

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

1 rank

Proteasome Macropain subunit MB1 : Homo sapiens

score: 8.696 on ChEMBL4662 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL3218825	0.761905	22.0	*
MFP1	CHEMBL3218825	0.757576	22.0	*
RDKit7	CHEMBL3218825	0.777778	22.0	*
Pattern	CHEMBL3218821	0.944056	25.0	*
AP_bits	CHEMBL3218825	0.651050	22.0	*
TT_bits	CHEMBL3218825	0.676923	22.0	*
FP2	CHEMBL3218825	0.754545	22.0	*
hybridization	CHEMBL3218825	0.677507	22.0	*
substructure	CHEMBL3218825	1.000000	22.0	*
graph	CHEMBL3218824	0.700000	5.4	
pubchem	CHEMBL3218825	0.904000	22.0	*
cdk_maccs	CHEMBL3218820	0.793103	50.0	
klekota_roth	CHEMBL3218841	0.790476	23.0	*

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

based on 11 locally validated fgps ---> 23.477

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

2 rank

Peptidase 1 : Dermatophagoides pteronyssinus

score: 7.327 on ChEMBL3351204 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL3679689	0.700000	7.85	*
MFP1	CHEMBL3360281	0.647059	9.00	*
RDKit7	CHEMBL3360284	0.682278	8.00	*
Pattern	CHEMBL3679689	0.939815	7.85	*
AP_bits	CHEMBL3360281	0.549834	9.00	*
TT_bits	CHEMBL3359775	0.514706	12.00	*
FP2	CHEMBL3360284	0.810526	8.00	*
hybridization	CHEMBL3360281	0.551913	9.00	
substructure	CHEMBL3359774	0.928571	9167.00	*
graph	CHEMBL3679690	0.678571	6.30	
pubchem	CHEMBL3360284	0.902439	8.00	*
cdk_maccs	CHEMBL3359775	0.696429	12.00	
klekota_roth	CHEMBL3360281	0.652174	9.00	*

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

based on 10 locally validated fgps ---> 466.790

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

3 rank

Cathepsin B : Homo sapiens

score: 7.228 on ChEMBL4072 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL3360294	0.681818	511.0	*
MFP1	CHEMBL3360281	0.647059	512.0	*
RDKit7	CHEMBL3360284	0.682278	242.0	*
Pattern	CHEMBL3360281	0.914414	512.0	*
AP_bits	CHEMBL3360281	0.549834	512.0	*
TT_bits	CHEMBL3359775	0.514706	50.0	*
FP2	CHEMBL3360284	0.810526	242.0	*
hybridization	CHEMBL3360281	0.551913	512.0	
substructure	CHEMBL3359776	0.866667	378.0	*
graph	CHEMBL3359780	0.676056	628.0	
pubchem	CHEMBL3360284	0.902439	242.0	*
cdk_maccs	CHEMBL3359775	0.696429	50.0	

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klekota_roth  CHEMBL133016          0.658120    59000.0      *
*** ic50 ACTIVITY *** value prediction
based on 10 locally validated fgps ---> 4293.936
["TT_bits", "substructure", "Pattern", "FP2", "MFP1", "klekota_roth",
"pubchem", "AP_bits", "FeatMFP1", "RDKit7"]

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4 rank

ADAM17 : Homo sapiens

score: 6.864 on ChEMBL3706 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL358770		0.809524	9.00	*
MFP1	CHEMBL358770		0.540541	9.00	*
RDKit7	CHEMBL358770		0.621590	9.00	
Pattern	CHEMBL144001		0.900452	0.57	*
AP_bits	CHEMBL144206		0.566007	2.80	*
TT_bits	CHEMBL314024		0.381579	2200.00	
FP2	CHEMBL358770		0.747664	9.00	*
hybridization	CHEMBL358770		0.517045	9.00	
substructure	CHEMBL144169		0.928571	3.30	*
graph	CHEMBL67311		0.711864	3592.00	
pubchem	CHEMBL358770		0.941176	9.00	*
cdk_maccs	CHEMBL144001		0.816667	0.57	*
klekota_roth	CHEMBL16520		0.613445	20.00	*

