

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

1 rank

Homeodomain-interacting protein kinase 4 : Homo sapiens

score: 12.707 on ChEMBL1075167 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL1975121		1.000000	794.33	*
MFP1	ChEMBL1975121		1.000000	794.33	*
RDKit7	ChEMBL1975121		1.000000	794.33	*
Pattern	ChEMBL1975121		1.000000	794.33	*
AP_bits	ChEMBL1975121		1.000000	794.33	*
TT_bits	ChEMBL1975121		1.000000	794.33	*
FP2	ChEMBL1975121		1.000000	794.33	*
hybridization	ChEMBL1975121		0.877451	794.33	*
substructure	ChEMBL1969049		1.000000	398.11	*
graph	ChEMBL1969049		0.829268	398.11	*
pubchem	ChEMBL1970217		1.000000	1258.93	*
cdk_maccs	ChEMBL1975121		1.000000	794.33	*
klekota_roth	ChEMBL1975121		1.000000	794.33	*

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

based on 13 locally validated fgps ---> 1176.319

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

2 rank

Serine/threonine-protein kinase AKT2 : Homo sapiens

score: 12.707 on ChEMBL2431 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL1975121		1.000000	2511.89	*
MFP1	ChEMBL1975121		1.000000	2511.89	*
RDKit7	ChEMBL1975121		1.000000	2511.89	*
Pattern	ChEMBL1975121		1.000000	2511.89	*
AP_bits	ChEMBL1975121		1.000000	2511.89	*
TT_bits	ChEMBL1975121		1.000000	2511.89	*
FP2	ChEMBL1975121		1.000000	2511.89	*
hybridization	ChEMBL1975121		0.877451	2511.89	*
substructure	ChEMBL1969049		1.000000	3981.07	*
graph	ChEMBL1969049		0.829268	3981.07	*
pubchem	ChEMBL1970217		1.000000	1258.93	*
cdk_maccs	ChEMBL1975121		1.000000	2511.89	*
klekota_roth	ChEMBL1975121		1.000000	2511.89	*

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

based on 13 locally validated fgps ---> 2572.927

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

3 rank

Glycogen synthase kinase-3 beta : Homo sapiens

score: 12.707 on ChEMBL262 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL1975121		1.000000	630.96	*
MFP1	ChEMBL1975121		1.000000	630.96	*
RDKit7	ChEMBL1975121		1.000000	630.96	*
Pattern	ChEMBL1975121		1.000000	630.96	*
AP_bits	ChEMBL1975121		1.000000	630.96	*
TT_bits	ChEMBL1975121		1.000000	630.96	*
FP2	ChEMBL1975121		1.000000	630.96	*
hybridization	ChEMBL1975121		0.877451	630.96	*
substructure	ChEMBL1969049		1.000000	100.00	*
graph	ChEMBL1969049		0.829268	100.00	*

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pubchem CHEMBL1970217 1.000000 251.19 *
cdk_maccs CHEMBL1975121 1.000000 630.96 *
klekota_roth CHEMBL1975121 1.000000 630.96 *
*** ki ACTIVITY *** value prediction
based on 13 locally validated fgps ---> 581.682
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

4 rank
Glycogen synthase kinase-3 alpha : Homo sapiens
score: 12.707 on CHEMBL2850 based on 13 fingerprints
Fingerprint type Ligand Tanimoto Similarity activity Valid fg
FeatMFP1 CHEMBL1975121 1.000000 630.96 *
MFP1 CHEMBL1975121 1.000000 630.96 *
RDKit7 CHEMBL1975121 1.000000 630.96 *
Pattern CHEMBL1975121 1.000000 630.96 *
AP_bits CHEMBL1975121 1.000000 630.96 *
TT_bits CHEMBL1975121 1.000000 630.96 *
FP2 CHEMBL1975121 1.000000 630.96 *
hybridization CHEMBL1975121 0.877451 630.96 *
substructure CHEMBL1969049 1.000000 251.19 *
graph CHEMBL1969049 0.829268 251.19 *
pubchem CHEMBL1970217 1.000000 501.19 *
cdk_maccs CHEMBL1975121 1.000000 630.96 *
klekota_roth CHEMBL1975121 1.000000 630.96 *
*** ki ACTIVITY *** value prediction
based on 13 locally validated fgps ---> 786.432
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

