

## MuSSEL Prediction $k_i$ :

1 rank

Protease : Human immunodeficiency virus 1

score: 9.261 on ChEMBL2366517 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL2165884		0.806452	11.390	*
MFP1	ChEMBL1276099		0.625000	0.026	*
RDKit7	ChEMBL2165897		0.788600	0.303	*
Pattern	ChEMBL1276099		0.875668	0.026	*
AP_bits	ChEMBL3605642		0.658711	0.012	*
TT_bits	ChEMBL1958486		0.551402	0.020	*
FP2	ChEMBL2165893		0.771930	0.027	*
hybridization	ChEMBL2165887		0.796502	3.375	*
substructure	ChEMBL2165898		0.869565	0.230	*
graph	ChEMBL2165897		0.778098	0.303	
pubchem	ChEMBL2165890		0.858447	0.217	*
cdk_maccs	ChEMBL1276099		0.925532	0.026	*
klekota_roth	ChEMBL1819298		0.733333	12.500	*

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

based on 12 locally validated fgps ---> 3.045

["TT\_bits", "substructure", "cdk\_maccs", "Pattern", "FP2", "MFP1",  
"klekota\_roth", "pubchem", "AP\_bits", "FeatMFP1", "RDKit7",  
"hybridization"]

2 rank

Human immunodeficiency virus type 1 protease : Human immunodeficiency virus 1

score: 2.811 on ChEMBL243 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL377249		0.666667	5.300	
MFP1	ChEMBL213012		0.620690	0.140	*
RDKit7	ChEMBL213012		0.644537	0.140	
Pattern	ChEMBL330404		0.827901	190.000	
AP_bits	ChEMBL220078		0.606459	0.235	*
TT_bits	ChEMBL213012		0.530000	0.140	
FP2	ChEMBL213012		0.601732	0.140	
hybridization	ChEMBL1323		0.654466	0.014	
substructure	ChEMBL120843		0.791667	38.000	
graph	ChEMBL213012		0.586301	0.140	
pubchem	ChEMBL330404		0.764192	190.000	
cdk_maccs	ChEMBL219288		0.873684	10.700	*
klekota_roth	ChEMBL213012		0.710345	0.140	*

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

based on 4 locally validated fgps ---> 1.971

["AP\_bits", "klekota\_roth", "MFP1", "cdk\_maccs"]

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

1 rank

Protease : Human immunodeficiency virus 1

score: 5.629 on ChEMBL2366517 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	ChEMBL2041942	0.818182	1.5	*
MFP1	ChEMBL254349	0.620690	1.8	*
RDKit7	ChEMBL507319	0.700464	10.0	*
Pattern	ChEMBL2041942	0.838752	1.5	
AP_bits	ChEMBL2041942	0.681490	1.5	*
TT_bits	ChEMBL254349	0.524752	1.8	*
FP2	ChEMBL507319	0.612903	10.0	
hybridization	ChEMBL2041942	0.685210	1.5	*
substructure	ChEMBL503571	0.760000	6.0	
graph	ChEMBL507319	0.644068	10.0	
pubchem	ChEMBL163	0.707113	0.6	
cdk_maccs	ChEMBL2041942	0.885417	1.5	*
klekota_roth	ChEMBL509137	0.713287	3.8	*

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

based on 8 locally validated fgps ---> 5.079

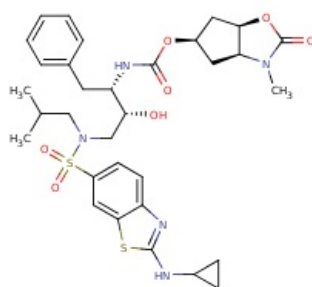
["TT\_bits", "cdk\_maccs", "AP\_bits", "MFP1", "klekota\_roth", "FeatMFP1", "RDKit7", "hybridization"]