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*** ic50 ACTIVITY *** value prediction
based on 9 locally validated fgps ---> 5.780
["substructure", "Pattern", "AP_bits", "MFP1", "pubchem", "FP2",
"FeatMFP1", "klekota_roth", "cdk_maccs"]

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5 rank

Matrix metalloproteinase-2 : Homo sapiens

score: 6.668 on ChEMBL333 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1090647		0.761905	0.70	*
MFP1	CHEMBL11306		0.571429	0.70	*
RDKit7	CHEMBL347673		0.527950	100.00	
Pattern	CHEMBL152531		0.947368	15.00	*
AP_bits	CHEMBL492599		0.569044	320.00	*
TT_bits	CHEMBL3355723		0.465753	12.50	
FP2	CHEMBL347673		0.635514	100.00	*
hybridization	CHEMBL3827934		0.569492	100.00	
substructure	CHEMBL196647		0.857143	197.00	*
graph	CHEMBL3827831		0.773913	0.20	*
pubchem	CHEMBL3355723		0.918033	12.50	*
cdk_maccs	CHEMBL152267		0.793103	25.70	
klekota_roth	CHEMBL153914		0.634146	0.38	*

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*** ic50 ACTIVITY *** value prediction
based on 9 locally validated fgps ---> 84.434
["substructure", "Pattern", "AP_bits", "MFP1", "pubchem", "graph", "FP2",
"FeatMFP1", "klekota_roth"]

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6 rank

Matrix metalloproteinase-1 : Homo sapiens

score: 6.140 on ChEMBL332 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1090647		0.761905	196.0	*
MFP1	CHEMBL96654		0.666667	30.0	*
RDKit7	CHEMBL133303		0.529114	500.0	
Pattern	CHEMBL286698		0.925059	110.0	*
AP_bits	CHEMBL162128		0.573668	488.0	*
TT_bits	CHEMBL57551		0.483871	147.0	

	FP2	CHEMBL144568	0.625954	2.2	
hybridization	CHEMBL96654	0.502732	30.0		
substructure	CHEMBL196647	0.857143	10000.0		*
graph	CHEMBL315898	0.686957	26.0		
pubchem	CHEMBL19623	0.883333	92.0		*
cdk_maccs	CHEMBL96654	0.839286	30.0		*
klekota_roth	CHEMBL94155	0.633028	7000.0		*

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
based on 8 locally validated fgps ---> 2389.582  
["substructure", "Pattern", "MFP1", "pubchem", "AP\_bits", "FeatMFP1",  
"klekota\_roth", "cdk\_maccs"]

7 rank

Matrix metalloproteinase 3 : Homo sapiens

score: 5.922 on CHEMBL283 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL154040	0.761905	120.00		*
MFP1	CHEMBL11306	0.571429	43.00		*
RDKit7	CHEMBL133303	0.529114	10800.00		
Pattern	CHEMBL152531	0.947368	21.88		*
AP_bits	CHEMBL162128	0.573668	2340.00		*
TT_bits	CHEMBL133303	0.454545	10800.00		
FP2	CHEMBL74670	0.692982	9.10		*
hybridization	CHEMBL154040	0.535714	120.00		
substructure	CHEMBL3617400	0.857143	450.00		*
graph	CHEMBL420259	0.690476	665.00		
pubchem	CHEMBL19623	0.883333	17.00		*
cdk_maccs	CHEMBL152267	0.793103	570.00		
klekota_roth	CHEMBL153914	0.634146	9.00		*

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
based on 8 locally validated fgps ---> 1553.075  
["substructure", "Pattern", "AP\_bits", "MFP1", "pubchem", "FP2",  
"FeatMFP1", "klekota\_roth"]

