

MuSSEL Prediction IC₅₀:

1 rank

Tyrosine-protein kinase SRC : Homo sapiens

score: 6.857 on ChEMBL267 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL355269		0.735294	63.1	*
MFP1	CHEMBL168656		0.584906	270.0	*
RDKit7	CHEMBL355891		0.748187	50.0	*
Pattern	CHEMBL169043		0.811350	24.0	
AP_bits	CHEMBL352619		0.517544	400.0	*
TT_bits	CHEMBL168656		0.592105	270.0	*
FP2	CHEMBL168656		0.669856	270.0	*
hybridization	CHEMBL169043		0.671031	24.0	*
substructure	CHEMBL1873475		0.739130	262.6	
graph	CHEMBL395665		0.565217	19700.0	
pubchem	CHEMBL168656		0.833333	270.0	*
cdk_maccs	CHEMBL395664		0.833333	14400.0	*
klekota_roth	CHEMBL1873475		0.671053	262.6	*

*** ic50 ACTIVITY *** value prediction

based on 10 locally validated fgps ---> 1888.354

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

2 rank

Epidermal growth factor receptor erbB1 : Homo sapiens

score: 6.812 on ChEMBL203 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL355269		0.735294	750.0	*
MFP1	CHEMBL168656		0.584906	2100.0	*
RDKit7	CHEMBL355891		0.748187	830.0	*
Pattern	CHEMBL168656		0.801858	2100.0	
AP_bits	CHEMBL355891		0.511312	830.0	*
TT_bits	CHEMBL168656		0.592105	2100.0	*
FP2	CHEMBL168656		0.669856	2100.0	*
hybridization	CHEMBL168656		0.653846	2100.0	*
substructure	CHEMBL1272222		0.772727	20.0	
graph	CHEMBL3416437		0.641221	153.0	
pubchem	CHEMBL168656		0.833333	2100.0	*
cdk_maccs	CHEMBL3647970		0.802817	48.8	*
klekota_roth	CHEMBL3647973		0.680000	60.9	*

*** ic50 ACTIVITY *** value prediction

based on 10 locally validated fgps ---> 1057.807

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

3 rank

Fibroblast growth factor receptor 2 : Homo sapiens

score: 6.388 on ChEMBL4142 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3701258		0.750000	0.4	*
MFP1	CHEMBL3701258		0.607843	0.4	*
RDKit7	CHEMBL3701278		0.689006	0.3	*
Pattern	CHEMBL3701259		0.846034	3.2	*
AP_bits	CHEMBL3701258		0.531915	0.4	*
TT_bits	CHEMBL3701258		0.608108	0.4	*
FP2	CHEMBL3701258		0.585586	0.4	
hybridization	CHEMBL3701258		0.650238	0.4	*
substructure	CHEMBL3701240		0.791667	6.9	
graph	CHEMBL3701258		0.656250	0.4	
pubchem	CHEMBL3701259		0.796610	3.2	
cdk_maccs	CHEMBL3701258		0.861538	0.4	*

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    klekota_roth CHEMBL3701258          0.842857      0.4      *
    *** ic50 ACTIVITY *** value prediction
    based on 9 locally validated fgps ---> 3.089
    ["TT_bits", "cdk_maccs", "Pattern", "MFP1", "klekota_roth", "AP_bits",
    "FeatMFP1", "RDKit7", "hybridization"]

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4 rank

Tyrosine-protein kinase SRC : Gallus gallus

score: 6.141 on ChEMBL3655 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL168382	0.733333	2.0	*
MFP1	CHEMBL168656	0.584906	4400.0	*
RDKit7	CHEMBL355019	0.738929	700.0	*
Pattern	CHEMBL169043	0.811350	3300.0	
AP_bits	CHEMBL352619	0.517544	400.0	*
TT_bits	CHEMBL168656	0.592105	4400.0	*
FP2	CHEMBL168656	0.669856	4400.0	*
hybridization	CHEMBL169043	0.671031	3300.0	*
substructure	CHEMBL168382	0.681818	2.0	
graph	CHEMBL169043	0.537594	3300.0	
pubchem	CHEMBL168656	0.833333	4400.0	*
cdk_maccs	CHEMBL168656	0.800000	4400.0	*
klekota_roth	CHEMBL168656	0.516854	4400.0	

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    *** ic50 ACTIVITY *** value prediction
    based on 8 locally validated fgps ---> 2500.662
    ["TT_bits", "AP_bits", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
    "hybridization"]

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5 rank

Tyrosine-protein kinase LCK : Homo sapiens

score: 5.131 on ChEMBL258 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL66102	0.709677	6.0	*
MFP1	CHEMBL262276	0.528302	290.0	*
RDKit7	CHEMBL297278	0.698466	240.0	*
Pattern	CHEMBL3786567	0.787834	7400.0	
AP_bits	CHEMBL1873475	0.494929	2.0	*
TT_bits	CHEMBL172514	0.545455	620.0	*
FP2	CHEMBL297278	0.640000	240.0	*
hybridization	CHEMBL3786167	0.588509	4900.0	
substructure	CHEMBL1873475	0.739130	2.0	
graph	CHEMBL397143	0.582707	20800.0	
pubchem	CHEMBL297278	0.791304	240.0	
cdk_maccs	CHEMBL233540	0.842857	2950.0	*
klekota_roth	CHEMBL1873475	0.671053	2.0	*

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    *** ic50 ACTIVITY *** value prediction
    based on 8 locally validated fgps ---> 352.557
    ["TT_bits", "AP_bits", "MFP1", "klekota_roth", "FP2", "FeatMFP1",
    "RDKit7", "cdk_maccs"]

