

MuSSEL Prediction k_i:

1 rank

Vascular endothelial growth factor receptor 3 : Homo sapiens

score: 7.106 on ChEMBL1955 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL939		0.750000	6309.57	*
MFP1	ChEMBL939		0.688889	6309.57	*
RDKit7	ChEMBL939		0.805133	6309.57	*
Pattern	ChEMBL124660		0.861301	3162.28	*
AP_bits	ChEMBL215152		0.516266	1258.93	
TT_bits	ChEMBL939		0.635135	6309.57	*
FP2	ChEMBL939		0.782313	6309.57	*
hybridization	ChEMBL939		0.816471	6309.57	*
substructure	ChEMBL1825138		0.818182	1584.89	
graph	ChEMBL939		0.777778	6309.57	
pubchem	ChEMBL939		0.925764	6309.57	*
cdk_maccs	ChEMBL939		0.840580	6309.57	*
klekota_roth	ChEMBL939		0.600000	6309.57	

*** ki ACTIVITY *** value prediction

based on 9 locally validated fgps ---> 5792.373

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

2 rank

Tyrosine-protein kinase LCK : Homo sapiens

score: 6.797 on ChEMBL258 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL939		0.750000	398.11	*
MFP1	ChEMBL939		0.688889	398.11	*
RDKit7	ChEMBL939		0.805133	398.11	*
Pattern	ChEMBL202721		0.856637	63.10	
AP_bits	ChEMBL202721		0.547865	63.10	*
TT_bits	ChEMBL939		0.635135	398.11	*
FP2	ChEMBL939		0.782313	398.11	*
hybridization	ChEMBL939		0.816471	398.11	*
substructure	ChEMBL230686		0.850000	29.40	
graph	ChEMBL939		0.777778	398.11	
pubchem	ChEMBL939		0.925764	398.11	*
cdk_maccs	ChEMBL24828		0.845070	39.81	*
klekota_roth	ChEMBL939		0.600000	398.11	

*** ki ACTIVITY *** value prediction

based on 9 locally validated fgps ---> 340.928

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

3 rank

Mitogen-activated protein kinase kinase kinase 5 : Homo sapiens

score: 6.797 on ChEMBL4852 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL939		0.750000	1584.89	*
MFP1	ChEMBL939		0.688889	1584.89	*
RDKit7	ChEMBL939		0.805133	1584.89	*
Pattern	ChEMBL202721		0.856637	31.62	
AP_bits	ChEMBL202721		0.547865	31.62	*
TT_bits	ChEMBL939		0.635135	1584.89	*
FP2	ChEMBL939		0.782313	1584.89	*
hybridization	ChEMBL939		0.816471	1584.89	*
substructure	ChEMBL95692		0.850000	1584.89	
graph	ChEMBL939		0.777778	1584.89	
pubchem	ChEMBL939		0.925764	1584.89	*
cdk_maccs	ChEMBL24828		0.845070	316.23	*

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    klekota_roth      CHEMBL939      0.600000    1584.89
    *** ki ACTIVITY *** value prediction
    based on 9 locally validated fgps ---> 1341.636
    ["TT_bits", "cdk_maccs", "AP_bits", "MFP1", "pubchem", "FP2", "FeatMFP1",
    "RDKit7", "hybridization"]

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4 rank

MAP kinase p38 alpha : Homo sapiens

score: 6.249 on ChEMBL260 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL939		0.750000	501.19		*
MFP1	CHEMBL939		0.688889	501.19		*
RDKit7	CHEMBL939		0.805133	501.19		*
Pattern	CHEMBL939		0.822785	501.19		
AP_bits	CHEMBL1256039		0.509091	885.00		
TT_bits	CHEMBL939		0.635135	501.19		*
FP2	CHEMBL939		0.782313	501.19		*
hybridization	CHEMBL939		0.816471	501.19		*
substructure	CHEMBL95692		0.850000	36.00		
graph	CHEMBL939		0.777778	501.19		
pubchem	CHEMBL939		0.925764	501.19		*
cdk_maccs	CHEMBL24828		0.845070	2511.89		*
klekota_roth	CHEMBL939		0.600000	501.19		

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    *** ki ACTIVITY *** value prediction
    based on 8 locally validated fgps ---> 627.194
    ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
    "hybridization"]

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5 rank

Tyrosine-protein kinase receptor UFO : Homo sapiens

score: 6.249 on ChEMBL4895 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL939		0.750000	1584.890		*
MFP1	CHEMBL939		0.688889	1584.890		*
RDKit7	CHEMBL939		0.805133	1584.890		*
Pattern	CHEMBL1983268		0.824959	39.810		
AP_bits	CHEMBL939		0.507317	1584.890		
TT_bits	CHEMBL939		0.635135	1584.890		*
FP2	CHEMBL939		0.782313	1584.890		*
hybridization	CHEMBL939		0.816471	1584.890		*
substructure	CHEMBL1825138		0.818182	5.012		
graph	CHEMBL939		0.777778	1584.890		
pubchem	CHEMBL939		0.925764	1584.890		*
cdk_maccs	CHEMBL24828		0.845070	251.190		*
klekota_roth	CHEMBL939		0.600000	1584.890		

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    *** ki ACTIVITY *** value prediction
    based on 8 locally validated fgps ---> 1501.312
    ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
    "hybridization"]

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6 rank

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

score: 6.249 on ChEMBL6166 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL939		0.750000	1000.00		*
MFP1	CHEMBL939		0.688889	1000.00		*
RDKit7	CHEMBL939		0.805133	1000.00		*
Pattern	CHEMBL1983268		0.824959	1995.26		
AP_bits	CHEMBL215152		0.516266	3162.28		
TT_bits	CHEMBL939		0.635135	1000.00		*

FP2	CHEMBL939	0.782313	1000.00	*
hybridization	CHEMBL939	0.816471	1000.00	*
substructure	CHEMBL95692	0.850000	794.33	
graph	CHEMBL939	0.777778	1000.00	
pubchem	CHEMBL939	0.925764	1000.00	*
cdk_maccs	CHEMBL24828	0.845070	158.49	*
klekota_roth	CHEMBL939	0.600000	1000.00	

*** ki ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 947.266
 ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
 "hybridization"]

7 rank

Homeodomain-interacting protein kinase 4 : Homo sapiens

score: 6.244 on CHEMBL1075167 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	1258.93	*
MFP1	CHEMBL939	0.688889	1258.93	*
RDKit7	CHEMBL939	0.805133	1258.93	*
Pattern	CHEMBL1968705	0.829787	5011.87	
AP_bits	CHEMBL939	0.507317	1258.93	
TT_bits	CHEMBL939	0.635135	1258.93	*
FP2	CHEMBL939	0.782313	1258.93	*
hybridization	CHEMBL939	0.816471	1258.93	*
substructure	CHEMBL939	0.750000	1258.93	
graph	CHEMBL939	0.777778	1258.93	
pubchem	CHEMBL939	0.925764	1258.93	*
cdk_maccs	CHEMBL939	0.840580	1258.93	*
klekota_roth	CHEMBL939	0.600000	1258.93	

*** ki ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 1258.930
 ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
 "hybridization"]

8 rank

Receptor protein-tyrosine kinase erbB-2 : Homo sapiens

score: 6.244 on CHEMBL1824 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	25.120	*
MFP1	CHEMBL939	0.688889	25.120	*
RDKit7	CHEMBL939	0.805133	25.120	*
Pattern	CHEMBL554	0.855025	1.585	
AP_bits	CHEMBL939	0.507317	25.120	
TT_bits	CHEMBL939	0.635135	25.120	*
FP2	CHEMBL939	0.782313	25.120	*
hybridization	CHEMBL939	0.816471	25.120	*
substructure	CHEMBL554	0.809524	1.585	
graph	CHEMBL939	0.777778	25.120	
pubchem	CHEMBL939	0.925764	25.120	*
cdk_maccs	CHEMBL939	0.840580	25.120	*
klekota_roth	CHEMBL939	0.600000	25.120	

*** ki ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 23.760
 ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
 "hybridization"]

9 rank

Epidermal growth factor receptor erbB1 : Homo sapiens

score: 6.244 on CHEMBL203 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	CHEMBL939	0.750000	0.40	*
MFP1	CHEMBL939	0.688889	0.40	*
RDKit7	CHEMBL939	0.805133	0.40	*
Pattern	CHEMBL1999749	0.825040	6.31	
AP_bits	CHEMBL215152	0.516266	501.19	
TT_bits	CHEMBL939	0.635135	0.40	*
FP2	CHEMBL939	0.782313	0.40	*
hybridization	CHEMBL939	0.816471	0.40	*
substructure	CHEMBL1682560	0.761905	8.00	
graph	CHEMBL939	0.777778	0.40	
pubchem	CHEMBL939	0.925764	0.40	*
cdk_maccs	CHEMBL939	0.840580	0.40	*
klekota_roth	CHEMBL939	0.600000	0.40	

*** ki ACTIVITY *** value prediction
based on 8 locally validated fgps ---> 0.400
["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7", "hybridization"]

10 rank

Serine/threonine-protein kinase PIM1 : Homo sapiens

score: 6.244 on ChEMBL2147 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	1995.26	*
MFP1	CHEMBL939	0.688889	1995.26	*
RDKit7	CHEMBL939	0.805133	1995.26	*
Pattern	CHEMBL939	0.822785	1995.26	
AP_bits	CHEMBL939	0.507317	1995.26	
TT_bits	CHEMBL939	0.635135	1995.26	*
FP2	CHEMBL939	0.782313	1995.26	*
hybridization	CHEMBL939	0.816471	1995.26	*
substructure	CHEMBL3634777	0.850000	3.40	
graph	CHEMBL939	0.777778	1995.26	
pubchem	CHEMBL939	0.925764	1995.26	*
cdk_maccs	CHEMBL939	0.840580	1995.26	*
klekota_roth	CHEMBL939	0.600000	1995.26	

