	105 / 53	Membrane receptor

Polypharmacology Browser 2 Prediction:

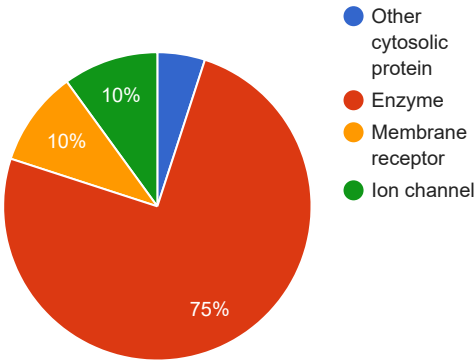
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL3880 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3880)	Heat shock protein HSP 90-alpha	Show NN
2	CHEMBL2971 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2971)	Tyrosine-protein kinase JAK2	Show NN
3	CHEMBL2835 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2835)	Tyrosine-protein kinase JAK1	Show NN
4	CHEMBL2599 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2599)	Tyrosine-protein kinase SYK	Show NN
5	CHEMBL240 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL240)	HERG	Show NN
6	CHEMBL4235 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4235)	11-beta-hydroxysteroid dehydrogenase 1	Show NN
7	CHEMBL260 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL260)	MAP kinase p38 alpha	Show NN
8	CHEMBL2148 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2148)	Tyrosine-protein kinase JAK3	Show NN
9	CHEMBL2276 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2276)	c-Jun N-terminal kinase 1	Show NN
10	CHEMBL1974 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1974)	Tyrosine-protein kinase receptor FLT3	Show NN
11	CHEMBL4247 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4247)	ALK tyrosine kinase receptor	Show NN
12	CHEMBL4794 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4794)	Vanilloid receptor	Show NN
13	CHEMBL1075104 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1075104)	Leucine-rich repeat serine/threonine-protein kinase 2	Show NN
14	CHEMBL284 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL284)	Dipeptidyl peptidase IV	Show NN
15	CHEMBL253 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL253)	Cannabinoid CB2 receptor	Show NN
16	CHEMBL1991 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1991)	Inhibitor of nuclear factor kappa B kinase beta subunit	Show NN
17	CHEMBL213 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL213)	Beta-1 adrenergic receptor	Show NN

18	CHEMBL262 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL262)	Glycogen synthase kinase-3 beta	Show NN
19	CHEMBL2147 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2147)	Serine/threonine-protein kinase PIM1	Show NN
20	CHEMBL5314 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL5314)	Tyrosine-protein kinase receptor TYRO3	Show NN