

MuSSEL Prediction IC₅₀:

1 rank

Vascular endothelial growth factor receptor 2 : Homo sapiens

score: 6.544 on ChEMBL279 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3754556		0.680000	86.67	*
MFP1	CHEMBL3746595		0.560976	4.00	*
RDKit7	CHEMBL612137		0.516364	40.00	
Pattern	CHEMBL470483		0.881696	470.00	*
AP_bits	CHEMBL1242977		0.576497	3270.00	*
TT_bits	CHEMBL272670		0.454545	19.95	
FP2	CHEMBL272670		0.633987	19.95	*
hybridization	CHEMBL182283		0.658046	630.00	*
substructure	CHEMBL577742		0.842105	13.00	
graph	CHEMBL183504		0.841808	2040.00	*
pubchem	CHEMBL3814321		0.871287	120.00	*
cdk_maccs	CHEMBL600398		0.839286	860.00	*
klekota_roth	CHEMBL243916		0.555556	2.60	

*** ic50 ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 645.383

["Pattern", "AP_bits", "MFP1", "pubchem", "graph", "FP2", "cdk_maccs", "hybridization"]

2 rank

MAP kinase signal-integrating kinase 2 : Homo sapiens

score: 5.958 on ChEMBL4204 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3805074		0.636364	22.0	
MFP1	CHEMBL3805074		0.636364	22.0	*
RDKit7	CHEMBL3805094		0.706952	760.0	*
Pattern	CHEMBL3805094		0.855422	760.0	*
AP_bits	CHEMBL3805094		0.444444	760.0	
TT_bits	CHEMBL3805094		0.597015	760.0	*
FP2	CHEMBL3805094		0.774194	760.0	*
hybridization	CHEMBL3805094		0.630653	760.0	*
substructure	CHEMBL3804952		0.761905	8.0	
graph	CHEMBL3805094		0.826347	760.0	*
pubchem	CHEMBL3805094		0.931034	760.0	*
cdk_maccs	CHEMBL3698947		0.700000	11.0	
klekota_roth	CHEMBL3805094		0.493151	760.0	

*** ic50 ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 531.260

["TT_bits", "Pattern", "MFP1", "pubchem", "graph", "FP2", "RDKit7", "hybridization"]

3 rank

Epidermal growth factor receptor erbB1 : Homo sapiens

score: 5.022 on ChEMBL203 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3754556		0.680000	71.82	*
MFP1	CHEMBL1928946		0.600000	108.00	*
RDKit7	CHEMBL1928956		0.506826	627.00	
Pattern	CHEMBL387187		0.905192	21.00	*
AP_bits	CHEMBL3814846		0.514943	3.96	*
TT_bits	CHEMBL1928946		0.477612	108.00	
FP2	CHEMBL1928956		0.639785	627.00	*
hybridization	CHEMBL247228		0.476804	10000.00	
substructure	CHEMBL2335018		0.833333	12800.00	
graph	CHEMBL1928954		0.692308	1671.00	
pubchem	CHEMBL14627		0.833333	74.00	*
cdk_maccs	CHEMBL1928956		0.849057	627.00	*

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klekota_roth CHEMBL3774451      0.404255      582.17
  *** ic50 ACTIVITY *** value prediction
    based on 6 locally validated fgps ---> 576.366
["Pattern", "AP_bits", "MFP1", "pubchem", "FP2", "cdk_maccs"]
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MuSSEL Prediction k_i:

1 rank

Leucine-rich repeat serine/threonine-protein kinase 2 : Homo sapiens
score: 3.810 on ChEMBL1075104 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581		0.615385	1584.890	
MFP1	CHEMBL574738		0.590909	1000.000	*
RDKit7	CHEMBL574738		0.602683	1000.000	
Pattern	CHEMBL3641887		0.873391	5.200	*
AP_bits	CHEMBL1988076		0.441667	2511.890	
TT_bits	CHEMBL574738		0.567164	1000.000	*
FP2	CHEMBL574738		0.614458	1000.000	
hybridization	CHEMBL574738		0.504902	1000.000	
substructure	CHEMBL1983111		0.882353	0.631	*
graph	CHEMBL574738		0.733333	1000.000	
pubchem	CHEMBL574738		0.896040	1000.000	*
cdk_maccs	CHEMBL3641833		0.762712	5.200	
klekota_roth	CHEMBL1992581		0.450980	1584.890	

*** ki ACTIVITY *** value prediction

based on 5 locally validated fgps ---> 600.887

["Pattern", "TT_bits", "MFP1", "substructure", "pubchem"]

2 rank

Tyrosine-protein kinase ABL : Homo sapiens

score: 3.483 on ChEMBL1862 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581		0.615385	199.53	
MFP1	CHEMBL574738		0.590909	25.12	*
RDKit7	CHEMBL574738		0.602683	25.12	
Pattern	CHEMBL1992306		0.855580	630.96	
AP_bits	CHEMBL1992306		0.546539	630.96	*
TT_bits	CHEMBL574738		0.567164	25.12	*
FP2	CHEMBL574738		0.614458	25.12	
hybridization	CHEMBL574738		0.504902	25.12	
substructure	CHEMBL1983111		0.882353	251.19	*
graph	CHEMBL574738		0.733333	25.12	
pubchem	CHEMBL574738		0.896040	25.12	*
cdk_maccs	CHEMBL1336		0.750000	158.49	
klekota_roth	CHEMBL1973178		0.460000	199.53	