*** ki ACTIVITY *** value prediction
based on 8 locally validated fgps ---> 1995.260
["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7", "hybridization"]

11 rank

Tyrosine-protein kinase BLK : Homo sapiens

score: 6.244 on ChEMBL2250 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	1000.00	*
MFP1	CHEMBL939	0.688889	1000.00	*
RDKit7	CHEMBL939	0.805133	1000.00	*
Pattern	CHEMBL1999749	0.825040	12.59	
AP_bits	CHEMBL215152	0.516266	630.96	
TT_bits	CHEMBL939	0.635135	1000.00	*
FP2	CHEMBL939	0.782313	1000.00	*
hybridization	CHEMBL939	0.816471	1000.00	*
substructure	CHEMBL1825138	0.818182	630.96	
graph	CHEMBL939	0.777778	1000.00	
pubchem	CHEMBL939	0.925764	1000.00	*
cdk_maccs	CHEMBL939	0.840580	1000.00	*
klekota_roth	CHEMBL939	0.600000	1000.00	

*** ki ACTIVITY *** value prediction
based on 8 locally validated fgps ---> 1000.000

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

12 rank

Phosphorylase kinase gamma subunit 2 : Homo sapiens

score: 6.244 on ChEMBL2349 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	ChEMBL939	0.750000	3162.28	*
MFP1	ChEMBL939	0.688889	3162.28	*
RDKit7	ChEMBL939	0.805133	3162.28	*
Pattern	ChEMBL1968705	0.829787	630.96	
AP_bits	ChEMBL939	0.507317	3162.28	
TT_bits	ChEMBL939	0.635135	3162.28	*
FP2	ChEMBL939	0.782313	3162.28	*
hybridization	ChEMBL939	0.816471	3162.28	*
substructure	ChEMBL1825138	0.818182	3162.28	
graph	ChEMBL939	0.777778	3162.28	
pubchem	ChEMBL939	0.925764	3162.28	*
cdk_maccs	ChEMBL939	0.840580	3162.28	*
klekota_roth	ChEMBL939	0.600000	3162.28	

*** ki ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 3162.280

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

13 rank

Serine/threonine-protein kinase Chk2 : Homo sapiens

score: 6.244 on ChEMBL2527 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	ChEMBL939	0.750000	630.96	*
MFP1	ChEMBL939	0.688889	630.96	*
RDKit7	ChEMBL939	0.805133	630.96	*
Pattern	ChEMBL1968705	0.829787	1000.00	
AP_bits	ChEMBL215152	0.516266	1995.26	
TT_bits	ChEMBL939	0.635135	630.96	*
FP2	ChEMBL939	0.782313	630.96	*
hybridization	ChEMBL939	0.816471	630.96	*
substructure	ChEMBL491473	0.772727	2511.89	
graph	ChEMBL939	0.777778	630.96	
pubchem	ChEMBL939	0.925764	630.96	*
cdk_maccs	ChEMBL939	0.840580	630.96	*
klekota_roth	ChEMBL939	0.600000	630.96	

*** ki ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 630.960

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

14 rank

Protein kinase C nu : Homo sapiens

score: 6.244 on ChEMBL2595 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	ChEMBL939	0.750000	1258.93	*
MFP1	ChEMBL939	0.688889	1258.93	*
RDKit7	ChEMBL939	0.805133	1258.93	*
Pattern	ChEMBL1968705	0.829787	1584.89	
AP_bits	ChEMBL939	0.507317	1258.93	
TT_bits	ChEMBL939	0.635135	1258.93	*
FP2	ChEMBL939	0.782313	1258.93	*
hybridization	ChEMBL939	0.816471	1258.93	*
substructure	ChEMBL95692	0.850000	3162.28	

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graph CHEMBL939 0.777778 1258.93
pubchem CHEMBL939 0.925764 1258.93 *
cdk_maccs CHEMBL939 0.840580 1258.93 *
klekota_roth CHEMBL939 0.600000 1258.93
*** ki ACTIVITY *** value prediction
based on 8 locally validated fgps ---> 1258.930
["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
"hybridization"]

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15 rank

c-Jun N-terminal kinase 3 : Homo sapiens

score: 6.244 on CHEMBL2637 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	794.33	*
MFP1	CHEMBL939	0.688889	794.33	*
RDKit7	CHEMBL939	0.805133	794.33	*
Pattern	CHEMBL939	0.822785	794.33	
AP_bits	CHEMBL939	0.507317	794.33	
TT_bits	CHEMBL939	0.635135	794.33	*
FP2	CHEMBL939	0.782313	794.33	*
hybridization	CHEMBL939	0.816471	794.33	*
substructure	CHEMBL939	0.750000	794.33	
graph	CHEMBL939	0.777778	794.33	
pubchem	CHEMBL939	0.925764	794.33	*
cdk_maccs	CHEMBL939	0.840580	794.33	*
klekota_roth	CHEMBL939	0.600000	794.33	

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*** ki ACTIVITY *** value prediction
based on 8 locally validated fgps ---> 794.330
["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
"hybridization"]

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16 rank

CaM kinase II delta : Homo sapiens

score: 6.244 on CHEMBL2801 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	2511.89	*
MFP1	CHEMBL939	0.688889	2511.89	*
RDKit7	CHEMBL939	0.805133	2511.89	*
Pattern	CHEMBL1968705	0.829787	1000.00	
AP_bits	CHEMBL939	0.507317	2511.89	
TT_bits	CHEMBL939	0.635135	2511.89	*
FP2	CHEMBL939	0.782313	2511.89	*
hybridization	CHEMBL939	0.816471	2511.89	*
substructure	CHEMBL1965702	0.800000	1995.26	
graph	CHEMBL939	0.777778	2511.89	
pubchem	CHEMBL939	0.925764	2511.89	*
cdk_maccs	CHEMBL939	0.840580	2511.89	*
klekota_roth	CHEMBL939	0.600000	2511.89	

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*** ki ACTIVITY *** value prediction
based on 8 locally validated fgps ---> 2511.890
["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
"hybridization"]

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17 rank

Casein kinase I delta : Homo sapiens

score: 6.244 on CHEMBL2828 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	7943.28	*
MFP1	CHEMBL939	0.688889	7943.28	*
RDKit7	CHEMBL939	0.805133	7943.28	*

Pattern	CHEMBL939	0.822785	7943.28	
AP_bits	CHEMBL215152	0.516266	5011.87	
TT_bits	CHEMBL939	0.635135	7943.28	*
FP2	CHEMBL939	0.782313	7943.28	*
hybridization	CHEMBL939	0.816471	7943.28	*
substructure	CHEMBL95692	0.850000	19.95	
graph	CHEMBL939	0.777778	7943.28	
pubchem	CHEMBL939	0.925764	7943.28	*
cdk_maccs	CHEMBL939	0.840580	7943.28	*
klekota_roth	CHEMBL939	0.600000	7943.28	

*** ki ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 7943.280
 ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
 "hybridization"]

18 rank

Receptor protein-tyrosine kinase erbB-4 : Homo sapiens

score: 6.244 on ChEMBL3009 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	158.49	*
MFP1	CHEMBL939	0.688889	158.49	*
RDKit7	CHEMBL939	0.805133	158.49	*
Pattern	CHEMBL554	0.855025	25.12	
AP_bits	CHEMBL215152	0.516266	199.53	
TT_bits	CHEMBL939	0.635135	158.49	*
FP2	CHEMBL939	0.782313	158.49	*
hybridization	CHEMBL939	0.816471	158.49	*
substructure	CHEMBL554	0.809524	25.12	
graph	CHEMBL939	0.777778	158.49	
pubchem	CHEMBL939	0.925764	158.49	*
cdk_maccs	CHEMBL939	0.840580	158.49	*
klekota_roth	CHEMBL939	0.600000	158.49	

*** ki ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 150.784
 ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
 "hybridization"]

19 rank

Tyrosine-protein kinase HCK : Homo sapiens

score: 6.244 on ChEMBL3234 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	2511.89	*
MFP1	CHEMBL939	0.688889	2511.89	*
RDKit7	CHEMBL939	0.805133	2511.89	*
Pattern	CHEMBL939	0.822785	2511.89	
AP_bits	CHEMBL939	0.507317	2511.89	
TT_bits	CHEMBL939	0.635135	2511.89	*
FP2	CHEMBL939	0.782313	2511.89	*
hybridization	CHEMBL939	0.816471	2511.89	*
substructure	CHEMBL939	0.750000	2511.89	
graph	CHEMBL939	0.777778	2511.89	
pubchem	CHEMBL939	0.925764	2511.89	*
cdk_maccs	CHEMBL939	0.840580	2511.89	*
klekota_roth	CHEMBL939	0.600000	2511.89	

*** ki ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 2511.890
 ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
 "hybridization"]

20 rank

Interleukin-1 receptor-associated kinase 1 : Homo sapiens

score: 6.244 on ChEMBL3357 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL939		0.750000	316.23		*
MFP1	CHEMBL939		0.688889	316.23		*
RDKit7	CHEMBL939		0.805133	316.23		*
Pattern	CHEMBL939		0.822785	316.23		
AP_bits	CHEMBL939		0.507317	316.23		
TT_bits	CHEMBL939		0.635135	316.23		*
FP2	CHEMBL939		0.782313	316.23		*
hybridization	CHEMBL939		0.816471	316.23		*
substructure	CHEMBL1825138		0.818182	199.53		
graph	CHEMBL939		0.777778	316.23		
pubchem	CHEMBL939		0.925764	316.23		*
cdk_maccs	CHEMBL939		0.840580	316.23		*
klekota_roth	CHEMBL939		0.600000	316.23		