8 rank

Matrix metalloproteinase 9 : Homo sapiens

score: 5.922 on CHEMBL321 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1090647	0.761905	8.60		*
MFP1	CHEMBL11306	0.571429	0.38		*
RDKit7	CHEMBL162128	0.519016	49.00		
Pattern	CHEMBL3355723	0.933486	31.50		*
AP_bits	CHEMBL162128	0.573668	49.00		*
TT_bits	CHEMBL57551	0.483871	80.00		
FP2	CHEMBL74670	0.692982	4.30		*
hybridization	CHEMBL117225	0.494624	840.00		
substructure	CHEMBL196647	0.857143	983.00		*
graph	CHEMBL550961	0.717742	0.60		
pubchem	CHEMBL3355723	0.918033	31.50		*
cdk_maccs	CHEMBL3355722	0.779661	19.50		
klekota_roth	CHEMBL16520	0.613445	12.00		*

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
based on 8 locally validated fgps ---> 91.630  
["substructure", "Pattern", "AP\_bits", "MFP1", "pubchem", "FP2",  
"FeatMFP1", "klekota\_roth"]

9 rank

Histone deacetylase 6 : Homo sapiens

score: 5.861 on CHEMBL1865 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
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Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL2431863	0.842105	79.0	*
MFP1	CHEMBL2431863	0.580645	79.0	*
RDKit7	CHEMBL3356933	0.551867	139.0	
Pattern	CHEMBL227170	0.871332	9.0	*
AP_bits	CHEMBL570041	0.547546	4900.0	*
TT_bits	CHEMBL2333341	0.509804	7.0	*
FP2	CHEMBL481718	0.678899	170.0	*
hybridization	CHEMBL3356933	0.486486	139.0	
substructure	CHEMBL3309286	0.928571	130.0	*
graph	CHEMBL3415628	0.741667	18.0	
pubchem	CHEMBL481718	0.901639	170.0	*
cdk_maccs	CHEMBL3693774	0.716667	7.0	
klekota_roth	CHEMBL402363	0.554688	12000.0	

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
based on 8 locally validated fgps ---> 4825.007  
["TT\_bits", "substructure", "Pattern", "AP\_bits", "MFP1", "pubchem", "FP2", "FeatMFP1"]

10 rank

Cathepsin L : Homo sapiens

score: 5.781 on ChEMBL3837 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL123571	0.727273	4300.00	*
MFP1	CHEMBL123571	0.567568	4300.00	*
RDKit7	CHEMBL122513	0.582960	42.00	
Pattern	CHEMBL377285	0.864745	342.00	*
AP_bits	CHEMBL258148	0.524922	34000.00	*
TT_bits	CHEMBL550246	0.423729	251.19	
FP2	CHEMBL122513	0.572816	42.00	
hybridization	CHEMBL518284	0.463277	10.00	
substructure	CHEMBL51314	0.857143	500.00	*
graph	CHEMBL123571	0.620438	4300.00	
pubchem	CHEMBL200884	0.842975	55.00	*
cdk_maccs	CHEMBL123571	0.803571	4300.00	*
klekota_roth	CHEMBL125553	0.593220	23.00	*

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
based on 8 locally validated fgps ---> 3324.267  
["substructure", "Pattern", "MFP1", "pubchem", "AP\_bits", "FeatMFP1", "klekota\_roth", "cdk\_maccs"]

11 rank

Histone deacetylase 8 : Homo sapiens

score: 5.740 on ChEMBL3192 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL1083439	0.750000	608.0	*
MFP1	CHEMBL2333341	0.551724	1030.0	*
RDKit7	CHEMBL3356933	0.551867	23.0	
Pattern	CHEMBL227170	0.871332	2060.0	*
AP_bits	CHEMBL572044	0.547619	9700.0	*
TT_bits	CHEMBL2333341	0.509804	1030.0	*
FP2	CHEMBL481718	0.678899	2340.0	*
hybridization	CHEMBL3356933	0.486486	23.0	
substructure	CHEMBL3309286	0.928571	59.0	*
graph	CHEMBL3415628	0.741667	76.0	
pubchem	CHEMBL481718	0.901639	2340.0	*
cdk_maccs	CHEMBL589246	0.700000	12170.0	
klekota_roth	CHEMBL402363	0.554688	3700.0	