*** ki ACTIVITY *** value prediction

based on 5 locally validated fgps ---> 166.683

["AP_bits", "TT_bits", "MFP1", "substructure", "pubchem"]

3 rank

Tyrosine-protein kinase receptor RET : Homo sapiens

score: 3.483 on ChEMBL2041 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581		0.615385	199.530	
MFP1	CHEMBL574738		0.590909	6.310	*
RDKit7	CHEMBL574738		0.602683	6.310	
Pattern	CHEMBL1992306		0.855580	7.943	
AP_bits	CHEMBL1992306		0.546539	7.943	*
TT_bits	CHEMBL574738		0.567164	6.310	*
FP2	CHEMBL574738		0.614458	6.310	
hybridization	CHEMBL574738		0.504902	6.310	
substructure	CHEMBL1983111		0.882353	3.162	*
graph	CHEMBL574738		0.733333	6.310	
pubchem	CHEMBL574738		0.896040	6.310	*
cdk_maccs	CHEMBL1982660		0.754717	100.000	
klekota_roth	CHEMBL1992581		0.450980	199.530	

*** ki ACTIVITY *** value prediction

based on 5 locally validated fgps ---> 6.007
["AP_bits", "TT_bits", "MFP1", "substructure", "pubchem"]

4 rank

Tyrosine-protein kinase LCK : Homo sapiens

score: 3.483 on ChEMBL258 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581		0.615385	3162.28	
MFP1	CHEMBL574738		0.590909	15.85	*
RDKit7	CHEMBL574738		0.602683	15.85	
Pattern	CHEMBL1992306		0.855580	251.19	
AP_bits	CHEMBL1992306		0.546539	251.19	*
TT_bits	CHEMBL574738		0.567164	15.85	*
FP2	CHEMBL574738		0.614458	15.85	
hybridization	CHEMBL574738		0.504902	15.85	
substructure	CHEMBL1983111		0.882353	199.53	*
graph	CHEMBL574738		0.733333	15.85	
pubchem	CHEMBL574738		0.896040	15.85	*
cdk_maccs	CHEMBL2170582		0.803279	116.00	
klekota_roth	CHEMBL1973178		0.460000	31.62	

*** ki ACTIVITY *** value prediction

based on 5 locally validated fgps ---> 99.654

["AP_bits", "TT_bits", "MFP1", "substructure", "pubchem"]

5 rank

Tyrosine-protein kinase JAK2 : Homo sapiens

score: 3.483 on ChEMBL2971 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL2420821		0.576923	310.000	
MFP1	CHEMBL574738		0.590909	1000.000	*
RDKit7	CHEMBL574738		0.602683	1000.000	
Pattern	CHEMBL1992306		0.855580	630.960	
AP_bits	CHEMBL1992306		0.546539	630.960	*
TT_bits	CHEMBL574738		0.567164	1000.000	*
FP2	CHEMBL574738		0.614458	1000.000	
hybridization	CHEMBL574738		0.504902	1000.000	
substructure	CHEMBL1983111		0.882353	3.981	*
graph	CHEMBL574738		0.733333	1000.000	
pubchem	CHEMBL574738		0.896040	1000.000	*
cdk_maccs	CHEMBL2170582		0.803279	130.000	
klekota_roth	CHEMBL2002723		0.431818	1995.260	

*** ki ACTIVITY *** value prediction

based on 5 locally validated fgps ---> 727.890

["AP_bits", "TT_bits", "MFP1", "substructure", "pubchem"]

6 rank

Serine/threonine-protein kinase Aurora-A : Homo sapiens

score: 3.483 on ChEMBL4722 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1976455		0.576923	1995.260	
MFP1	CHEMBL574738		0.590909	1584.890	*
RDKit7	CHEMBL574738		0.602683	1584.890	
Pattern	CHEMBL1992306		0.855580	501.190	
AP_bits	CHEMBL1992306		0.546539	501.190	*
TT_bits	CHEMBL574738		0.567164	1584.890	*
FP2	CHEMBL574738		0.614458	1584.890	
hybridization	CHEMBL574738		0.504902	1584.890	
substructure	CHEMBL1983111		0.882353	3.981	*
graph	CHEMBL574738		0.733333	1584.890	
pubchem	CHEMBL574738		0.896040	1584.890	*

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    cdk_maccs      CHEMBL1336          0.750000    794.330
    klekota_roth   CHEMBL2002723        0.431818   1584.890
    *** ki ACTIVITY *** value prediction
    based on 5 locally validated fgps ---> 904.998
["AP_bits", "TT_bits", "MFP1", "substructure", "pubchem"]