*** ki ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 316.230

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

21 rank

Interleukin-1 receptor-associated kinase 4 : Homo sapiens

score: 6.244 on ChEMBL3778 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL939		0.750000	1000.00		*
MFP1	CHEMBL939		0.688889	1000.00		*
RDKit7	CHEMBL939		0.805133	1000.00		*
Pattern	CHEMBL939		0.822785	1000.00		
AP_bits	CHEMBL939		0.507317	1000.00		
TT_bits	CHEMBL939		0.635135	1000.00		*
FP2	CHEMBL939		0.782313	1000.00		*
hybridization	CHEMBL939		0.816471	1000.00		*
substructure	CHEMBL1996155		0.842105	3162.28		
graph	CHEMBL939		0.777778	1000.00		
pubchem	CHEMBL939		0.925764	1000.00		*
cdk_maccs	CHEMBL939		0.840580	1000.00		*
klekota_roth	CHEMBL939		0.600000	1000.00		

*** ki ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 1000.000

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

22 rank

CaM kinase II gamma : Homo sapiens

score: 6.244 on ChEMBL3829 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL939		0.750000	3162.28		*
MFP1	CHEMBL939		0.688889	3162.28		*
RDKit7	CHEMBL939		0.805133	3162.28		*
Pattern	CHEMBL1968705		0.829787	3162.28		
AP_bits	CHEMBL939		0.507317	3162.28		
TT_bits	CHEMBL939		0.635135	3162.28		*
FP2	CHEMBL939		0.782313	3162.28		*
hybridization	CHEMBL939		0.816471	3162.28		*
substructure	CHEMBL939		0.750000	3162.28		
graph	CHEMBL939		0.777778	3162.28		
pubchem	CHEMBL939		0.925764	3162.28		*
cdk_maccs	CHEMBL939		0.840580	3162.28		*
klekota_roth	CHEMBL939		0.600000	3162.28		

*** ki ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 3162.280
 ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
 "hybridization"]

23 rank

LIM domain kinase 1 : Homo sapiens

score: 6.244 on ChEMBL3836 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL939		0.750000	3981.07		*
MFP1	ChEMBL939		0.688889	3981.07		*
RDKit7	ChEMBL939		0.805133	3981.07		*
Pattern	ChEMBL939		0.822785	3981.07		
AP_bits	ChEMBL939		0.507317	3981.07		
TT_bits	ChEMBL939		0.635135	3981.07		*
FP2	ChEMBL939		0.782313	3981.07		*
hybridization	ChEMBL939		0.816471	3981.07		*
substructure	ChEMBL1996155		0.842105	5011.87		
graph	ChEMBL939		0.777778	3981.07		
pubchem	ChEMBL939		0.925764	3981.07		*
cdk_maccs	ChEMBL939		0.840580	3981.07		*
klekota_roth	ChEMBL939		0.600000	3981.07		

*** ki ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 3981.070
 ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
 "hybridization"]

24 rank

Tyrosine-protein kinase Lyn : Homo sapiens

score: 6.244 on ChEMBL3905 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL939		0.750000	158.49		*
MFP1	ChEMBL939		0.688889	158.49		*
RDKit7	ChEMBL939		0.805133	158.49		*
Pattern	ChEMBL1999749		0.825040	63.10		
AP_bits	ChEMBL215152		0.516266	1000.00		
TT_bits	ChEMBL939		0.635135	158.49		*
FP2	ChEMBL939		0.782313	158.49		*
hybridization	ChEMBL939		0.816471	158.49		*
substructure	ChEMBL230686		0.850000	25.90		
graph	ChEMBL939		0.777778	158.49		
pubchem	ChEMBL939		0.925764	158.49		*
cdk_maccs	ChEMBL939		0.840580	158.49		*
klekota_roth	ChEMBL939		0.600000	158.49		

*** ki ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 158.490
 ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
 "hybridization"]

25 rank

c-Jun N-terminal kinase 2 : Homo sapiens

score: 6.244 on ChEMBL4179 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL939		0.750000	2511.89		*
MFP1	ChEMBL939		0.688889	2511.89		*
RDKit7	ChEMBL939		0.805133	2511.89		*
Pattern	ChEMBL939		0.822785	2511.89		
AP_bits	ChEMBL939		0.507317	2511.89		
TT_bits	ChEMBL939		0.635135	2511.89		*
FP2	ChEMBL939		0.782313	2511.89		*

hybridization	CHEMBL939	0.816471	2511.89	*
substructure	CHEMBL101311	0.761905	1584.89	
graph	CHEMBL939	0.777778	2511.89	
pubchem	CHEMBL939	0.925764	2511.89	*
cdk_maccs	CHEMBL939	0.840580	2511.89	*
klekota_roth	CHEMBL939	0.600000	2511.89	

*** ki ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 2511.890
 ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
 "hybridization"]

26 rank

Serine/threonine-protein kinase 2 : Homo sapiens

score: 6.244 on ChEMBL4202 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	398.11		*
MFP1	CHEMBL939	0.688889	398.11		*
RDKit7	CHEMBL939	0.805133	398.11		*
Pattern	CHEMBL1968705	0.829787	6309.57		
AP_bits	CHEMBL939	0.507317	398.11		
TT_bits	CHEMBL939	0.635135	398.11		*
FP2	CHEMBL939	0.782313	398.11		*
hybridization	CHEMBL939	0.816471	398.11		*
substructure	CHEMBL1825138	0.818182	31.62		
graph	CHEMBL939	0.777778	398.11		
pubchem	CHEMBL939	0.925764	398.11		*
cdk_maccs	CHEMBL939	0.840580	398.11		*
klekota_roth	CHEMBL939	0.600000	398.11		

*** ki ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 398.110
 ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
 "hybridization"]

27 rank

MAP kinase signal-integrating kinase 2 : Homo sapiens

score: 6.244 on ChEMBL4204 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	398.11		*
MFP1	CHEMBL939	0.688889	398.11		*
RDKit7	CHEMBL939	0.805133	398.11		*
Pattern	CHEMBL1968705	0.829787	7943.28		
AP_bits	CHEMBL939	0.507317	398.11		
TT_bits	CHEMBL939	0.635135	398.11		*
FP2	CHEMBL939	0.782313	398.11		*
hybridization	CHEMBL939	0.816471	398.11		*
substructure	CHEMBL939	0.750000	398.11		
graph	CHEMBL939	0.777778	398.11		
pubchem	CHEMBL939	0.925764	398.11		*
cdk_maccs	CHEMBL939	0.840580	398.11		*
klekota_roth	CHEMBL939	0.600000	398.11		

*** ki ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 398.110
 ["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
 "hybridization"]

28 rank

Tyrosine-protein kinase FRK : Homo sapiens

score: 6.244 on ChEMBL4223 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	251.19		*

MFP1	CHEMBL939	0.688889	251.19	*
RDKit7	CHEMBL939	0.805133	251.19	*
Pattern	CHEMBL1973961	0.826014	1258.93	
AP_bits	CHEMBL939	0.507317	251.19	
TT_bits	CHEMBL939	0.635135	251.19	*
FP2	CHEMBL939	0.782313	251.19	*
hybridization	CHEMBL939	0.816471	251.19	*
substructure	CHEMBL1825138	0.818182	199.53	
graph	CHEMBL939	0.777778	251.19	
pubchem	CHEMBL939	0.925764	251.19	*
cdk_maccs	CHEMBL939	0.840580	251.19	*
klekota_roth	CHEMBL939	0.600000	251.19	

*** ki ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 251.190

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

29 rank

Serine/threonine-protein kinase D2 : Homo sapiens

score: 6.244 on ChEMBL4900 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939		0.750000	2511.89	*
MFP1	CHEMBL939		0.688889	2511.89	*
RDKit7	CHEMBL939		0.805133	2511.89	*
Pattern	CHEMBL1968705		0.829787	7943.28	
AP_bits	CHEMBL939		0.507317	2511.89	
TT_bits	CHEMBL939		0.635135	2511.89	*
FP2	CHEMBL939		0.782313	2511.89	*
hybridization	CHEMBL939		0.816471	2511.89	*
substructure	CHEMBL1996155		0.842105	398.11	
graph	CHEMBL939		0.777778	2511.89	
pubchem	CHEMBL939		0.925764	2511.89	*
cdk_maccs	CHEMBL939		0.840580	2511.89	*
klekota_roth	CHEMBL939		0.600000	2511.89	

*** ki ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 2511.890

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

30 rank

Serine/threonine-protein kinase PIM3 : Homo sapiens

score: 6.244 on ChEMBL5407 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939		0.750000	1258.93	*
MFP1	CHEMBL939		0.688889	1258.93	*
RDKit7	CHEMBL939		0.805133	1258.93	*
Pattern	CHEMBL1968705		0.829787	3981.07	
AP_bits	CHEMBL939		0.507317	1258.93	
TT_bits	CHEMBL939		0.635135	1258.93	*
FP2	CHEMBL939		0.782313	1258.93	*
hybridization	CHEMBL939		0.816471	1258.93	*
substructure	CHEMBL3634777		0.850000	0.11	
graph	CHEMBL939		0.777778	1258.93	
pubchem	CHEMBL939		0.925764	1258.93	*
cdk_maccs	CHEMBL939		0.840580	1258.93	*
klekota_roth	CHEMBL939		0.600000	1258.93	