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
based on 8 locally validated fgps ---> 1575.219

["TT\_bits", "substructure", "Pattern", "AP\_bits", "MFP1", "pubchem",  
"FP2", "FeatMFP1"]

12 rank

Histone deacetylase 2 : Homo sapiens

score: 5.727 on ChEMBL1937 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3098687		0.750000	956.0	*
MFP1	CHEMBL2333341		0.551724	381.0	*
RDKit7	CHEMBL3356933		0.551867	1770.0	
Pattern	CHEMBL227170		0.871332	205.0	*
AP_bits	CHEMBL2012815		0.535022	290.0	*
TT_bits	CHEMBL2333341		0.509804	381.0	*
FP2	CHEMBL481718		0.678899	5540.0	*
hybridization	CHEMBL3356933		0.486486	1770.0	
substructure	CHEMBL3309286		0.928571	100.0	*
graph	CHEMBL140525		0.714286	200.0	
pubchem	CHEMBL481718		0.901639	5540.0	*
cdk_maccs	CHEMBL3309290		0.687500	100.0	
klekota_roth	CHEMBL2063396		0.563492	1400.0	

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

based on 8 locally validated fgps ---> 1959.524

["TT\_bits", "substructure", "Pattern", "AP\_bits", "MFP1", "pubchem",  
"FP2", "FeatMFP1"]

13 rank

Histone deacetylase 1 : Homo sapiens

score: 5.398 on ChEMBL325 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL246391		0.842105	93.0	*
MFP1	CHEMBL246391		0.656250	93.0	*
RDKit7	CHEMBL235702		0.616519	560.0	
Pattern	CHEMBL227170		0.871332	36.9	*
AP_bits	CHEMBL570041		0.547546	200.0	*
TT_bits	CHEMBL246391		0.466667	93.0	
FP2	CHEMBL246391		0.637255	93.0	*
hybridization	CHEMBL246391		0.557576	93.0	
substructure	CHEMBL3309286		0.928571	43.0	*
graph	CHEMBL3415628		0.741667	6020.0	
pubchem	CHEMBL246391		0.915254	93.0	*
cdk_maccs	CHEMBL246391		0.741379	93.0	
klekota_roth	CHEMBL2063396		0.563492	680.0	

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

based on 7 locally validated fgps ---> 8910.543

["substructure", "Pattern", "AP\_bits", "MFP1", "pubchem", "FP2",  
"FeatMFP1"]

14 rank

Immunoglobulin epsilon Fc receptor : Homo sapiens

score: 5.254 on ChEMBL2940 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL96654		0.761905	1900.0	*
MFP1	CHEMBL96654		0.666667	1900.0	*
RDKit7	CHEMBL420077		0.465278	200.0	
Pattern	CHEMBL325608		0.914352	210.0	*
AP_bits	CHEMBL112228		0.556114	3700.0	*
TT_bits	CHEMBL94155		0.459016	5000.0	
FP2	CHEMBL94368		0.586207	1600.0	
hybridization	CHEMBL96654		0.502732	1900.0	
substructure	CHEMBL11306		0.714286	1000.0	

graph	CHEMBL330625	0.601449	5000.0	
pubchem	CHEMBL96654	0.882353	1900.0	*
cdk_maccs	CHEMBL96654	0.839286	1900.0	*
klekota_roth	CHEMBL94155	0.633028	5000.0	*

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 7 locally validated fgps ---> 3785.606  
 ["Pattern", "MFP1", "pubchem", "AP\_bits", "FeatMFP1", "klekota\_roth",  
 "cdk\_maccs"]