7 rank
Neurotrophic tyrosine kinase receptor type 2 : Homo sapiens
score: 3.483 on CHEMBL4898 based on 5 fingerprints
Fingerprint type      Ligand      Tanimoto Similarity  activity Valid fg
FeatMFP1  CHEMBL1992581          0.615385    251.19
MFP1      CHEMBL574738          0.590909    251.19      *
RDKit7    CHEMBL574738          0.602683    251.19
Pattern   CHEMBL1992306          0.855580    125.89
AP_bits   CHEMBL1992306          0.546539    125.89      *
TT_bits   CHEMBL574738          0.567164    251.19      *
FP2       CHEMBL574738          0.614458    251.19
hybridization CHEMBL574738          0.504902    251.19
substructure CHEMBL1983111          0.882353     31.62      *
graph     CHEMBL574738          0.733333    251.19
pubchem   CHEMBL574738          0.896040    251.19      *
cdk_maccs CHEMBL1336          0.750000    630.96
klekota_roth CHEMBL1992581          0.450980    251.19
    *** ki ACTIVITY *** value prediction
    based on 5 locally validated fgps ---> 182.216
["AP_bits", "TT_bits", "MFP1", "substructure", "pubchem"]

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8 rank
Serine/threonine-protein kinase TAO1 : Homo sapiens
score: 3.483 on CHEMBL5261 based on 5 fingerprints
Fingerprint type      Ligand      Tanimoto Similarity  activity Valid fg
FeatMFP1  CHEMBL1992306          0.571429     79.43
MFP1      CHEMBL574738          0.590909    501.19      *
RDKit7    CHEMBL574738          0.602683    501.19
Pattern   CHEMBL1992306          0.855580     79.43
AP_bits   CHEMBL1992306          0.546539     79.43      *
TT_bits   CHEMBL574738          0.567164    501.19      *
FP2       CHEMBL574738          0.614458    501.19
hybridization CHEMBL574738          0.504902    501.19
substructure CHEMBL1983111          0.882353    100.00      *
graph     CHEMBL574738          0.733333    501.19
pubchem   CHEMBL574738          0.896040    501.19      *
cdk_maccs CHEMBL1336          0.750000    398.11
klekota_roth CHEMBL2002723          0.431818   5011.87
    *** ki ACTIVITY *** value prediction
    based on 5 locally validated fgps ---> 336.600
["AP_bits", "TT_bits", "MFP1", "substructure", "pubchem"]

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9 rank
Tyrosine-protein kinase receptor TYRO3 : Homo sapiens
score: 3.483 on CHEMBL5314 based on 5 fingerprints
Fingerprint type      Ligand      Tanimoto Similarity  activity Valid fg
FeatMFP1  CHEMBL1986756          0.629630    251.19
MFP1      CHEMBL574738          0.590909   1584.89      *
RDKit7    CHEMBL574738          0.602683   1584.89
Pattern   CHEMBL1992306          0.855580    316.23
AP_bits   CHEMBL1992306          0.546539    316.23      *
TT_bits   CHEMBL574738          0.567164   1584.89      *
FP2       CHEMBL574738          0.614458   1584.89
hybridization CHEMBL574738          0.504902   1584.89

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substructure CHEMBL1983111      0.882353    125.89      *
graph CHEMBL574738             0.733333    1584.89
pubchem CHEMBL574738           0.896040    1584.89      *
cdk_maccs CHEMBL1992306        0.740741     316.23
klekota_roth CHEMBL2002723      0.431818    1258.93
*** ki ACTIVITY *** value prediction
based on 5 locally validated fgps ---> 1039.358
["AP_bits", "TT_bits", "MFP1", "substructure", "pubchem"]

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10 rank

Proto-oncogene tyrosine-protein kinase ROS : Homo sapiens

score: 3.483 on CHEMBL5568 based on 5 fingerprints

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Fingerprint type      Ligand      Tanimoto Similarity activity Valid fg
FeatMFP1 CHEMBL1992306      0.571429    1000.00
MFP1 CHEMBL574738          0.590909    1995.26      *
RDKit7 CHEMBL574738          0.602683    1995.26
Pattern CHEMBL1992306        0.855580    1000.00
AP_bits CHEMBL1992306        0.546539    1000.00      *
TT_bits CHEMBL574738          0.567164    1995.26      *
FP2 CHEMBL574738            0.614458    1995.26
hybridization CHEMBL574738      0.504902    1995.26
substructure CHEMBL1983111      0.882353     31.62      *
graph CHEMBL574738            0.733333    1995.26
pubchem CHEMBL574738            0.896040    1995.26      *
cdk_maccs CHEMBL1982660        0.754717     63.10
klekota_roth CHEMBL1992306      0.413793    1000.00
*** ki ACTIVITY *** value prediction
based on 5 locally validated fgps ---> 1403.480
["AP_bits", "TT_bits", "MFP1", "substructure", "pubchem"]