*** ki ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 1258.930

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

31 rank

Misshapen-like kinase 1 : Homo sapiens

score: 6.244 on ChEMBL5518 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939		0.750000	5011.87	*
MFP1	CHEMBL939		0.688889	5011.87	*
RDKit7	CHEMBL939		0.805133	5011.87	*
Pattern	CHEMBL939		0.822785	5011.87	
AP_bits	CHEMBL939		0.507317	5011.87	
TT_bits	CHEMBL939		0.635135	5011.87	*
FP2	CHEMBL939		0.782313	5011.87	*
hybridization	CHEMBL939		0.816471	5011.87	*
substructure	CHEMBL95692		0.850000	3981.07	
graph	CHEMBL939		0.777778	5011.87	
pubchem	CHEMBL939		0.925764	5011.87	*
cdk_maccs	CHEMBL939		0.840580	5011.87	*
klekota_roth	CHEMBL939		0.600000	5011.87	

*** ki ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 5011.870

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

32 rank

BR serine/threonine-protein kinase 1 : Homo sapiens

score: 6.244 on ChEMBL5650 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939		0.750000	3162.28	*
MFP1	CHEMBL939		0.688889	3162.28	*
RDKit7	CHEMBL939		0.805133	3162.28	*
Pattern	CHEMBL939		0.822785	3162.28	
AP_bits	CHEMBL939		0.507317	3162.28	
TT_bits	CHEMBL939		0.635135	3162.28	*
FP2	CHEMBL939		0.782313	3162.28	*
hybridization	CHEMBL939		0.816471	3162.28	*
substructure	CHEMBL939		0.750000	3162.28	
graph	CHEMBL939		0.777778	3162.28	
pubchem	CHEMBL939		0.925764	3162.28	*
cdk_maccs	CHEMBL939		0.840580	3162.28	*
klekota_roth	CHEMBL939		0.600000	3162.28	

*** ki ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 3162.280

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

33 rank

Serine/threonine-protein kinase SIK2 : Homo sapiens

score: 6.244 on ChEMBL5699 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939		0.750000	316.23	*
MFP1	CHEMBL939		0.688889	316.23	*
RDKit7	CHEMBL939		0.805133	316.23	*
Pattern	CHEMBL939		0.822785	316.23	
AP_bits	CHEMBL939		0.507317	316.23	
TT_bits	CHEMBL939		0.635135	316.23	*
FP2	CHEMBL939		0.782313	316.23	*
hybridization	CHEMBL939		0.816471	316.23	*
substructure	CHEMBL939		0.750000	316.23	
graph	CHEMBL939		0.777778	316.23	
pubchem	CHEMBL939		0.925764	316.23	*

```

    cdk_maccs CHEMBL939          0.840580    316.23      *
    klekota_roth CHEMBL939        0.600000    316.23
    *** ki ACTIVITY *** value prediction
    based on 8 locally validated fgps ---> 316.230
["TT_bits", "cdk_maccs", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7",
"hybridization"]

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34 rank

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

score: 3.640 on ChEMBL2185 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL24828		0.676471	2511.89	
MFP1	CHEMBL202721		0.540000	79.43	
RDKit7	CHEMBL202721		0.717813	79.43	
Pattern	CHEMBL386310		0.875415	1.00	*
AP_bits	CHEMBL386310		0.608054	1.00	*
TT_bits	CHEMBL217804		0.609756	2.00	*
FP2	CHEMBL202721		0.619048	79.43	
hybridization	CHEMBL554		0.701826	1995.26	*
substructure	CHEMBL1825138		0.818182	39.81	
graph	CHEMBL24828		0.668293	2511.89	
pubchem	CHEMBL24828		0.848739	2511.89	
cdk_maccs	CHEMBL24828		0.845070	2511.89	*
klekota_roth	CHEMBL491473		0.585366	1258.93	

*** ki ACTIVITY *** value prediction

based on 5 locally validated fgps ---> 902.132

["Pattern", "hybridization", "TT_bits", "cdk_maccs", "AP_bits"]

35 rank

Platelet-derived growth factor receptor alpha : Homo sapiens

score: 3.105 on ChEMBL2007 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL24828		0.676471	158.49	
MFP1	CHEMBL202721		0.540000	398.11	
RDKit7	CHEMBL202721		0.717813	398.11	
Pattern	CHEMBL124660		0.861301	63.10	*
AP_bits	CHEMBL202721		0.547865	398.11	*
TT_bits	CHEMBL202721		0.529412	398.11	
FP2	CHEMBL202721		0.619048	398.11	
hybridization	CHEMBL202721		0.685714	398.11	
substructure	CHEMBL24828		0.809524	158.49	
graph	CHEMBL24828		0.668293	158.49	
pubchem	CHEMBL124660		0.851064	63.10	*
cdk_maccs	CHEMBL24828		0.845070	158.49	*
klekota_roth	CHEMBL491473		0.585366	10.00	

*** ki ACTIVITY *** value prediction

based on 4 locally validated fgps ---> 170.700

["Pattern", "cdk_maccs", "pubchem", "AP_bits"]

MuSSEL Prediction IC₅₀:

1 rank

Epidermal growth factor receptor erbB1 : Homo sapiens

score: 10.901 on ChEMBL203 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL56936		0.812500	2.00	*
MFP1	CHEMBL939		0.688889	0.10	*
RDKit7	CHEMBL598799		0.915222	9.08	*
Pattern	CHEMBL598799		0.926786	9.08	*
AP_bits	CHEMBL598799		0.675595	9.08	*
TT_bits	CHEMBL598799		0.760000	9.08	*
FP2	CHEMBL2334003		0.855072	13.60	*
hybridization	CHEMBL598799		0.841871	9.08	*
substructure	CHEMBL247709		0.950000	48.00	*
graph	CHEMBL3355883		0.911917	38.30	*
pubchem	CHEMBL2334003		0.950893	13.60	*
cdk_maccs	CHEMBL291514		0.911765	79.00	*
klekota_roth	CHEMBL247709		0.700000	48.00	*

*** ic50 ACTIVITY *** value prediction

based on 13 locally validated fgps ---> 58.254

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

2 rank

Receptor protein-tyrosine kinase erbB-2 : Homo sapiens

score: 10.719 on ChEMBL1824 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3814812		0.777778	12.1	*
MFP1	CHEMBL939		0.688889	240.0	*
RDKit7	CHEMBL598799		0.915222	10.1	*
Pattern	CHEMBL598799		0.926786	10.1	*
AP_bits	CHEMBL598799		0.675595	10.1	*
TT_bits	CHEMBL598799		0.760000	10.1	*
FP2	CHEMBL197640		0.836735	2.0	*
hybridization	CHEMBL598799		0.841871	10.1	*
substructure	CHEMBL247709		0.950000	41.0	*
graph	CHEMBL2408050		0.835897	264.0	*
pubchem	CHEMBL939		0.925764	240.0	*
cdk_maccs	CHEMBL197640		0.884058	2.0	*
klekota_roth	CHEMBL247709		0.700000	41.0	*

*** ic50 ACTIVITY *** value prediction

based on 13 locally validated fgps ---> 125.194

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

3 rank

Vascular endothelial growth factor receptor 2 : Homo sapiens

score: 10.262 on ChEMBL279 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1202477		0.787879	9.0	*
MFP1	CHEMBL939		0.688889	1900.0	*
RDKit7	CHEMBL939		0.805133	1900.0	*
Pattern	CHEMBL3758749		0.898067	1810.0	*
AP_bits	CHEMBL3133754		0.603198	8568.0	*
TT_bits	CHEMBL169797		0.643836	1110.0	*
FP2	CHEMBL1744347		0.787671	20.0	*
hybridization	CHEMBL939		0.816471	1900.0	*
substructure	CHEMBL147180		0.947368	40.0	*
graph	CHEMBL3706823		0.782609	1.0	*

```

        pubchem  CHEMBL1744347          0.934211      20.0      *
        cdk_maccs CHEMBL1744347          0.900000      20.0      *
        klekota_roth CHEMBL2448067        0.666667      30.0      *
        *** ic50 ACTIVITY *** value prediction
        based on 13 locally validated fgps ---> 1332.325
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

```

4 rank

Tyrosine-protein kinase SRC : Homo sapiens

score: 10.050 on CHEMBL267 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL128158	0.764706	1.1	*
MFP1	CHEMBL939	0.688889	1100.0	*
RDKit7	CHEMBL939	0.805133	1100.0	*
Pattern	CHEMBL426148	0.879581	600.0	*
AP_bits	CHEMBL201307	0.572005	3000.0	*
TT_bits	CHEMBL169797	0.643836	37.0	*
FP2	CHEMBL939	0.782313	1100.0	*
hybridization	CHEMBL939	0.816471	1100.0	*
substructure	CHEMBL217977	0.894737	540.0	*
graph	CHEMBL939	0.777778	1100.0	*
pubchem	CHEMBL939	0.925764	1100.0	*
cdk_maccs	CHEMBL128158	0.898551	1.1	*
klekota_roth	CHEMBL939	0.600000	1100.0	*

```

        *** ic50 ACTIVITY *** value prediction
        based on 13 locally validated fgps ---> 701.377
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

```

5 rank

Tyrosine-protein kinase receptor RET : Homo sapiens

score: 10.028 on CHEMBL2041 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL3797261	0.800000	5.0	*
MFP1	CHEMBL939	0.688889	1700.0	*
RDKit7	CHEMBL939	0.805133	1700.0	*
Pattern	CHEMBL3800348	0.855615	29.0	*
AP_bits	CHEMBL939	0.507317	1700.0	*
TT_bits	CHEMBL939	0.635135	1700.0	*
FP2	CHEMBL939	0.782313	1700.0	*
hybridization	CHEMBL939	0.816471	1700.0	*
substructure	CHEMBL3797261	0.857143	5.0	*
graph	CHEMBL939	0.777778	1700.0	*
pubchem	CHEMBL939	0.925764	1700.0	*
cdk_maccs	CHEMBL3797261	0.914286	5.0	*
klekota_roth	CHEMBL3799971	0.662338	11.0	*