15 rank

Aminopeptidase N : Sus scrofa

score: 5.182 on ChEMBL2590 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL2036146		0.761905	4100.0		*
MFP1	CHEMBL2036144		0.666667	21000.0		*
RDKit7	CHEMBL597936		0.551646	6700.0		
Pattern	CHEMBL597332		0.855580	4300.0		*
AP_bits	CHEMBL599356		0.512712	33100.0		*
TT_bits	CHEMBL594961		0.473684	65100.0		
FP2	CHEMBL575029		0.601695	4300.0		
hybridization	CHEMBL594961		0.629508	65100.0		
substructure	CHEMBL593542		0.800000	36000.0		
graph	CHEMBL594848		0.651515	18500.0		
pubchem	CHEMBL594961		0.905983	65100.0		*
cdk_maccs	CHEMBL594961		0.821429	65100.0		*
klekota_roth	CHEMBL594961		0.657407	65100.0		*

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 7 locally validated fgps ---> 34298.205  
 ["Pattern", "MFP1", "pubchem", "AP\_bits", "FeatMFP1", "klekota\_roth",  
 "cdk\_maccs"]

16 rank

Matrix metalloproteinase 14 : Homo sapiens

score: 5.102 on ChEMBL3869 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1090647		0.761905	34.0		*
MFP1	CHEMBL20154		0.540541	1.9		*
RDKit7	CHEMBL117225		0.456816	1900.0		
Pattern	CHEMBL117225		0.876333	1900.0		*
AP_bits	CHEMBL492599		0.569044	1100.0		*
TT_bits	CHEMBL267603		0.439024	80000.0		
FP2	CHEMBL19843		0.575221	56.0		
hybridization	CHEMBL117225		0.494624	1900.0		
substructure	CHEMBL196647		0.857143	1490.0		*
graph	CHEMBL1392507		0.620968	26700.0		
pubchem	CHEMBL19623		0.883333	105.0		*
cdk_maccs	CHEMBL117225		0.770492	1900.0		
klekota_roth	CHEMBL16520		0.613445	1.9		*

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 7 locally validated fgps ---> 421.389  
 ["substructure", "Pattern", "MFP1", "pubchem", "AP\_bits", "FeatMFP1",  
 "klekota\_roth"]

17 rank

Matrix metalloproteinase 13 : Homo sapiens

score: 5.008 on ChEMBL280 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL2048512		0.681818	6.40		*
MFP1	CHEMBL2048512		0.555556	6.40		*
RDKit7	CHEMBL117225		0.456816	73.00		

Pattern	CHEMBL516206	0.920561	0.10	*
AP_bits	CHEMBL250266	0.550960	2300.00	*
TT_bits	CHEMBL1796289	0.372881	39810.72	
FP2	CHEMBL278366	0.552632	1590.00	
hybridization	CHEMBL117225	0.494624	73.00	
substructure	CHEMBL3617400	0.857143	4.60	*
graph	CHEMBL2048512	0.652174	6.40	
pubchem	CHEMBL117225	0.830769	73.00	*
cdk_maccs	CHEMBL117225	0.770492	73.00	
klekota_roth	CHEMBL117225	0.611111	73.00	*

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 7 locally validated fgps ---> 272.868  
 ["substructure", "Pattern", "MFP1", "pubchem", "AP\_bits", "FeatMFP1",  
 "klekota\_roth"]

18 rank

Neprilysin : Rattus norvegicus

score: 4.979 on ChEMBL3369 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL16791	0.714286	600.0	*
MFP1	CHEMBL16046	0.588235	2.0	*
RDKit7	CHEMBL314626	0.418704	1270.0	
Pattern	CHEMBL358338	0.863341	28.0	*
AP_bits	CHEMBL23598	0.503145	800.0	*
TT_bits	CHEMBL146594	0.435484	3.0	
FP2	CHEMBL16975	0.642202	1.2	*
hybridization	CHEMBL16975	0.500000	1.2	
substructure	CHEMBL16467	0.714286	800.0	
graph	CHEMBL16467	0.666667	800.0	
pubchem	CHEMBL16568	0.842975	750.0	*
cdk_maccs	CHEMBL16568	0.824561	750.0	*
klekota_roth	CHEMBL16975	0.547170	1.2	