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11 rank

NT-3 growth factor receptor : Homo sapiens

score: 3.483 on CHEMBL5608 based on 5 fingerprints

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Fingerprint type      Ligand      Tanimoto Similarity activity Valid fg
FeatMFP1 CHEMBL1992581      0.615385     630.96
MFP1 CHEMBL574738          0.590909    1000.00      *
RDKit7 CHEMBL574738          0.602683    1000.00
Pattern CHEMBL1992306        0.855580     15.85
AP_bits CHEMBL1992306        0.546539     15.85      *
TT_bits CHEMBL574738          0.567164    1000.00      *
FP2 CHEMBL574738            0.614458    1000.00
hybridization CHEMBL574738      0.504902    1000.00
substructure CHEMBL1983111      0.882353     39.81      *
graph CHEMBL574738            0.733333    1000.00
pubchem CHEMBL574738            0.896040    1000.00      *
cdk_maccs CHEMBL1336          0.750000     398.11
klekota_roth CHEMBL1992581      0.450980     630.96
*** ki ACTIVITY *** value prediction
based on 5 locally validated fgps ---> 611.132
["AP_bits", "TT_bits", "MFP1", "substructure", "pubchem"]

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12 rank

Mitogen-activated protein kinase kinase kinase kinase 4 : Homo sapiens

score: 3.483 on CHEMBL6166 based on 5 fingerprints

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Fingerprint type      Ligand      Tanimoto Similarity activity Valid fg
FeatMFP1 CHEMBL1992581      0.615385    1000.00
MFP1 CHEMBL574738          0.590909    158.49      *
RDKit7 CHEMBL574738          0.602683    158.49
Pattern CHEMBL1992306        0.855580   10000.00
AP_bits CHEMBL1992306        0.546539   10000.00      *

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TT_bits	CHEMBL574738	0.567164	158.49	*
FP2	CHEMBL574738	0.614458	158.49	
hybridization	CHEMBL574738	0.504902	158.49	
substructure	CHEMBL1983111	0.882353	100.00	*
graph	CHEMBL574738	0.733333	158.49	
pubchem	CHEMBL574738	0.896040	158.49	*
cdk_maccs	CHEMBL1982660	0.754717	63.10	
klekota_roth	CHEMBL1992581	0.450980	1000.00	

*** ki ACTIVITY *** value prediction

based on 5 locally validated fgps ---> 2115.094

["AP_bits", "TT_bits", "MFP1", "substructure", "pubchem"]

13 rank

Macrophage colony stimulating factor receptor : Homo sapiens

score: 2.936 on ChEMBL1844 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581	0.615385	1584.890	
MFP1	CHEMBL574738	0.590909	50.120	*
RDKit7	CHEMBL574738	0.602683	50.120	
Pattern	CHEMBL1988838	0.828753	316.230	
AP_bits	CHEMBL1336	0.507795	158.490	
TT_bits	CHEMBL574738	0.567164	50.120	*
FP2	CHEMBL574738	0.614458	50.120	
hybridization	CHEMBL574738	0.504902	50.120	
substructure	CHEMBL1983111	0.882353	63.100	*
graph	CHEMBL574738	0.733333	50.120	
pubchem	CHEMBL574738	0.896040	50.120	*
cdk_maccs	CHEMBL1336	0.750000	158.490	
klekota_roth	CHEMBL1973178	0.460000	5.012	

*** ki ACTIVITY *** value prediction

based on 4 locally validated fgps ---> 53.365

["TT_bits", "MFP1", "substructure", "pubchem"]

14 rank

Vascular endothelial growth factor receptor 1 : Homo sapiens

score: 2.936 on ChEMBL1868 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581	0.615385	316.230	
MFP1	CHEMBL574738	0.590909	31.620	*
RDKit7	CHEMBL574738	0.602683	31.620	
Pattern	CHEMBL1988838	0.828753	79.430	
AP_bits	CHEMBL1336	0.507795	316.230	
TT_bits	CHEMBL574738	0.567164	31.620	*
FP2	CHEMBL574738	0.614458	31.620	
hybridization	CHEMBL574738	0.504902	31.620	
substructure	CHEMBL1983111	0.882353	10.000	*
graph	CHEMBL574738	0.733333	31.620	
pubchem	CHEMBL574738	0.896040	31.620	*
cdk_maccs	CHEMBL1982660	0.754717	125.890	
klekota_roth	CHEMBL1973178	0.460000	0.631	

*** ki ACTIVITY *** value prediction

based on 4 locally validated fgps ---> 26.215

["TT_bits", "MFP1", "substructure", "pubchem"]

15 rank

Platelet-derived growth factor receptor beta : Homo sapiens

score: 2.936 on ChEMBL1913 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581	0.615385	1995.260	
MFP1	CHEMBL574738	0.590909	7.943	*

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
RDKit7	CHEMBL574738	0.602683	7.943	
Pattern	CHEMBL574738	0.827381	7.943	
AP_bits	CHEMBL1336	0.507795	3.981	
TT_bits	CHEMBL574738	0.567164	7.943	*
FP2	CHEMBL574738	0.614458	7.943	
hybridization	CHEMBL574738	0.504902	7.943	
substructure	CHEMBL1983111	0.882353	63.100	*
graph	CHEMBL574738	0.733333	7.943	
pubchem	CHEMBL574738	0.896040	7.943	*
cdk_maccs	CHEMBL1336	0.750000	3.981	
klekota_roth	CHEMBL1992581	0.450980	1995.260	

*** ki ACTIVITY *** value prediction
based on 4 locally validated fgps ---> 21.732
["TT_bits", "MFP1", "substructure", "pubchem"]

