

MuSSEL Prediction IC₅₀:

1 rank

Neuraminidase : Influenza A virus

score: 11.797 on ChEMBL1667684 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL3342471		0.923077	7.1	*
MFP1	ChEMBL3342471		0.918919	7.1	*
RDKit7	ChEMBL3342471		0.929990	7.1	*
Pattern	ChEMBL3342478		0.965753	1.9	*
AP_bits	ChEMBL3342478		0.792363	1.9	*
TT_bits	ChEMBL3342471		0.830189	7.1	*
FP2	ChEMBL3342471		0.891892	7.1	*
hybridization	ChEMBL3342485		0.966469	2.1	*
substructure	ChEMBL3342471		0.920000	7.1	*
graph	ChEMBL3342485		0.921053	2.1	*
pubchem	ChEMBL3342485		0.892405	2.1	*
cdk_maccs	ChEMBL3342478		0.913793	1.9	*
klekota_roth	ChEMBL3342478		0.930693	1.9	*

*** ic50 ACTIVITY *** value prediction

based on 13 locally validated fgps ---> 7.924

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

2 rank

Neuraminidase : Influenza A virus (strain A/USSR/90/1977 H1N1)

score: 11.797 on ChEMBL3559643 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL3342471		0.923077	19.0	*
MFP1	ChEMBL3342471		0.918919	19.0	*
RDKit7	ChEMBL3342471		0.929990	19.0	*
Pattern	ChEMBL3342478		0.965753	3.8	*
AP_bits	ChEMBL3342478		0.792363	3.8	*
TT_bits	ChEMBL3342471		0.830189	19.0	*
FP2	ChEMBL3342471		0.891892	19.0	*
hybridization	ChEMBL3342485		0.966469	4.3	*
substructure	ChEMBL3342471		0.920000	19.0	*
graph	ChEMBL3342485		0.921053	4.3	*
pubchem	ChEMBL3342485		0.892405	4.3	*
cdk_maccs	ChEMBL3342478		0.913793	3.8	*
klekota_roth	ChEMBL3342478		0.930693	3.8	*

*** ic50 ACTIVITY *** value prediction

based on 13 locally validated fgps ---> 18.838

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

3 rank

Neuraminidase : Influenza A virus (A/Puerto Rico/8/1934(H1N1))

score: 7.557 on ChEMBL2051 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL310217		0.814815	620.0	*
MFP1	ChEMBL79499		0.714286	12.0	*
RDKit7	ChEMBL674		0.774295	1.0	*
Pattern	ChEMBL81083		0.912644	90.0	*
AP_bits	ChEMBL81083		0.545652	90.0	*
TT_bits	ChEMBL79499		0.573770	12.0	*
FP2	ChEMBL79499		0.725000	12.0	*
hybridization	ChEMBL81717		0.760748	0.5	*
substructure	ChEMBL310217		0.846154	620.0	
graph	ChEMBL53768		0.672043	1500.0	

pubchem	CHEMBL81083	0.846667	90.0	*
cdk_maccs	CHEMBL53336	0.771930	2300.0	
klekota_roth	CHEMBL674	0.888889	1.0	*

*** ic50 ACTIVITY *** value prediction
 based on 10 locally validated fgps ---> 21.359
 ["TT_bits", "Pattern", "FP2", "MFP1", "klekota_roth", "pubchem",
 "AP_bits", "FeatMFP1", "RDKit7", "hybridization"]

4 rank

Neuraminidase : Influenza B virus (strain B/Lee/1940)

score: 6.560 on ChEMBL3377 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL79499		0.814815	35.0	*
MFP1	CHEMBL79499		0.714286	35.0	*
RDKit7	CHEMBL674		0.774295	3.0	*
Pattern	CHEMBL98906		0.822811	1.6	
AP_bits	CHEMBL352318		0.532946	0.3	*
TT_bits	CHEMBL79499		0.573770	35.0	*
FP2	CHEMBL79499		0.725000	35.0	*
hybridization	CHEMBL674		0.698189	3.0	*
substructure	CHEMBL79499		0.846154	35.0	
graph	CHEMBL311273		0.656085	36000.0	
pubchem	CHEMBL79499		0.837838	35.0	*
cdk_maccs	CHEMBL674		0.771930	3.0	
klekota_roth	CHEMBL674		0.888889	3.0	*