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

based on 7 locally validated fgps ---> 393.619

["Pattern", "AP\_bits", "MFP1", "pubchem", "FP2", "FeatMFP1", "cdk\_maccs"]

## MuSSEL Prediction k<sub>i</sub>:

1 rank

Matrix metalloproteinase 8 : Homo sapiens

score: 5.439 on ChEMBL4588 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL103480		0.800000	380.0	*
MFP1	ChEMBL71800		0.647059	3.6	*
RDKit7	ChEMBL324522		0.559840	55000.0	
Pattern	ChEMBL70406		0.941176	13.0	*
AP_bits	ChEMBL70406		0.548061	13.0	*
TT_bits	ChEMBL71800		0.477612	3.6	
FP2	ChEMBL324522		0.770000	55000.0	*
hybridization	ChEMBL324522		0.555556	55000.0	
substructure	ChEMBL102373		0.846154	1100.0	
graph	ChEMBL324522		0.722689	55000.0	
pubchem	ChEMBL430838		0.890756	30.0	*
cdk_maccs	ChEMBL117503		0.842105	25000.0	*
klekota_roth	ChEMBL334065		0.657658	50000.0	

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

based on 7 locally validated fgps ---> 9645.068

["Pattern", "AP\_bits", "MFP1", "pubchem", "FP2", "FeatMFP1", "cdk\_maccs"]

2 rank

Matrix metalloproteinase-2 : Homo sapiens

score: 3.743 on ChEMBL333 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL415074		0.761905	0.10	*
MFP1	ChEMBL72337		0.628571	18.00	*
RDKit7	ChEMBL295798		0.471090	91.00	
Pattern	ChEMBL70406		0.941176	25.00	*
AP_bits	ChEMBL70406		0.548061	25.00	*
TT_bits	ChEMBL72337		0.455882	18.00	
FP2	ChEMBL77057		0.573913	0.02	
hybridization	ChEMBL308228		0.503958	1.90	
substructure	ChEMBL74040		0.733333	0.01	
graph	ChEMBL77057		0.682759	0.02	
pubchem	ChEMBL70406		0.862903	25.00	*
cdk_maccs	ChEMBL72337		0.824561	18.00	
klekota_roth	ChEMBL72337		0.572581	18.00	

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

based on 5 locally validated fgps ---> 15.267

["FeatMFP1", "Pattern", "MFP1", "pubchem", "AP\_bits"]

3 rank

Matrix metalloproteinase 3 : Homo sapiens

score: 3.130 on ChEMBL283 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL415074		0.761905	5.44	*
MFP1	ChEMBL430838		0.583333	91.20	
RDKit7	ChEMBL112864		0.482465	120.00	
Pattern	ChEMBL269334		0.926773	15.00	*
AP_bits	ChEMBL112864		0.550544	120.00	*
TT_bits	ChEMBL430838		0.439394	91.20	
FP2	ChEMBL77057		0.573913	5.87	
hybridization	ChEMBL167232		0.468672	168.00	
substructure	ChEMBL313207		0.733333	16.00	
graph	ChEMBL77057		0.682759	5.87	
pubchem	ChEMBL430838		0.890756	91.20	*
cdk_maccs	ChEMBL77754		0.810345	25.30	
klekota_roth	ChEMBL16520		0.613445	310.00	

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



based on 4 locally validated fgps ---> 72.839  
["FeatMFP1", "Pattern", "pubchem", "AP\_bits"]

4 rank

Matrix metalloproteinase-1 : Homo sapiens

score: 3.119 on ChEMBL332 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL415074		0.761905	5120.0		*
MFP1	ChEMBL430838		0.583333	9600.0		
RDKit7	ChEMBL112864		0.482465	1090.0		
Pattern	ChEMBL167232		0.915332	282.0		*
AP_bits	ChEMBL112864		0.550544	1090.0		*
TT_bits	ChEMBL430838		0.439394	9600.0		
FP2	ChEMBL77057		0.573913	313.0		
hybridization	ChEMBL167232		0.468672	282.0		
substructure	ChEMBL313207		0.733333	350.0		
graph	ChEMBL77057		0.682759	313.0		
pubchem	ChEMBL430838		0.890756	9600.0		*
cdk_maccs	ChEMBL77754		0.810345	7.8		
klekota_roth	ChEMBL16520		0.613445	2.0		