16 rank

Stem cell growth factor receptor : Homo sapiens

score: 2.936 on ChEMBL1936 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL2000934	0.629630	199.530	
MFP1	CHEMBL574738	0.590909	1584.890	*
RDKit7	CHEMBL574738	0.602683	1584.890	
Pattern	CHEMBL574738	0.827381	1584.890	
AP_bits	CHEMBL2004438	0.492857	158.490	
TT_bits	CHEMBL574738	0.567164	1584.890	*
FP2	CHEMBL574738	0.614458	1584.890	
hybridization	CHEMBL574738	0.504902	1584.890	
substructure	CHEMBL1983111	0.882353	251.190	*
graph	CHEMBL574738	0.733333	1584.890	
pubchem	CHEMBL574738	0.896040	1584.890	*
cdk_maccs	CHEMBL1971943	0.649123	316.230	
klekota_roth	CHEMBL1973178	0.460000	1.585	

*** ki ACTIVITY *** value prediction
based on 4 locally validated fgps ---> 1251.465
["TT_bits", "MFP1", "substructure", "pubchem"]

17 rank

Platelet-derived growth factor receptor alpha : Homo sapiens

score: 2.936 on ChEMBL2007 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL574738	0.558824	79.43	
MFP1	CHEMBL574738	0.590909	79.43	*
RDKit7	CHEMBL574738	0.602683	79.43	
Pattern	CHEMBL574738	0.827381	79.43	
AP_bits	CHEMBL1336	0.507795	1000.00	
TT_bits	CHEMBL574738	0.567164	79.43	*
FP2	CHEMBL574738	0.614458	79.43	
hybridization	CHEMBL574738	0.504902	79.43	
substructure	CHEMBL1983111	0.882353	100.00	*
graph	CHEMBL574738	0.733333	79.43	
pubchem	CHEMBL574738	0.896040	79.43	*
cdk_maccs	CHEMBL1336	0.750000	1000.00	
klekota_roth	CHEMBL1336	0.387097	1000.00	

*** ki ACTIVITY *** value prediction
based on 4 locally validated fgps ---> 84.573
["TT_bits", "MFP1", "substructure", "pubchem"]

18 rank

Death-associated protein kinase 3 : Homo sapiens

score: 2.936 on ChEMBL2468 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL574738		0.558824	3981.07	
MFP1	CHEMBL574738		0.590909	3981.07	*
RDKit7	CHEMBL574738		0.602683	3981.07	
Pattern	CHEMBL1988838		0.828753	316.23	
AP_bits	CHEMBL411903		0.476695	794.33	
TT_bits	CHEMBL574738		0.567164	3981.07	*
FP2	CHEMBL574738		0.614458	3981.07	
hybridization	CHEMBL574738		0.504902	3981.07	
substructure	CHEMBL1983111		0.882353	251.19	*
graph	CHEMBL574738		0.733333	3981.07	
pubchem	CHEMBL574738		0.896040	3981.07	*
cdk_maccs	CHEMBL475251		0.698413	79.43	
klekota_roth	CHEMBL1084546		0.388060	1000.00	

*** ki ACTIVITY *** value prediction
based on 4 locally validated fgps ---> 3048.600
["TT_bits", "MFP1", "substructure", "pubchem"]

19 rank

Vascular endothelial growth factor receptor 2 : Homo sapiens

score: 2.936 on ChEMBL279 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1254007		0.620690	0.024	
MFP1	CHEMBL574738		0.590909	2.512	*
RDKit7	CHEMBL574738		0.602683	2.512	
Pattern	CHEMBL400512		0.845011	8.000	
AP_bits	CHEMBL394826		0.509009	9.000	
TT_bits	CHEMBL574738		0.567164	2.512	*
FP2	CHEMBL574738		0.614458	2.512	
hybridization	CHEMBL574738		0.504902	2.512	
substructure	CHEMBL1983111		0.882353	15.850	*
graph	CHEMBL574738		0.733333	2.512	
pubchem	CHEMBL574738		0.896040	2.512	*
cdk_maccs	CHEMBL248978		0.811321	23.000	
klekota_roth	CHEMBL236205		0.489796	80.000	

*** ki ACTIVITY *** value prediction
based on 4 locally validated fgps ---> 5.846
["TT_bits", "MFP1", "substructure", "pubchem"]

20 rank

Nerve growth factor receptor Trk-A : Homo sapiens

score: 2.936 on ChEMBL2815 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581		0.615385	10000.00	
MFP1	CHEMBL574738		0.590909	1584.89	*
RDKit7	CHEMBL574738		0.602683	1584.89	
Pattern	CHEMBL1988838		0.828753	125.89	
AP_bits	CHEMBL1336		0.507795	1584.89	
TT_bits	CHEMBL574738		0.567164	1584.89	*
FP2	CHEMBL574738		0.614458	1584.89	
hybridization	CHEMBL574738		0.504902	1584.89	
substructure	CHEMBL1983111		0.882353	100.00	*
graph	CHEMBL574738		0.733333	1584.89	
pubchem	CHEMBL574738		0.896040	1584.89	*
cdk_maccs	CHEMBL1336		0.750000	1584.89	
klekota_roth	CHEMBL1992581		0.450980	10000.00	