*** ic50 ACTIVITY *** value prediction
 based on 9 locally validated fgps ---> 40.557
 ["TT_bits", "AP_bits", "MFP1", "klekota_roth", "pubchem", "FP2",
 "FeatMFP1", "RDKit7", "hybridization"]

5 rank

Neuraminidase : Influenza A virus (strain A/Wilson-Smith/1933 H1N1)

(Influenza A virus(strain A/WS/1933 H1N1))

score: 5.582 on ChEMBL1287610 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL674		0.730769	2.6	*
MFP1	CHEMBL674		0.675000	2.6	*
RDKit7	CHEMBL674		0.774295	2.6	*
Pattern	CHEMBL3357205		0.817181	6946.0	
AP_bits	CHEMBL3263942		0.498099	24.6	*
TT_bits	CHEMBL3357205		0.593750	6946.0	*
FP2	CHEMBL674		0.722973	2.6	*
hybridization	CHEMBL674		0.698189	2.6	*
substructure	CHEMBL674		0.807692	2.6	
graph	CHEMBL674		0.650273	2.6	
pubchem	CHEMBL3357202		0.776316	1010.0	
cdk_maccs	CHEMBL674		0.771930	2.6	
klekota_roth	CHEMBL674		0.888889	2.6	*

*** ic50 ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 1425.604
 ["TT_bits", "AP_bits", "MFP1", "klekota_roth", "FP2", "FeatMFP1",
 "RDKit7", "hybridization"]

6 rank

Neuraminidase : Influenza A virus

score: 5.505 on ChEMBL6135 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL674		0.730769	0.4	*
MFP1	CHEMBL674		0.675000	0.4	*
RDKit7	CHEMBL674		0.774295	0.4	*

Pattern	CHEMBL3263942	0.772277	3.2	
AP_bits	CHEMBL3263939	0.515267	1.7	*
TT_bits	CHEMBL674	0.500000	0.4	*
FP2	CHEMBL674	0.722973	0.4	*
hybridization	CHEMBL674	0.698189	0.4	*
substructure	CHEMBL674	0.807692	0.4	
graph	CHEMBL674	0.650273	0.4	
pubchem	CHEMBL3263938	0.673203	1.8	
cdk_maccs	CHEMBL674	0.771930	0.4	
klekota_roth	CHEMBL674	0.888889	0.4	*

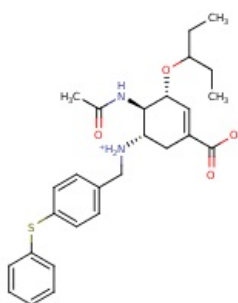
*** ic50 ACTIVITY *** value prediction
based on 8 locally validated fgps ---> 0.649
["TT_bits", "AP_bits", "MFP1", "klekota_roth", "FP2", "FeatMFP1",
"RDKit7", "hybridization"]

SwissTargetPrediction report:

Reference:

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

Query Molecule



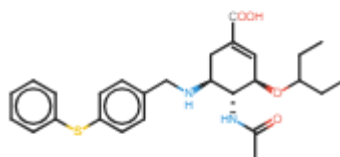
Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
5-hydroxytryptamine receptor 2A	P28223	HTR2A	CHEMBL224	<div><div></div></div>	16 / 13	Membrane receptor
5-hydroxytryptamine receptor 2C (by homology)	P28335	HTR2C	CHEMBL225	<div><div></div></div>	4 / 13	Membrane receptor
5-hydroxytryptamine receptor 2B (by homology)	P41595	HTR2B	CHEMBL1833	<div><div></div></div>	4 / 13	Membrane receptor
Activation peptide fragment 1	P00734	F2	CHEMBL204	<div><div></div></div>	49 / 4	Serine Protease
Muscleblind-like protein 1	Q9NR56	MBNL1	CHEMBL1293317	<div><div></div></div>	24 / 6	Unclassified
Muscleblind-like protein 2 (by homology)	Q5VZF2	MBNL2		<div><div></div></div>	24 / 6	Unclassified
Muscleblind-like protein 3 (by homology)	Q9NUK0	MBNL3		<div><div></div></div>	24 / 6	Unclassified
Factor X light chain	P00742	F10	CHEMBL244	<div><div></div></div>	45 / 3	Serine Protease
Coagulation factor VII	P08709	F7	CHEMBL3991	<div><div></div></div>	45 / 3	Serine Protease
Coagulation factor IXa heavy chain (by homology)	P00740	F9	CHEMBL2016	<div><div></div></div>	45 / 3	Serine Protease
Microtubule-associated protein tau	P10636	MAPT	CHEMBL1293224	<div><div></div></div>	52 / 9	Unclassified
Thromboxane A2 receptor	P21731	TBXA2R	CHEMBL2069	<div><div></div></div>	139 / 6	Membrane receptor
Alpha-trypsin chain 1	P07477	PRSS1	CHEMBL209	<div><div></div></div>	10 / 2	Serine Protease
Trypsin-2 (by homology)	P07478	PRSS2	CHEMBL3159	<div><div></div></div>	10 / 2	Serine Protease
Trypsin-3 (by homology)	P35030	PRSS3	CHEMBL4551	<div><div></div></div>	10 / 2	Serine Protease

Polypharmacology Browser 2 Prediction:

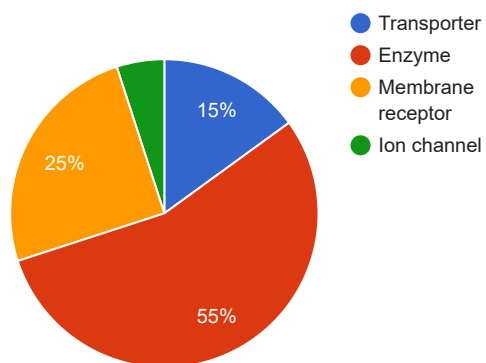
Targets predicted using NN(ECfp4) + NB(ECfp4).

[Save Table](#)



Query molecule

Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL332 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL332)	Matrix metalloproteinase-1	Show NN
2	CHEMBL333 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL333)	Matrix metalloproteinase-2	Show NN
3	CHEMBL338 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL338)	Dopamine transporter	Show NN
4	CHEMBL313 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL313)	Serotonin transporter	Show NN
5	CHEMBL280 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL280)	Matrix metalloproteinase 13	Show NN
6	CHEMBL4822 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4822)	Beta-secretase 1	Show NN
7	CHEMBL2625 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2625)	Angiotensin-converting enzyme	Show NN
8	CHEMBL283 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL283)	Matrix metalloproteinase 3	Show NN
9	CHEMBL321 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL321)	Matrix metalloproteinase 9	Show NN
10	CHEMBL304 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL304)	Norepinephrine transporter	Show NN
11	CHEMBL233 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL233)	Mu opioid receptor	Show NN
12	CHEMBL236 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL236)	Delta opioid receptor	Show NN
13	CHEMBL1944 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1944)	Neprilysin	Show NN
14	CHEMBL240 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL240)	HERG	Show NN
15	CHEMBL2581 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2581)	Cathepsin D	Show NN
16	CHEMBL3369 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3369)	Neprilysin	Show NN
17	CHEMBL1945 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1945)	Melatonin receptor 1A	Show NN
18	CHEMBL217 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL217)	Dopamine D2 receptor	Show NN

19	CHEMBL4588 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4588)	Matrix metalloproteinase 8	Show NN
20	CHEMBL249 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL249)	Neurokinin 1 receptor	Show NN