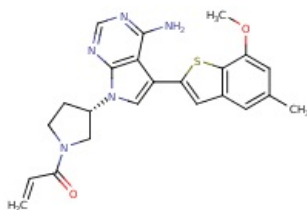
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SwissTargetPrediction report:

Reference:

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

Query Molecule



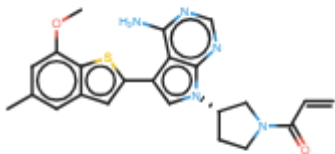
Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
Tyrosine-protein kinase Lck	P06239	LCK	CHEMBL258	<div><div></div></div>	117 / 53	Tyr Kinase
Tyrosine-protein kinase Lyn (<i>by homology</i>)	P07948	LYN	CHEMBL3905	<div><div></div></div>	117 / 53	Tyr Kinase
Tyrosine-protein kinase HCK (<i>by homology</i>)	P08631	HCK	CHEMBL3234	<div><div></div></div>	117 / 53	Tyr Kinase
Tyrosine-protein kinase Blk (<i>by homology</i>)	P51451	BLK	CHEMBL2250	<div><div></div></div>	117 / 53	Tyr Kinase
Epidermal growth factor receptor	P00533	EGFR	CHEMBL203	<div><div></div></div>	134 / 46	Tyr Kinase
Receptor tyrosine-protein kinase erbB-2	P04626	ERBB2	CHEMBL1824	<div><div></div></div>	133 / 46	Tyr Kinase
ERBB4 intracellular domain (<i>by homology</i>)	Q15303	ERBB4	CHEMBL3009	<div><div></div></div>	133 / 46	Tyr Kinase
Receptor tyrosine-protein kinase erbB-3 (<i>by homology</i>)	P21860	ERBB3	CHEMBL5838	<div><div></div></div>	133 / 46	Tyr Kinase
Tyrosine-protein kinase Fyn (<i>by homology</i>)	P06241	FYN	CHEMBL1841	<div><div></div></div>	82 / 122	Tyr Kinase
Tyrosine-protein kinase Yes (<i>by homology</i>)	P07947	YES1	CHEMBL2073	<div><div></div></div>	82 / 122	Tyr Kinase
Tyrosine-protein kinase Fgr (<i>by homology</i>)	P09769	FGR	CHEMBL4454	<div><div></div></div>	82 / 122	Tyr Kinase
Proto-oncogene tyrosine-protein kinase Src	P12931	SRC	CHEMBL267	<div><div></div></div>	82 / 122	Tyr Kinase
Tyrosine-protein kinase FRK (<i>by homology</i>)	P42685	FRK	CHEMBL4223	<div><div></div></div>	82 / 122	Tyr Kinase
Macrophage colony-stimulating factor 1 receptor	P07333	CSF1R	CHEMBL1844	<div><div></div></div>	134 / 3	Tyr Kinase
Mast/stem cell growth factor receptor Kit	P10721	KIT	CHEMBL1936	<div><div></div></div>	134 / 3	Tyr Kinase

Polypharmacology Browser 2 Prediction:

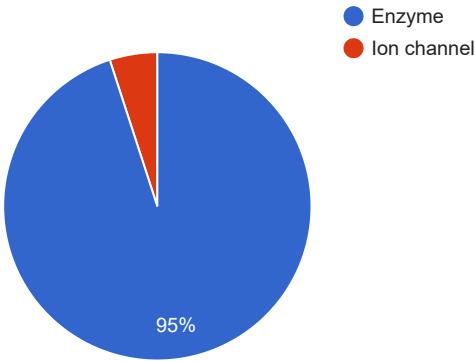
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL203 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL203)	Epidermal growth factor receptor erbB1	Show NN
2	CHEMBL267 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL267)	Tyrosine-protein kinase SRC	Show NN
3	CHEMBL279 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL279)	Vascular endothelial growth factor receptor 2	Show NN
4	CHEMBL3650 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3650)	Fibroblast growth factor receptor 1	Show NN
5	CHEMBL4128 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4128)	Tyrosine-protein kinase TIE-2	Show NN
6	CHEMBL258 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL258)	Tyrosine-protein kinase LCK	Show NN
7	CHEMBL1981 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1981)	Insulin receptor	Show NN
8	CHEMBL1957 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1957)	Insulin-like growth factor I receptor	Show NN
9	CHEMBL3905 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3905)	Tyrosine-protein kinase Lyn	Show NN
10	CHEMBL2742 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2742)	Fibroblast growth factor receptor 3	Show NN
11	CHEMBL4142 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4142)	Fibroblast growth factor receptor 2	Show NN
12	CHEMBL2959 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2959)	Tyrosine-protein kinase ITK/TSK	Show NN
13	CHEMBL240 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL240)	HERG	Show NN
14	CHEMBL2185 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2185)	Serine/threonine-protein kinase Aurora-B	Show NN
15	CHEMBL2148 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2148)	Tyrosine-protein kinase JAK3	Show NN
16	CHEMBL3835 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3835)	Serine/threonine-protein kinase NEK2	Show NN
17	CHEMBL5251 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL5251)	Tyrosine-protein kinase BTK	Show NN
18	CHEMBL1974 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1974)	Tyrosine-protein kinase receptor FLT3	Show NN

19	CHEMBL3267 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3267)	PI3-kinase p110-gamma subunit	Show NN
20	CHEMBL1862 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1862)	Tyrosine-protein kinase ABL	Show NN