```

        *** ic50 ACTIVITY *** value prediction
        based on 13 locally validated fgps ---> 740.419
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

```

6 rank

Receptor protein-tyrosine kinase erbB-4 : Homo sapiens

score: 9.883 on CHEMBL3009 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	476.0	*

MFP1	CHEMBL939	0.688889	476.0	*
RDKit7	CHEMBL939	0.805133	476.0	*
Pattern	CHEMBL3680375	0.891753	61.5	*
AP_bits	CHEMBL1645462	0.519411	190.0	*
TT_bits	CHEMBL939	0.635135	476.0	*
FP2	CHEMBL939	0.782313	476.0	*
hybridization	CHEMBL939	0.816471	476.0	*
substructure	CHEMBL3828092	0.850000	1603.0	*
graph	CHEMBL939	0.777778	476.0	*
pubchem	CHEMBL939	0.925764	476.0	*
cdk_maccs	CHEMBL939	0.840580	476.0	*
klekota_roth	CHEMBL939	0.600000	476.0	*

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 352.929

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

7 rank

Vascular endothelial growth factor receptor 1 : Homo sapiens

score: 9.188 on ChEMBL1868 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1202477	0.787879	550.0	*	
MFP1	CHEMBL24137	0.617021	200.0	*	
RDKit7	CHEMBL1744347	0.792329	600.0	*	
Pattern	CHEMBL2448066	0.872302	20.0	*	
AP_bits	CHEMBL453737	0.538462	45.0	*	
TT_bits	CHEMBL2448067	0.586667	200.0	*	
FP2	CHEMBL1744347	0.787671	600.0	*	
hybridization	CHEMBL1744347	0.757506	600.0	*	
substructure	CHEMBL147180	0.947368	300.0	*	
graph	CHEMBL1744347	0.766497	600.0	*	
pubchem	CHEMBL1744347	0.934211	600.0	*	
cdk_maccs	CHEMBL1744347	0.900000	600.0	*	
klekota_roth	CHEMBL2448067	0.666667	200.0	*	

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 426.218

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

8 rank

Fibroblast growth factor receptor 1 : Homo sapiens

score: 9.165 on ChEMBL3650 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1202477	0.787879	2000.0	*	
MFP1	CHEMBL24137	0.617021	6700.0	*	
RDKit7	CHEMBL1744347	0.792329	2100.0	*	
Pattern	CHEMBL2448066	0.872302	900.0	*	
AP_bits	CHEMBL3691340	0.515843	11.5	*	
TT_bits	CHEMBL2419762	0.586667	63.0	*	
FP2	CHEMBL1744347	0.787671	2100.0	*	
hybridization	CHEMBL1744347	0.757506	2100.0	*	
substructure	CHEMBL147180	0.947368	9400.0	*	
graph	CHEMBL1744347	0.766497	2100.0	*	
pubchem	CHEMBL1744347	0.934211	2100.0	*	
cdk_maccs	CHEMBL1744347	0.900000	2100.0	*	
klekota_roth	CHEMBL2448067	0.666667	4200.0	*	

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 4262.451

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

9 rank

Serine/threonine-protein kinase B-raf : Homo sapiens

score: 9.154 on ChEMBL5145 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939		0.750000	30000.0	*
MFP1	CHEMBL939		0.688889	30000.0	*
RDKit7	CHEMBL939		0.805133	30000.0	*
Pattern	CHEMBL3133753		0.912892	31.0	*
AP_bits	CHEMBL3133753		0.618911	31.0	*
TT_bits	CHEMBL939		0.635135	30000.0	*
FP2	CHEMBL939		0.782313	30000.0	*
hybridization	CHEMBL939		0.816471	30000.0	*
substructure	CHEMBL1079785		0.809524	8.7	
graph	CHEMBL939		0.777778	30000.0	*
pubchem	CHEMBL939		0.925764	30000.0	*
cdk_maccs	CHEMBL939		0.840580	30000.0	*
klekota_roth	CHEMBL939		0.600000	30000.0	*

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 16597.534

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

10 rank

Ephrin type-B receptor 4 : Homo sapiens

score: 9.036 on ChEMBL5147 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939		0.750000	1000.0	*
MFP1	CHEMBL939		0.688889	1000.0	*
RDKit7	CHEMBL939		0.805133	1000.0	*
Pattern	CHEMBL288441		0.823430	5.5	
AP_bits	CHEMBL939		0.507317	1000.0	*
TT_bits	CHEMBL939		0.635135	1000.0	*
FP2	CHEMBL939		0.782313	1000.0	*
hybridization	CHEMBL939		0.816471	1000.0	*
substructure	CHEMBL3544983		0.900000	50.0	*
graph	CHEMBL939		0.777778	1000.0	*
pubchem	CHEMBL939		0.925764	1000.0	*
cdk_maccs	CHEMBL288441		0.847222	5.5	*
klekota_roth	CHEMBL939		0.600000	1000.0	*

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 704.900

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

11 rank

Tyrosine-protein kinase ABL : Homo sapiens

score: 9.022 on ChEMBL1862 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939		0.750000	1200.0	*
MFP1	CHEMBL939		0.688889	1200.0	*
RDKit7	CHEMBL939		0.805133	1200.0	*
Pattern	CHEMBL1630109		0.886010	5300.0	*
AP_bits	CHEMBL939		0.507317	1200.0	*
TT_bits	CHEMBL939		0.635135	1200.0	*
FP2	CHEMBL939		0.782313	1200.0	*

hybridization	CHEMBL939	0.816471	1200.0	*
substructure	CHEMBL601719	0.818182	24.0	
graph	CHEMBL939	0.777778	1200.0	*
pubchem	CHEMBL939	0.925764	1200.0	*
cdk_maccs	CHEMBL288441	0.847222	0.5	*
klekota_roth	CHEMBL939	0.600000	1200.0	*

*** ic50 ACTIVITY *** value prediction
based on 12 locally validated fgps ---> 1769.360
["TT_bits", "cdk_maccs", "Pattern", "FP2", "MFP1", "klekota_roth",
"pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7", "hybridization"]

12 rank

Tyrosine kinase non-receptor protein 2 : Homo sapiens

score: 8.986 on ChEMBL4599 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939		0.750000	2300.0	*
MFP1	CHEMBL939		0.688889	2300.0	*
RDKit7	CHEMBL939		0.805133	2300.0	*
Pattern	CHEMBL1983268		0.824959	70.0	
AP_bits	CHEMBL939		0.507317	2300.0	*
TT_bits	CHEMBL939		0.635135	2300.0	*
FP2	CHEMBL939		0.782313	2300.0	*
hybridization	CHEMBL939		0.816471	2300.0	*
substructure	CHEMBL247468		0.850000	98.0	*
graph	CHEMBL939		0.777778	2300.0	*
pubchem	CHEMBL939		0.925764	2300.0	*
cdk_maccs	CHEMBL288441		0.847222	2.7	*
klekota_roth	CHEMBL939		0.600000	2300.0	*

*** ic50 ACTIVITY *** value prediction
based on 11 locally validated fgps ---> 1919.949
["TT_bits", "cdk_maccs", "AP_bits", "MFP1", "klekota_roth", "pubchem",
"graph", "FP2", "FeatMFP1", "RDKit7", "hybridization"]

13 rank

ATP-binding cassette sub-family G member 2 : Homo sapiens

score: 8.986 on ChEMBL5393 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL939		0.750000	400.0	*
MFP1	CHEMBL939		0.688889	400.0	*
RDKit7	CHEMBL939		0.805133	400.0	*
Pattern	CHEMBL3809832		0.856373	1710.0	*
AP_bits	CHEMBL939		0.507317	400.0	*
TT_bits	CHEMBL939		0.635135	400.0	*
FP2	CHEMBL939		0.782313	400.0	*
hybridization	CHEMBL939		0.816471	400.0	*
substructure	CHEMBL939		0.750000	400.0	
graph	CHEMBL939		0.777778	400.0	*
pubchem	CHEMBL939		0.925764	400.0	*
cdk_maccs	CHEMBL939		0.840580	400.0	*
klekota_roth	CHEMBL939		0.600000	400.0	*

*** ic50 ACTIVITY *** value prediction
based on 12 locally validated fgps ---> 4402.171
["TT_bits", "cdk_maccs", "Pattern", "FP2", "MFP1", "klekota_roth",
"pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7", "hybridization"]

14 rank

Platelet-derived growth factor receptor beta : Homo sapiens

score: 8.899 on ChEMBL1913 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL593274		0.742857	3600.0	*

MFP1	CHEMBL593274	0.588235	3600.0	*
RDKit7	CHEMBL301018	0.750727	3000.0	*
Pattern	CHEMBL1630109	0.886010	2500.0	*
AP_bits	CHEMBL604893	0.609078	7700.0	*
TT_bits	CHEMBL1630109	0.587500	2500.0	*
FP2	CHEMBL301018	0.710145	3000.0	*
hybridization	CHEMBL1630113	0.747788	3900.0	*
substructure	CHEMBL593909	0.900000	9200.0	*
graph	CHEMBL1630113	0.734694	3900.0	*
pubchem	CHEMBL301018	0.910714	3000.0	*
cdk_maccs	CHEMBL24828	0.845070	477.0	*
klekota_roth	CHEMBL593909	0.620690	9200.0	*

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 4335.226

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

15 rank

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

score: 8.875 on ChEMBL4722 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL593274		0.742857	27.00		*
MFP1	CHEMBL593274		0.588235	27.00		*
RDKit7	CHEMBL301018		0.750727	6500.00		*
Pattern	CHEMBL382667		0.880750	0.15		*
AP_bits	CHEMBL604893		0.609078	690.00		*
TT_bits	CHEMBL217804		0.609756	220.00		*
FP2	CHEMBL301018		0.710145	6500.00		*
hybridization	CHEMBL604893		0.700787	690.00		*
substructure	CHEMBL593909		0.900000	85.00		*
graph	CHEMBL301018		0.713514	6500.00		*
pubchem	CHEMBL301018		0.910714	6500.00		*
cdk_maccs	CHEMBL203945		0.851351	0.80		*
klekota_roth	CHEMBL593909		0.620690	85.00		*

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 4089.889

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

16 rank

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

score: 8.835 on ChEMBL2185 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL593274		0.742857	78.0		*
MFP1	CHEMBL593274		0.588235	78.0		*
RDKit7	CHEMBL301018		0.750727	7400.0		*
Pattern	CHEMBL3685239		0.873684	6.5		*
AP_bits	CHEMBL604893		0.609078	4800.0		*
TT_bits	CHEMBL217804		0.609756	2.0		*
FP2	CHEMBL301018		0.710145	7400.0		*
hybridization	CHEMBL604893		0.700787	4800.0		*
substructure	CHEMBL593909		0.900000	90.0		*
graph	CHEMBL301018		0.713514	7400.0		*
pubchem	CHEMBL301018		0.910714	7400.0		*
cdk_maccs	CHEMBL593909		0.818182	90.0		*
klekota_roth	CHEMBL593909		0.620690	90.0		*

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 1930.037

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

17 rank

Vascular endothelial growth factor receptor 3 : Homo sapiens

score: 8.714 on ChEMBL1955 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL593274	0.742857	470.0	*
MFP1	CHEMBL593274	0.588235	470.0	*
RDKit7	CHEMBL301018	0.750727	2400.0	*
Pattern	CHEMBL1934327	0.851590	9.6	*
AP_bits	CHEMBL593274	0.569602	470.0	*
TT_bits	CHEMBL301018	0.541667	2400.0	*
FP2	CHEMBL301018	0.710145	2400.0	*
hybridization	CHEMBL593274	0.682879	470.0	*
substructure	CHEMBL593909	0.900000	3000.0	*
graph	CHEMBL301018	0.713514	2400.0	*
pubchem	CHEMBL301018	0.910714	2400.0	*
cdk_maccs	CHEMBL24828	0.845070	233.0	*
klekota_roth	CHEMBL593909	0.620690	3000.0	*

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 1711.813

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

18 rank

Tyrosine-protein kinase HCK : Homo sapiens

score: 8.136 on ChEMBL3234 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	110.0	*
MFP1	CHEMBL939	0.688889	110.0	*
RDKit7	CHEMBL939	0.805133	110.0	*
Pattern	CHEMBL288441	0.823430	3.2	*
AP_bits	CHEMBL939	0.507317	110.0	*
TT_bits	CHEMBL939	0.635135	110.0	*
FP2	CHEMBL939	0.782313	110.0	*
hybridization	CHEMBL939	0.816471	110.0	*
substructure	CHEMBL288441	0.772727	3.2	*
graph	CHEMBL939	0.777778	110.0	*
pubchem	CHEMBL939	0.925764	110.0	*
cdk_maccs	CHEMBL288441	0.847222	3.2	*
klekota_roth	CHEMBL939	0.600000	110.0	*

*** ic50 ACTIVITY *** value prediction

based on 11 locally validated fgps ---> 180.410

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

19 rank

Cruzipain : Trypanosoma cruzi

score: 8.129 on ChEMBL3563 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL939	0.750000	88000.0	*
MFP1	CHEMBL939	0.688889	88000.0	*
RDKit7	CHEMBL939	0.805133	88000.0	*
Pattern	CHEMBL939	0.822785	88000.0	*
AP_bits	CHEMBL939	0.507317	88000.0	*
TT_bits	CHEMBL939	0.635135	88000.0	*
FP2	CHEMBL939	0.782313	88000.0	*