# SwissTargetPrediction report:

## Reference:

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

## Query Molecule



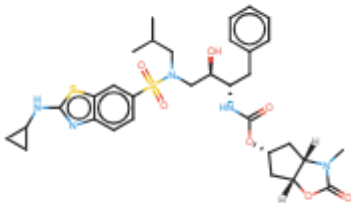
## Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
Cytochrome P450 3A4	P08684	CYP3A4	CHEMBL340	<div><div></div></div>	5 / 1	Enzyme
Thromboxane-A synthase	P24557	TBXAS1	CHEMBL1835	<div><div></div></div>	6 / 1	Enzyme
Cytochrome P450 3A5 (by homology)	P20815	CYP3A5	CHEMBL3019	<div><div></div></div>	5 / 1	Enzyme
Cytochrome P450 3A7 (by homology)	P24462	CYP3A7		<div><div></div></div>	5 / 1	Enzyme
Cytochrome P450 3A43 (by homology)	Q9HB55	CYP3A43	CHEMBL5792	<div><div></div></div>	5 / 1	Enzyme
Muscleblind-like protein 1	Q9NR56	MBNL1	CHEMBL1293317	<div><div></div></div>	177 / 2	Unclassified
Muscleblind-like protein 2 (by homology)	Q5VZF2	MBNL2		<div><div></div></div>	177 / 2	Unclassified
Muscleblind-like protein 3 (by homology)	Q9NUK0	MBNL3		<div><div></div></div>	177 / 2	Unclassified
Microtubule-associated protein tau	P10636	MAPT	CHEMBL1293224	<div><div></div></div>	181 / 13	Unclassified
Dual specificity tyrosine-phosphorylation-regulated kinase 1A	Q13627	DYRK1A	CHEMBL2292	<div><div></div></div>	10 / 12	Ser_Thr_Tyr Kinase
C-C chemokine receptor type 1 (by homology)	P32246	CCR1	CHEMBL2413	<div><div></div></div>	106 / 13	Membrane receptor
C-C chemokine receptor type 2 (by homology)	P41597	CCR2	CHEMBL4015	<div><div></div></div>	106 / 13	Membrane receptor
C-C chemokine receptor type 3	P51677	CCR3	CHEMBL3473	<div><div></div></div>	106 / 13	Membrane receptor
C-C chemokine receptor type 5	P51681	CCR5	CHEMBL274	<div><div></div></div>	106 / 13	Membrane receptor
C-C chemokine receptor-like 2 (by homology)	C9JP23	CCRL2		<div><div></div></div>	102 / 13	Membrane receptor

# Polypharmacology Browser 2 Prediction:

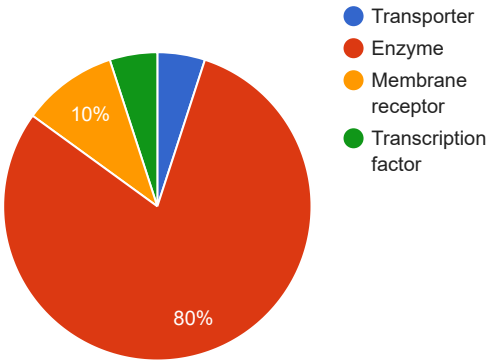
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL204 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL204">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL204</a> )	Thrombin	Show NN
2	CHEMBL283 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL283">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL283</a> )	Matrix metalloproteinase 3	Show NN
3	CHEMBL340 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL340">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL340</a> )	Cytochrome P450 3A4	Show NN
4	CHEMBL332 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL332">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL332</a> )	Matrix metalloproteinase-1	Show NN
5	CHEMBL2334 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2334">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2334</a> )	Caspase-3	Show NN
6	CHEMBL261 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL261">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL261</a> )	Carbonic anhydrase I	Show NN
7	CHEMBL205 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL205">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL205</a> )	Carbonic anhydrase II	Show NN
8	CHEMBL333 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL333">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL333</a> )	Matrix metalloproteinase-2	Show NN
9	CHEMBL3594 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3594">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3594</a> )	Carbonic anhydrase IX	Show NN
10	CHEMBL4561 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4561">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4561</a> )	Neuropeptide Y receptor type 5	Show NN
11	CHEMBL321 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL321">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL321</a> )	Matrix metalloproteinase 9	Show NN
12	CHEMBL4072 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4072">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4072</a> )	Cathepsin B	Show NN
13	CHEMBL280 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL280">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL280</a> )	Matrix metalloproteinase 13	Show NN
14	CHEMBL3242 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3242">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3242</a> )	Carbonic anhydrase XII	Show NN
15	CHEMBL4588 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4588">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4588</a> )	Matrix metalloproteinase 8	Show NN
16	CHEMBL3869 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3869">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3869</a> )	Matrix metalloproteinase 14	Show NN
17	CHEMBL3706 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3706">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3706</a> )	ADAM17	Show NN
18	CHEMBL1741186 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1741186">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1741186</a> )	Nuclear receptor ROR-gamma	Show NN

19	CHEMBL2871 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2871">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2871</a> )	Cholecystikin A receptor	Show NN
20	CHEMBL4076 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4076">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4076</a> )	Sodium/calcium exchanger 1	Show NN