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

based on 4 locally validated fgps ---> 3223.905  
["FeatMFP1", "Pattern", "pubchem", "AP\_bits"]

5 rank

Matrix metalloproteinase 9 : Homo sapiens

score: 3.009 on ChEMBL321 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL71800		0.727273	3.0		
MFP1	ChEMBL71800		0.647059	3.0		*
RDKit7	ChEMBL367959		0.523873	5500.0		
Pattern	ChEMBL70406		0.941176	6.3		*
AP_bits	ChEMBL70406		0.548061	6.3		*
TT_bits	ChEMBL71800		0.477612	3.0		
FP2	ChEMBL367959		0.609524	5500.0		
hybridization	ChEMBL69024		0.514905	1.5		
substructure	ChEMBL171466		0.785714	150.0		
graph	ChEMBL381189		0.666667	6600.0		
pubchem	ChEMBL369184		0.872881	900.0		*
cdk_maccs	ChEMBL71800		0.824561	3.0		
klekota_roth	ChEMBL16520		0.613445	2.0		

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

based on 4 locally validated fgps ---> 135.367  
["Pattern", "MFP1", "pubchem", "AP\_bits"]

6 rank

Cathepsin K : Homo sapiens

score: 3.001 on ChEMBL268 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL99288		0.583333	110.0		
MFP1	ChEMBL371466		0.529412	1500.0		
RDKit7	ChEMBL96987		0.606258	20.0		
Pattern	ChEMBL2316590		0.874172	11.5		*
AP_bits	ChEMBL97402		0.538188	111.0		*
TT_bits	ChEMBL200235		0.491525	300.0		
FP2	ChEMBL607169		0.730769	10.1		*
hybridization	ChEMBL96987		0.486957	20.0		
substructure	ChEMBL198612		0.812500	246.0		
graph	ChEMBL3605412		0.608333	114.0		
pubchem	ChEMBL371466		0.858333	1500.0		*

cdk_maccs	CHEMBL100482	0.693548	30.0
klekota_roth	CHEMBL1651359	0.530973	2.9

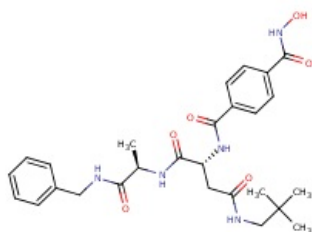
\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 4 locally validated fgps ---> 1844.626  
["Pattern", "FP2", "pubchem", "AP\_bits"]