*** ki ACTIVITY *** value prediction
based on 4 locally validated fgps ---> 1213.668
["TT_bits", "MFP1", "substructure", "pubchem"]

21 rank

Rho-associated protein kinase 2 : Homo sapiens

score: 2.936 on ChEMBL2973 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL574738		0.558824	501.19	
MFP1	CHEMBL574738		0.590909	501.19	*
RDKit7	CHEMBL574738		0.602683	501.19	
Pattern	CHEMBL1997554		0.831111	501.19	
AP_bits	CHEMBL1981410		0.506466	1584.89	
TT_bits	CHEMBL574738		0.567164	501.19	*
FP2	CHEMBL574738		0.614458	501.19	
hybridization	CHEMBL574738		0.504902	501.19	
substructure	CHEMBL1983111		0.882353	158.49	*
graph	CHEMBL574738		0.733333	501.19	
pubchem	CHEMBL574738		0.896040	501.19	*
cdk_maccs	CHEMBL1997554		0.673077	501.19	
klekota_roth	CHEMBL1984363		0.418182	158.49	

*** ki ACTIVITY *** value prediction

based on 4 locally validated fgps ---> 415.515

["TT_bits", "MFP1", "substructure", "pubchem"]

22 rank

Fibroblast growth factor receptor 1 : Homo sapiens

score: 2.936 on ChEMBL3650 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581		0.615385	794.33	
MFP1	CHEMBL574738		0.590909	501.19	*
RDKit7	CHEMBL574738		0.602683	501.19	
Pattern	CHEMBL1988838		0.828753	199.53	
AP_bits	CHEMBL1987910		0.478365	1258.93	
TT_bits	CHEMBL574738		0.567164	501.19	*
FP2	CHEMBL574738		0.614458	501.19	
hybridization	CHEMBL574738		0.504902	501.19	
substructure	CHEMBL1983111		0.882353	19.95	*
graph	CHEMBL574738		0.733333	501.19	
pubchem	CHEMBL574738		0.896040	501.19	*
cdk_maccs	CHEMBL1982660		0.754717	3981.07	
klekota_roth	CHEMBL1992581		0.450980	794.33	

*** ki ACTIVITY *** value prediction

based on 4 locally validated fgps ---> 380.880

["TT_bits", "MFP1", "substructure", "pubchem"]

23 rank

cAMP-dependent protein kinase alpha-catalytic subunit : Homo sapiens

score: 2.936 on ChEMBL4101 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3580669		0.592593	3000.00	
MFP1	CHEMBL574738		0.590909	199.53	*
RDKit7	CHEMBL574738		0.602683	199.53	
Pattern	CHEMBL1997554		0.831111	199.53	
AP_bits	CHEMBL1983393		0.445623	794.33	
TT_bits	CHEMBL574738		0.567164	199.53	*
FP2	CHEMBL574738		0.614458	199.53	
hybridization	CHEMBL574738		0.504902	199.53	
substructure	CHEMBL1983111		0.882353	125.89	*
graph	CHEMBL574738		0.733333	199.53	
pubchem	CHEMBL574738		0.896040	199.53	*
cdk_maccs	CHEMBL475251		0.698413	251.19	
klekota_roth	CHEMBL2002723		0.431818	1258.93	

*** ki ACTIVITY *** value prediction

based on 4 locally validated fgps ---> 181.120
["TT_bits", "MFP1", "substructure", "pubchem"]

24 rank

Dual specificity protein kinase CLK4 : Homo sapiens

score: 2.936 on ChEMBL4203 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1986756		0.629630	63.10	
MFP1	CHEMBL574738		0.590909	316.23	*
RDKit7	CHEMBL574738		0.602683	316.23	
Pattern	CHEMBL1988838		0.828753	251.19	
AP_bits	CHEMBL1981410		0.506466	2511.89	
TT_bits	CHEMBL574738		0.567164	316.23	*
FP2	CHEMBL574738		0.614458	316.23	
hybridization	CHEMBL574738		0.504902	316.23	
substructure	CHEMBL1983111		0.882353	199.53	*
graph	CHEMBL574738		0.733333	316.23	
pubchem	CHEMBL574738		0.896040	316.23	*
cdk_maccs	CHEMBL1979176		0.754717	15.85	
klekota_roth	CHEMBL1992581		0.450980	251.19	

*** ki ACTIVITY *** value prediction

based on 4 locally validated fgps ---> 287.055
["TT_bits", "MFP1", "substructure", "pubchem"]

25 rank

Dual specificity protein kinase CLK2 : Homo sapiens

score: 2.936 on ChEMBL4225 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581		0.615385	2511.89	
MFP1	CHEMBL574738		0.590909	3162.28	*
RDKit7	CHEMBL574738		0.602683	3162.28	
Pattern	CHEMBL1988838		0.828753	398.11	
AP_bits	CHEMBL1981410		0.506466	5011.87	
TT_bits	CHEMBL574738		0.567164	3162.28	*
FP2	CHEMBL574738		0.614458	3162.28	
hybridization	CHEMBL574738		0.504902	3162.28	
substructure	CHEMBL1983111		0.882353	630.96	*
graph	CHEMBL574738		0.733333	3162.28	
pubchem	CHEMBL574738		0.896040	3162.28	*
cdk_maccs	CHEMBL1979176		0.754717	1995.26	
klekota_roth	CHEMBL1992581		0.450980	2511.89	