```

hybridization CHEMBL939          0.816471  88000.0      *
substructure  CHEMBL939          0.750000  88000.0
graph         CHEMBL939          0.777778  88000.0      *
pubchem       CHEMBL939          0.925764  88000.0      *
cdk_maccs     CHEMBL939          0.840580  88000.0      *
klekota_roth  CHEMBL939          0.600000  88000.0      *
*** ic50 ACTIVITY *** value prediction
based on 11 locally validated fgps ---> 88000.000
["TT_bits", "cdk_maccs", "AP_bits", "MFP1", "klekota_roth", "pubchem",
"graph", "FP2", "FeatMFP1", "RDKit7", "hybridization"]

20 rank
Tyrosine-protein kinase BRK : Homo sapiens
score: 8.129 on CHEMBL4601 based on 11 fingerprints
Fingerprint type      Ligand  Tanimoto Similarity  activity Valid fg
FeatMFP1              CHEMBL939          0.750000    980.0      *
MFP1                  CHEMBL939          0.688889    980.0      *
RDKit7                CHEMBL939          0.805133    980.0      *
Pattern               CHEMBL1983268      0.824959    195.0
AP_bits               CHEMBL939          0.507317    980.0      *
TT_bits               CHEMBL939          0.635135    980.0      *
FP2                   CHEMBL939          0.782313    980.0      *
hybridization         CHEMBL939          0.816471    980.0      *
substructure          CHEMBL939          0.750000    980.0
graph                 CHEMBL939          0.777778    980.0      *
pubchem               CHEMBL939          0.925764    980.0      *
cdk_maccs             CHEMBL939          0.840580    980.0      *
klekota_roth          CHEMBL939          0.600000    980.0      *
*** ic50 ACTIVITY *** value prediction
based on 11 locally validated fgps ---> 945.203
["TT_bits", "cdk_maccs", "AP_bits", "MFP1", "klekota_roth", "pubchem",
"graph", "FP2", "FeatMFP1", "RDKit7", "hybridization"]

21 rank
Beta-secretase 1 : Homo sapiens
score: 8.129 on CHEMBL4822 based on 11 fingerprints
Fingerprint type      Ligand  Tanimoto Similarity  activity Valid fg
FeatMFP1              CHEMBL939          0.750000   20000.0    *
MFP1                  CHEMBL939          0.688889   20000.0    *
RDKit7                CHEMBL939          0.805133   20000.0    *
Pattern               CHEMBL939          0.822785   20000.0
AP_bits               CHEMBL939          0.507317   20000.0    *
TT_bits               CHEMBL939          0.635135   20000.0    *
FP2                   CHEMBL939          0.782313   20000.0    *
hybridization         CHEMBL939          0.816471   20000.0    *
substructure          CHEMBL2047223      0.842105    1700.0
graph                 CHEMBL939          0.777778   20000.0    *
pubchem               CHEMBL939          0.925764   20000.0    *
cdk_maccs             CHEMBL939          0.840580   20000.0    *
klekota_roth          CHEMBL939          0.600000   20000.0    *
*** ic50 ACTIVITY *** value prediction
based on 11 locally validated fgps ---> 19175.609
["TT_bits", "cdk_maccs", "AP_bits", "MFP1", "klekota_roth", "pubchem",
"graph", "FP2", "FeatMFP1", "RDKit7", "hybridization"]