# SwissTargetPrediction report:

## Reference:

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

## Query Molecule



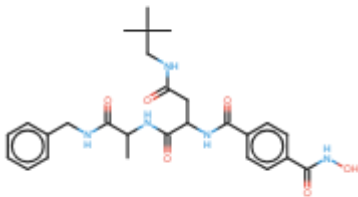
## Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
Cathepsin L2 ( <i>by homology</i> )	<a href="#">O60911</a>	<a href="#">CTSL2</a>	CHEMBL3272	<div><div></div></div>	77 / 150	Cysteine Protease
Cathepsin L1 light chain	<a href="#">P07711</a>	<a href="#">CTSL1</a>	CHEMBL3837	<div><div></div></div>	77 / 150	Cysteine Protease
Cathepsin S	<a href="#">P25774</a>	<a href="#">CTSS</a>	CHEMBL2954	<div><div></div></div>	77 / 150	Cysteine Protease
Cathepsin K	<a href="#">P43235</a>	<a href="#">CTSK</a>	CHEMBL268	<div><div></div></div>	77 / 150	Cysteine Protease
Microtubule-associated protein tau	<a href="#">P10636</a>	<a href="#">MAPT</a>	CHEMBL1293224	<div><div></div></div>	200 / 16	Unclassified
Disintegrin and metalloproteinase domain-containing protein 17	<a href="#">P78536</a>	<a href="#">ADAM17</a>	CHEMBL3706	<div><div></div></div>	236 / 39	Metallo Protease
22 kDa interstitial collagenase	<a href="#">P03956</a>	<a href="#">MMP1</a>	CHEMBL332	<div><div></div></div>	752 / 277	Metallo Protease
Stromelysin-1	<a href="#">P08254</a>	<a href="#">MMP3</a>	CHEMBL283	<div><div></div></div>	752 / 277	Metallo Protease
Stromelysin-2 ( <i>by homology</i> )	<a href="#">P09238</a>	<a href="#">MMP10</a>	CHEMBL4270	<div><div></div></div>	752 / 277	Metallo Protease
Neutrophil collagenase ( <i>by homology</i> )	<a href="#">P22894</a>	<a href="#">MMP8</a>	CHEMBL4588	<div><div></div></div>	684 / 273	Metallo Protease
Macrophage metalloelastase ( <i>by homology</i> )	<a href="#">P39900</a>	<a href="#">MMP12</a>	CHEMBL4393	<div><div></div></div>	696 / 241	Metallo Protease
Collagenase 3 ( <i>by homology</i> )	<a href="#">P45452</a>	<a href="#">MMP13</a>	CHEMBL280	<div><div></div></div>	697 / 241	Metallo Protease
Matrix metalloproteinase-27 ( <i>by homology</i> )	<a href="#">Q9H306</a>	<a href="#">MMP27</a>		<div><div></div></div>	752 / 277	Metallo Protease
Histone deacetylase 1 ( <i>by homology</i> )	<a href="#">Q13547</a>	<a href="#">HDAC1</a>	CHEMBL325	<div><div></div></div>	174 / 42	Enzyme
Histone deacetylase 2	<a href="#">Q92769</a>	<a href="#">HDAC2</a>	CHEMBL1937	<div><div></div></div>	174 / 42	Enzyme

# Polypharmacology Browser 2 Prediction:

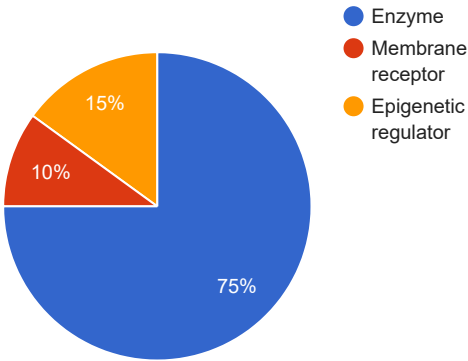
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL4662 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4662">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4662</a> )	Proteasome Macropain subunit MB1	Show NN
2	CHEMBL325 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL325">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL325</a> )	Histone deacetylase 1	Show NN
3	CHEMBL4822 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4822">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4822</a> )	Beta-secretase 1	Show NN
4	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
5	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
6	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
7	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
8	CHEMBL2954 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2954">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2954</a> )	Cathepsin S	Show NN
9	CHEMBL1865 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1865">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1865</a> )	Histone deacetylase 6	Show NN
10	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
11	CHEMBL3192 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3192">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3192</a> )	Histone deacetylase 8	Show NN
12	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
13	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
14	CHEMBL233 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL233">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL233</a> )	Mu opioid receptor	Show NN
15	CHEMBL3837 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3837">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3837</a> )	Cathepsin L	Show NN
16	CHEMBL268 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL268">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL268</a> )	Cathepsin K	Show NN
17	CHEMBL3286 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3286">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3286</a> )	Urokinase-type plasminogen activator	Show NN
18	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

19	CHEMBL236 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL236">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL236</a> )	Delta opioid receptor	Show NN
20	CHEMBL4801 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4801">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4801</a> )	Caspase-1	Show NN