*** ki ACTIVITY *** value prediction

based on 4 locally validated fgps ---> 2529.450
["TT_bits", "MFP1", "substructure", "pubchem"]

26 rank

Maternal embryonic leucine zipper kinase : Homo sapiens

score: 2.936 on ChEMBL4578 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL574738		0.558824	125.89	
MFP1	CHEMBL574738		0.590909	125.89	*
RDKit7	CHEMBL574738		0.602683	125.89	
Pattern	CHEMBL1988838		0.828753	1258.93	
AP_bits	CHEMBL1981410		0.506466	630.96	
TT_bits	CHEMBL574738		0.567164	125.89	*
FP2	CHEMBL574738		0.614458	125.89	
hybridization	CHEMBL574738		0.504902	125.89	
substructure	CHEMBL1983111		0.882353	199.53	*
graph	CHEMBL574738		0.733333	125.89	
pubchem	CHEMBL574738		0.896040	125.89	*

```

        cdk_maccs  CHEMBL2001239          0.672131      630.96
        klekota_roth CHEMBL1084546        0.388060       79.43
        *** ki ACTIVITY *** value prediction
        based on 4 locally validated fgps ---> 144.300
        ["TT_bits", "MFP1", "substructure", "pubchem"]

```

27 rank

Mitogen-activated protein kinase kinase kinase kinase 2 : Homo sapiens
score: 2.936 on CHEMBL5330 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581		0.615385	251.19	
MFP1	CHEMBL574738		0.590909	79.43	*
RDKit7	CHEMBL574738		0.602683	79.43	
Pattern	CHEMBL1988838		0.828753	398.11	
AP_bits	CHEMBL1981410		0.506466	1584.89	
TT_bits	CHEMBL574738		0.567164	79.43	*
FP2	CHEMBL574738		0.614458	79.43	
hybridization	CHEMBL574738		0.504902	79.43	
substructure	CHEMBL1983111		0.882353	39.81	*
graph	CHEMBL574738		0.733333	79.43	
pubchem	CHEMBL574738		0.896040	79.43	*
cdk_maccs	CHEMBL1979176		0.754717	3162.28	
klekota_roth	CHEMBL1992581		0.450980	251.19	

```

        *** ki ACTIVITY *** value prediction
        based on 4 locally validated fgps ---> 69.525
        ["TT_bits", "MFP1", "substructure", "pubchem"]

```

28 rank

Leukocyte tyrosine kinase receptor : Homo sapiens
score: 2.936 on CHEMBL5627 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581		0.615385	1995.26	
MFP1	CHEMBL574738		0.590909	630.96	*
RDKit7	CHEMBL574738		0.602683	630.96	
Pattern	CHEMBL574738		0.827381	630.96	
AP_bits	CHEMBL1965033		0.478571	794.33	
TT_bits	CHEMBL574738		0.567164	630.96	*
FP2	CHEMBL574738		0.614458	630.96	
hybridization	CHEMBL574738		0.504902	630.96	
substructure	CHEMBL1983111		0.882353	39.81	*
graph	CHEMBL574738		0.733333	630.96	
pubchem	CHEMBL574738		0.896040	630.96	*
cdk_maccs	CHEMBL574738		0.638889	630.96	
klekota_roth	CHEMBL1992581		0.450980	1995.26	

```

        *** ki ACTIVITY *** value prediction
        based on 4 locally validated fgps ---> 483.173
        ["TT_bits", "MFP1", "substructure", "pubchem"]

```

29 rank

Tyrosine-protein kinase FYN : Homo sapiens
score: 2.601 on CHEMBL1841 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1992581		0.615385	1584.89	
MFP1	CHEMBL574738		0.590909	158.49	*
RDKit7	CHEMBL574738		0.602683	158.49	
Pattern	CHEMBL1992306		0.855580	251.19	
AP_bits	CHEMBL1992306		0.546539	251.19	*
TT_bits	CHEMBL574738		0.567164	158.49	*
FP2	CHEMBL574738		0.614458	158.49	
hybridization	CHEMBL574738		0.504902	158.49	

substructure	CHEMBL1084546	0.764706	1995.26	
graph	CHEMBL574738	0.733333	158.49	
pubchem	CHEMBL574738	0.896040	158.49	*
cdk_maccs	CHEMBL1992306	0.740741	251.19	
klekota_roth	CHEMBL1973178	0.460000	79.43	

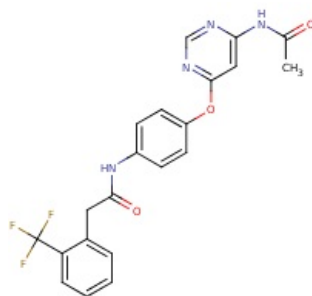
*** ki ACTIVITY *** value prediction
based on 4 locally validated fgps ---> 181.665
["AP_bits", "TT_bits", "MFP1", "pubchem"]