22 rank
Serine/threonine-protein kinase RIPK2 : Homo sapiens
score: 8.129 on CHEMBL5014 based on 11 fingerprints
Fingerprint type      Ligand  Tanimoto Similarity  activity Valid fg
FeatMFP1              CHEMBL939          0.750000     3.8      *

```

MFP1	CHEMBL939	0.688889	3.8	*
RDKit7	CHEMBL939	0.805133	3.8	*
Pattern	CHEMBL939	0.822785	3.8	
AP_bits	CHEMBL939	0.507317	3.8	*
TT_bits	CHEMBL939	0.635135	3.8	*
FP2	CHEMBL939	0.782313	3.8	*
hybridization	CHEMBL939	0.816471	3.8	*
substructure	CHEMBL939	0.750000	3.8	
graph	CHEMBL939	0.777778	3.8	*
pubchem	CHEMBL939	0.925764	3.8	*
cdk_maccs	CHEMBL939	0.840580	3.8	*
klekota_roth	CHEMBL939	0.600000	3.8	*

*** ic50 ACTIVITY *** value prediction

based on 11 locally validated fgps ---> 5.709

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

23 rank

HERG : Homo sapiens

score: 8.005 on ChEMBL240 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3623278		0.727273	17000.0	*
MFP1	CHEMBL3623278		0.583333	17000.0	*
RDKit7	CHEMBL193544		0.703361	5000.0	*
Pattern	CHEMBL554		0.855025	1000.0	*
AP_bits	CHEMBL1645462		0.519411	4000.0	*
TT_bits	CHEMBL554		0.533333	1000.0	*
FP2	CHEMBL193544		0.703030	5000.0	*
hybridization	CHEMBL193544		0.709812	5000.0	*
substructure	CHEMBL1916532		0.947368	3000.0	*
graph	CHEMBL193544		0.705314	5000.0	
pubchem	CHEMBL193544		0.858333	5000.0	*
cdk_maccs	CHEMBL1916533		0.864865	4000.0	*
klekota_roth	CHEMBL3359238		0.511905	1400.0	

*** ic50 ACTIVITY *** value prediction

based on 11 locally validated fgps ---> 6768.192

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

24 rank

Tyrosine-protein kinase TIE-2 : Homo sapiens

score: 7.922 on ChEMBL4128 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL593274		0.742857	37.0	*
MFP1	CHEMBL593274		0.588235	37.0	*
RDKit7	CHEMBL301018		0.750727	8300.0	*
Pattern	CHEMBL593971		0.829889	4000.0	
AP_bits	CHEMBL604893		0.609078	510.0	*
TT_bits	CHEMBL301018		0.541667	8300.0	*
FP2	CHEMBL301018		0.710145	8300.0	*
hybridization	CHEMBL604893		0.700787	510.0	*
substructure	CHEMBL593909		0.900000	615.0	*
graph	CHEMBL301018		0.713514	8300.0	
pubchem	CHEMBL301018		0.910714	8300.0	*
cdk_maccs	CHEMBL288441		0.847222	1191.0	*
klekota_roth	CHEMBL593909		0.620690	615.0	*

*** ic50 ACTIVITY *** value prediction

based on 11 locally validated fgps ---> 2424.601

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

25 rank

Ephrin type-A receptor 2 : Homo sapiens

score: 7.549 on ChEMBL2068 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3322983		0.705882	300.0	*
MFP1	CHEMBL3322981		0.541667	620.0	*
RDKit7	CHEMBL3322973		0.772433	1470.0	*
Pattern	CHEMBL3322972		0.846816	1190.0	*
AP_bits	CHEMBL1090360		0.461438	370.0	
TT_bits	CHEMBL3322978		0.531646	580.0	*
FP2	CHEMBL3322983		0.724359	300.0	*
hybridization	CHEMBL3322983		0.760000	300.0	*
substructure	CHEMBL3544983		0.900000	50.0	*
graph	CHEMBL3322973		0.738693	1470.0	
pubchem	CHEMBL3322973		0.908696	1470.0	*
cdk_maccs	CHEMBL3322987		0.857143	160.0	*
klekota_roth	CHEMBL3322987		0.455556	160.0	

*** ic50 ACTIVITY *** value prediction

based on 10 locally validated fgps ---> 627.315

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

26 rank

Insulin receptor : Homo sapiens

score: 7.203 on ChEMBL1981 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL2063926		0.685714	10000.0	*
MFP1	CHEMBL301018		0.547619	2600.0	*
RDKit7	CHEMBL301018		0.750727	2600.0	*
Pattern	CHEMBL1630109		0.886010	3600.0	*
AP_bits	CHEMBL502652		0.527043	100.0	*
TT_bits	CHEMBL1630109		0.587500	3600.0	*
FP2	CHEMBL301018		0.710145	2600.0	*
hybridization	CHEMBL1630113		0.747788	5500.0	*
substructure	CHEMBL3823045		0.850000	26.0	*
graph	CHEMBL1630113		0.734694	5500.0	
pubchem	CHEMBL301018		0.910714	2600.0	*
cdk_maccs	CHEMBL3785951		0.794872	93.0	
klekota_roth	CHEMBL3263965		0.526316	11805.0	

*** ic50 ACTIVITY *** value prediction

based on 9 locally validated fgps ---> 4380.344

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

27 rank

Tyrosine-protein kinase LCK : Homo sapiens

score: 7.025 on ChEMBL258 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL217092		0.694444	4.0	*
MFP1	CHEMBL541586		0.536585	10000.0	*
RDKit7	CHEMBL540068		0.752505	5000.0	*
Pattern	CHEMBL288441		0.823430	1.3	
AP_bits	CHEMBL453737		0.538462	4.0	*
TT_bits	CHEMBL541586		0.571429	10000.0	*
FP2	CHEMBL540068		0.669118	5000.0	*
hybridization	CHEMBL540068		0.667488	5000.0	*
substructure	CHEMBL247468		0.850000	9.0	*
graph	CHEMBL540068		0.705556	5000.0	
pubchem	CHEMBL540068		0.897321	5000.0	*

```

        cdk_maccs  CHEMBL288441          0.847222      1.3      *
    klekota_roth  CHEMBL288441          0.532609      1.3
    *** ic50 ACTIVITY *** value prediction
    based on 9 locally validated fgps ---> 4594.651
["TT_bits", "cdk_maccs", "AP_bits", "MFP1", "pubchem", "FP2", "FeatMFP1",
"RDKit7", "hybridization"]

```

28 rank

Cyclin-dependent kinase 2 : Homo sapiens

score: 6.537 on ChEMBL301 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL217092		0.694444	10000.0		*
MFP1	CHEMBL554		0.490909	11000.0		
RDKit7	CHEMBL1630110		0.694683	850.0		*
Pattern	CHEMBL1630109		0.886010	920.0		*
AP_bits	CHEMBL201307		0.572005	62000.0		*
TT_bits	CHEMBL1630109		0.587500	920.0		*
FP2	CHEMBL1630116		0.640000	1400.0		*
hybridization	CHEMBL1630113		0.747788	1900.0		*
substructure	CHEMBL2163984		0.850000	700.0		*
graph	CHEMBL1630113		0.734694	1900.0		
pubchem	CHEMBL127907		0.829694	1000.0		
cdk_maccs	CHEMBL186396		0.864865	812.0		*
klekota_roth	CHEMBL201307		0.480769	62000.0		

```

    *** ic50 ACTIVITY *** value prediction
    based on 8 locally validated fgps ---> 7359.761
["TT_bits", "cdk_maccs", "Pattern", "AP_bits", "FP2", "FeatMFP1",
"RDKit7", "hybridization"]

```

29 rank

Stem cell growth factor receptor : Homo sapiens

score: 6.036 on ChEMBL1936 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL217092		0.694444	200.00		*
MFP1	CHEMBL3594105		0.491803	38.20		
RDKit7	CHEMBL24828		0.708850	343.00		*
Pattern	CHEMBL330863		0.864177	21.00		*
AP_bits	CHEMBL3764279		0.555280	162.50		*
TT_bits	CHEMBL3628796		0.481481	3.00		
FP2	CHEMBL24828		0.617284	343.00		
hybridization	CHEMBL24828		0.654348	343.00		*
substructure	CHEMBL1945173		0.850000	1100.00		*
graph	CHEMBL24828		0.668293	343.00		
pubchem	CHEMBL102346		0.862069	50.00		*
cdk_maccs	CHEMBL288441		0.847222	6313.00		*
klekota_roth	CHEMBL3823520		0.566667	9.36		