SwissTargetPrediction report:

Reference:

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

Query Molecule



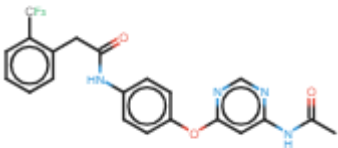
Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
Vascular endothelial growth factor receptor 1	P17948	FLT1	CHEMBL1868	<div><div></div></div>	287 / 90	Tyr Kinase
Vascular endothelial growth factor receptor 3	P35916	FLT4	CHEMBL1955	<div><div></div></div>	283 / 90	Tyr Kinase
Vascular endothelial growth factor receptor 2 (by homology)	P35968	KDR	CHEMBL279	<div><div></div></div>	283 / 90	Tyr Kinase
Macrophage colony-stimulating factor 1 receptor	P07333	CSF1R	CHEMBL1844	<div><div></div></div>	69 / 26	Tyr Kinase
Mast/stem cell growth factor receptor Kit	P10721	KIT	CHEMBL1936	<div><div></div></div>	69 / 26	Tyr Kinase
Receptor-type tyrosine-protein kinase FLT3	P36888	FLT3	CHEMBL1974	<div><div></div></div>	30 / 26	Tyr Kinase
Platelet-derived growth factor receptor beta	P09619	PDGFRB	CHEMBL1913	<div><div></div></div>	21 / 36	Tyr Kinase
Platelet-derived growth factor receptor alpha (by homology)	P16234	PDGFRA	CHEMBL2007	<div><div></div></div>	21 / 36	Tyr Kinase
Serine/threonine-protein kinase PLK1	P53350	PLK1	CHEMBL3024	<div><div></div></div>	60 / 1	Ser_Thr Kinase
Serine/threonine-protein kinase PLK3	Q9H4B4	PLK3	CHEMBL4897	<div><div></div></div>	60 / 1	Ser_Thr Kinase
Serine/threonine-protein kinase PLK2 (by homology)	Q9NYY3	PLK2	CHEMBL5938	<div><div></div></div>	60 / 1	Ser_Thr Kinase
RAF proto-oncogene serine/threonine-protein kinase	P04049	RAF1	CHEMBL1906	<div><div></div></div>	144 / 9	Ser_Thr_Tyr Kinase
Serine/threonine-protein kinase B-raf	P15056	BRAF	CHEMBL5145	<div><div></div></div>	144 / 9	Ser_Thr_Tyr Kinase
Serine/threonine-protein kinase A-Raf (by homology)	P10398	ARAF	CHEMBL1169596	<div><div></div></div>	144 / 9	Ser_Thr Kinase
Focal adhesion kinase 1	Q05397	PTK2	CHEMBL2695	<div><div></div></div>	44 / 2	Tyr Kinase

Polypharmacology Browser 2 Prediction:

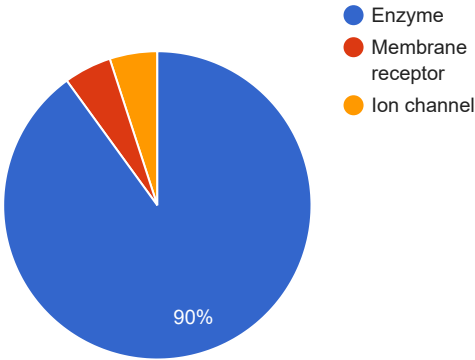
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL279 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL279)	Vascular endothelial growth factor receptor 2	Show NN
2	CHEMBL203 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL203)	Epidermal growth factor receptor erbB1	Show NN
3	CHEMBL2276 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2276)	c-Jun N-terminal kinase 1	Show NN
4	CHEMBL2637 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2637)	c-Jun N-terminal kinase 3	Show NN
5	CHEMBL1824 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1824)	Receptor protein-tyrosine kinase erbB-2	Show NN
6	CHEMBL1974 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1974)	Tyrosine-protein kinase receptor FLT3	Show NN
7	CHEMBL1844 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1844)	Macrophage colony stimulating factor receptor	Show NN
8	CHEMBL3717 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3717)	Hepatocyte growth factor receptor	Show NN
9	CHEMBL5102 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL5102)	Vanilloid receptor	Show NN
10	CHEMBL4722 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4722)	Serine/threonine-protein kinase Aurora-A	Show NN
11	CHEMBL258 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL258)	Tyrosine-protein kinase LCK	Show NN
12	CHEMBL260 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL260)	MAP kinase p38 alpha	Show NN
13	CHEMBL1868 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1868)	Vascular endothelial growth factor receptor 1	Show NN
14	CHEMBL256 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL256)	Adenosine A3 receptor	Show NN
15	CHEMBL267 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL267)	Tyrosine-protein kinase SRC	Show NN
16	CHEMBL1955 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1955)	Vascular endothelial growth factor receptor 3	Show NN
17	CHEMBL2815 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2815)	Nerve growth factor receptor Trk-A	Show NN
18	CHEMBL261 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL261)	Carbonic anhydrase I	Show NN

19	CHEMBL205 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL205)	Carbonic anhydrase II	Show NN
20	CHEMBL3229 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3229)	Anandamide amidohydrolase	Show NN