```

    *** ic50 ACTIVITY *** value prediction
    based on 7 locally validated fgps ---> 1090.081
["cdk_maccs", "Pattern", "pubchem", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

```

30 rank

Tyrosine-protein kinase receptor FLT3 : Homo sapiens

score: 5.851 on ChEMBL1974 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL3545311		0.615385	2.10		
MFP1	CHEMBL3594105		0.491803	134.00		
RDKit7	CHEMBL598797		0.708257	1500.00		*
Pattern	CHEMBL330863		0.864177	128.00		*
AP_bits	CHEMBL1940111		0.561080	10.00		*

TT_bits	CHEMBL598797	0.551282	1500.00	*
FP2	CHEMBL598797	0.580838	1500.00	
hybridization	CHEMBL598797	0.639413	1500.00	*
substructure	CHEMBL1915641	0.850000	61.00	*
graph	CHEMBL598797	0.661458	1500.00	
pubchem	CHEMBL102346	0.862069	230.00	*
cdk_maccs	CHEMBL3355065	0.814286	50.00	*
klekota_roth	CHEMBL3823520	0.566667	8.91	

*** ic50 ACTIVITY *** value prediction
based on 7 locally validated fgps ---> 638.262
["TT_bits", "cdk_maccs", "Pattern", "pubchem", "AP_bits", "RDKit7",
"hybridization"]

31 rank

MAP kinase p38 alpha : Homo sapiens

score: 5.775 on ChEMBL260 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL7917	0.612903	560.0		
MFP1	CHEMBL7917	0.500000	560.0		
RDKit7	CHEMBL7917	0.752505	560.0		*
Pattern	CHEMBL188114	0.860269	30.0		*
AP_bits	CHEMBL188167	0.529183	50.0		*
TT_bits	CHEMBL7917	0.549296	560.0		*
FP2	CHEMBL7917	0.669118	560.0		*
hybridization	CHEMBL7917	0.667488	560.0		*
substructure	CHEMBL95692	0.850000	19.0		*
graph	CHEMBL7917	0.705556	560.0		
pubchem	CHEMBL7917	0.897321	560.0		*
cdk_maccs	CHEMBL1946341	0.767123	2800.0		
klekota_roth	CHEMBL215289	0.456311	1300.0		

*** ic50 ACTIVITY *** value prediction
based on 7 locally validated fgps ---> 489.892
["TT_bits", "Pattern", "AP_bits", "pubchem", "FP2", "RDKit7",
"hybridization"]

32 rank

Histone deacetylase 1 : Homo sapiens

score: 5.762 on ChEMBL325 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3700343	0.657895	330.0		
MFP1	CHEMBL3700343	0.537037	330.0		*
RDKit7	CHEMBL3633769	0.725184	3.5		*
Pattern	CHEMBL1630109	0.886010	35.0		*
AP_bits	CHEMBL3700343	0.626844	330.0		*
TT_bits	CHEMBL1630109	0.587500	35.0		*
FP2	CHEMBL1630110	0.619318	650.0		
hybridization	CHEMBL1630107	0.742152	610.0		*
substructure	CHEMBL216300	0.695652	9.0		
graph	CHEMBL1630107	0.720812	610.0		
pubchem	CHEMBL3633769	0.832653	3.5		*
cdk_maccs	CHEMBL3700343	0.824324	330.0		*
klekota_roth	CHEMBL3700343	0.494737	330.0		

*** ic50 ACTIVITY *** value prediction
based on 8 locally validated fgps ---> 274.996
["TT_bits", "cdk_maccs", "Pattern", "MFP1", "pubchem", "AP_bits",
"RDKit7", "hybridization"]

33 rank

Macrophage colony stimulating factor receptor : Homo sapiens

score: 5.726 on ChEMBL1844 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL24828		0.676471	1600.0		
MFP1	CHEMBL481231		0.527273	7.0		*
RDKit7	CHEMBL24828		0.708850	1600.0		*
Pattern	CHEMBL125898		0.862779	1400.0		*
AP_bits	CHEMBL1940111		0.561080	400.0		*
TT_bits	CHEMBL1940267		0.487500	300.0		
FP2	CHEMBL553908		0.669118	1500.0		*
hybridization	CHEMBL553908		0.667488	1500.0		*
substructure	CHEMBL24828		0.809524	1600.0		
graph	CHEMBL553908		0.705556	1500.0		
pubchem	CHEMBL553908		0.883929	1500.0		*
cdk_maccs	CHEMBL24828		0.845070	1600.0		*
klekota_roth	CHEMBL481231		0.580645	7.0		

*** ic50 ACTIVITY *** value prediction
 based on 8 locally validated fgps ---> 1230.512
 ["cdk_maccs", "Pattern", "AP_bits", "MFP1", "pubchem", "FP2", "RDKit7",
 "hybridization"]

34 rank

C-C chemokine receptor type 4 : Homo sapiens

score: 5.426 on ChEMBL2414 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL488691		0.757576	150.0		*
MFP1	CHEMBL488691		0.480000	150.0		
RDKit7	CHEMBL488690		0.688946	92.0		*
Pattern	CHEMBL488855		0.881416	130.0		*
AP_bits	CHEMBL488855		0.496372	130.0		*
TT_bits	CHEMBL488704		0.395833	220.0		
FP2	CHEMBL488690		0.604938	92.0		
hybridization	CHEMBL488690		0.579798	92.0		
substructure	CHEMBL365155		0.894737	2000.0		*
graph	CHEMBL495736		0.648649	87.0		
pubchem	CHEMBL487665		0.882609	550.0		*
cdk_maccs	CHEMBL496151		0.824324	48.0		*
klekota_roth	CHEMBL488691		0.500000	150.0		

*** ic50 ACTIVITY *** value prediction
 based on 7 locally validated fgps ---> 300.844
 ["substructure", "Pattern", "pubchem", "AP_bits", "FeatMFP1", "RDKit7",
 "cdk_maccs"]

35 rank

Ephrin type-B receptor 2 : Homo sapiens

score: 4.791 on ChEMBL3290 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL288441		0.694444	8.5		*
MFP1	CHEMBL150315		0.477273	8500.0		
RDKit7	CHEMBL150315		0.712135	8500.0		*
Pattern	CHEMBL288441		0.823430	8.5		
AP_bits	CHEMBL288441		0.474648	8.5		*
TT_bits	CHEMBL127907		0.527778	1200.0		*
FP2	CHEMBL150315		0.641379	8500.0		*
hybridization	CHEMBL150315		0.611241	8500.0		
substructure	CHEMBL288441		0.772727	8.5		
graph	CHEMBL97771		0.666667	86000.0		
pubchem	CHEMBL150315		0.893805	8500.0		*
cdk_maccs	CHEMBL288441		0.847222	8.5		*
klekota_roth	CHEMBL288441		0.532609	8.5		

*** ic50 ACTIVITY *** value prediction
 based on 7 locally validated fgps ---> 9424.287

["TT_bits", "AP_bits", "pubchem", "FP2", "FeatMFP1", "RDKit7",
"cdk_maccs"]

36 rank

Tyrosine-protein kinase CSK : Homo sapiens

score: 4.774 on ChEMBL2634 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL369360		0.727273	7300.0	*
MFP1	CHEMBL369360		0.571429	7300.0	*
RDKit7	CHEMBL169186		0.696327	1700.0	*
Pattern	CHEMBL201307		0.839607	21000.0	
AP_bits	CHEMBL201307		0.572005	21000.0	*
TT_bits	CHEMBL201307		0.521739	21000.0	*
FP2	CHEMBL369360		0.588889	7300.0	
hybridization	CHEMBL369360		0.626894	7300.0	
substructure	CHEMBL169186		0.809524	1700.0	
graph	CHEMBL1614725		0.668224	4700.0	
pubchem	CHEMBL169186		0.838057	1700.0	*
cdk_maccs	CHEMBL288441		0.847222	63.0	*
klekota_roth	CHEMBL169186		0.558140	1700.0	

*** ic50 ACTIVITY *** value prediction

based on 7 locally validated fgps ---> 7459.712

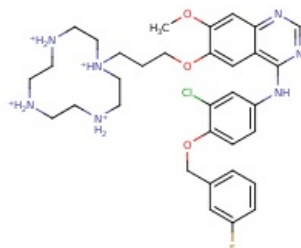
["TT_bits", "AP_bits", "MFP1", "pubchem", "FeatMFP1", "RDKit7",
"cdk_maccs"]

SwissTargetPrediction report:

Reference:

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

Query Molecule



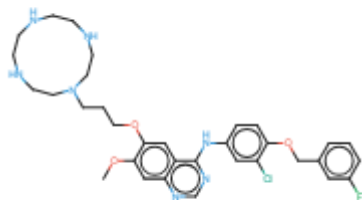
Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
Epidermal growth factor receptor	P00533	EGFR	CHEMBL203	<div><div></div></div>	27 / 755	Tyr Kinase
Receptor tyrosine-protein kinase erbB-2	P04626	ERBB2	CHEMBL1824	<div><div></div></div>	27 / 755	Tyr Kinase
Receptor tyrosine-protein kinase erbB-3 (<i>by homology</i>)	P21860	ERBB3	CHEMBL5838	<div><div></div></div>	27 / 755	Tyr Kinase
ERBB4 intracellular domain (<i>by homology</i>)	Q15303	ERBB4	CHEMBL3009	<div><div></div></div>	27 / 755	Tyr Kinase
Vascular endothelial growth factor receptor 1	P17948	FLT1	CHEMBL1868	<div><div></div></div>	24 / 216	Tyr Kinase
Vascular endothelial growth factor receptor 3 (<i>by homology</i>)	P35916	FLT4	CHEMBL1955	<div><div></div></div>	24 / 216	Tyr Kinase
Vascular endothelial growth factor receptor 2	P35968	KDR	CHEMBL279	<div><div></div></div>	24 / 216	Tyr Kinase
Serine/threonine-protein kinase Chk2	O96017	CHEK2	CHEMBL2527	<div><div></div></div>	5 / 17	Ser_Thr Kinase
Tyrosine-protein kinase ABL1	P00519	ABL1	CHEMBL1862	<div><div></div></div>	3 / 27	Tyr Kinase
Hepatocyte growth factor receptor	P08581	MET	CHEMBL3717	<div><div></div></div>	5 / 14	Tyr Kinase
Abelson tyrosine-protein kinase 2	P42684	ABL2	CHEMBL4014	<div><div></div></div>	3 / 27	Tyr Kinase
Mitogen-activated protein kinase 8 (<i>by homology</i>)	P45983	MAPK8	CHEMBL2276	<div><div></div></div>	6 / 27	Ser_Thr Kinase
Mitogen-activated protein kinase 9	P45984	MAPK9	CHEMBL4179	<div><div></div></div>	6 / 27	Ser_Thr Kinase
Mitogen-activated protein kinase 10	P53779	MAPK10	CHEMBL2637	<div><div></div></div>	6 / 27	Ser_Thr Kinase
Mitogen-activated protein kinase 14	Q16539	MAPK14	CHEMBL260	<div><div></div></div>	6 / 27	Ser_Thr Kinase

Polypharmacology Browser 2 Prediction:

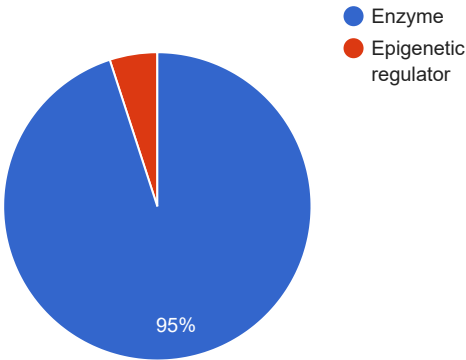
Targets predicted using NN(ECfp4) + NB(ECfp4).

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	CHEMBL1824 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1824)	Receptor protein-tyrosine kinase erbB-2	Show NN
3	CHEMBL1862 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1862)	Tyrosine-protein kinase ABL	Show NN
4	CHEMBL1981 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1981)	Insulin receptor	Show NN
5	CHEMBL1913 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1913)	Platelet-derived growth factor receptor beta	Show NN
6	CHEMBL279 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL279)	Vascular endothelial growth factor receptor 2	Show NN
7	CHEMBL267 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL267)	Tyrosine-protein kinase SRC	Show NN
8	CHEMBL258 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL258)	Tyrosine-protein kinase LCK	Show NN
9	CHEMBL1868 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1868)	Vascular endothelial growth factor receptor 1	Show NN
10	CHEMBL3009 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3009)	Receptor protein-tyrosine kinase erbB-4	Show NN
11	CHEMBL1974 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1974)	Tyrosine-protein kinase receptor FLT3	Show NN
12	CHEMBL2185 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2185)	Serine/threonine-protein kinase Aurora-B	Show NN
13	CHEMBL1955 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1955)	Vascular endothelial growth factor receptor 3	Show NN
14	CHEMBL1844 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1844)	Macrophage colony stimulating factor receptor	Show NN
15	CHEMBL3650 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3650)	Fibroblast growth factor receptor 1	Show NN
16	CHEMBL1936 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1936)	Stem cell growth factor receptor	Show NN
17	CHEMBL3024 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3024)	Serine/threonine-protein kinase PLK1	Show NN
18	CHEMBL2041 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2041)	Tyrosine-protein kinase receptor RET	Show NN

19	CHEMBL325 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL325)	Histone deacetylase 1	Show NN
20	CHEMBL2007 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2007)	Platelet-derived growth factor receptor alpha	Show NN