5 rank
cGMP-dependent protein kinase 2 : Homo sapiens
score: 12.707 on CHEMBL2896 based on 13 fingerprints
Fingerprint type Ligand Tanimoto Similarity activity Valid fg
FeatMFP1 CHEMBL1975121 1.000000 15.85 *
MFP1 CHEMBL1975121 1.000000 15.85 *
RDKit7 CHEMBL1975121 1.000000 15.85 *
Pattern CHEMBL1975121 1.000000 15.85 *
AP_bits CHEMBL1975121 1.000000 15.85 *
TT_bits CHEMBL1975121 1.000000 15.85 *
FP2 CHEMBL1975121 1.000000 15.85 *
hybridization CHEMBL1975121 0.877451 15.85 *
substructure CHEMBL1969049 1.000000 79.43 *
graph CHEMBL1969049 0.829268 79.43 *
pubchem CHEMBL1970217 1.000000 50.12 *
cdk_maccs CHEMBL1975121 1.000000 15.85 *
klekota_roth CHEMBL1975121 1.000000 15.85 *
*** ki ACTIVITY *** value prediction
based on 13 locally validated fgps ---> 48.815
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

6 rank
Protein kinase C gamma : Homo sapiens
score: 12.707 on CHEMBL2938 based on 13 fingerprints
Fingerprint type Ligand Tanimoto Similarity activity Valid fg
FeatMFP1 CHEMBL1975121 1.000000 1000.00 *
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MFP1	CHEMBL1975121	1.000000	1000.00	*
RDKit7	CHEMBL1975121	1.000000	1000.00	*
Pattern	CHEMBL1975121	1.000000	1000.00	*
AP_bits	CHEMBL1975121	1.000000	1000.00	*
TT_bits	CHEMBL1975121	1.000000	1000.00	*
FP2	CHEMBL1975121	1.000000	1000.00	*
hybridization	CHEMBL1975121	0.877451	1000.00	*
substructure	CHEMBL1970217	1.000000	794.33	*
graph	CHEMBL1970217	0.829268	794.33	*
pubchem	CHEMBL1970217	1.000000	794.33	*
cdk_maccs	CHEMBL1975121	1.000000	1000.00	*
klekota_roth	CHEMBL1975121	1.000000	1000.00	*

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

based on 13 locally validated fgps ---> 1173.481

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

7 rank

Rho-associated protein kinase 2 : Homo sapiens

score: 12.707 on ChEMBL2973 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1975121	1.000000	199.53	*	
MFP1	CHEMBL1975121	1.000000	199.53	*	
RDKit7	CHEMBL1975121	1.000000	199.53	*	
Pattern	CHEMBL1975121	1.000000	199.53	*	
AP_bits	CHEMBL1975121	1.000000	199.53	*	
TT_bits	CHEMBL1975121	1.000000	199.53	*	
FP2	CHEMBL1975121	1.000000	199.53	*	
hybridization	CHEMBL1975121	0.877451	199.53	*	
substructure	CHEMBL1975121	1.000000	199.53	*	
graph	CHEMBL1975121	0.829268	199.53	*	
pubchem	CHEMBL1975121	1.000000	199.53	*	
cdk_maccs	CHEMBL1975121	1.000000	199.53	*	
klekota_roth	CHEMBL1975121	1.000000	199.53	*	

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

based on 13 locally validated fgps ---> 122.606

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

8 rank

Protein kinase C delta : Homo sapiens

score: 12.707 on ChEMBL2996 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1975121	1.000000	63.10	*	
MFP1	CHEMBL1975121	1.000000	63.10	*	
RDKit7	CHEMBL1975121	1.000000	63.10	*	
Pattern	CHEMBL1975121	1.000000	63.10	*	
AP_bits	CHEMBL1975121	1.000000	63.10	*	
TT_bits	CHEMBL1975121	1.000000	63.10	*	
FP2	CHEMBL1975121	1.000000	63.10	*	
hybridization	CHEMBL1975121	0.877451	63.10	*	
substructure	CHEMBL1969049	1.000000	125.89	*	
graph	CHEMBL1969049	0.829268	125.89	*	
pubchem	CHEMBL1970217	1.000000	39.81	*	
cdk_maccs	CHEMBL1975121	1.000000	63.10	*	
klekota_roth	CHEMBL1975121	1.000000	63.10	*	

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

based on 13 locally validated fgps ---> 159.905

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

9 rank

Cyclin-dependent kinase 2 : Homo sapiens

score: 12.707 on ChEMBL301 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL1975121		1.000000	2511.89	*
MFP1	ChEMBL1975121		1.000000	2511.89	*
RDKit7	ChEMBL1975121		1.000000	2511.89	*
Pattern	ChEMBL1975121		1.000000	2511.89	*
AP_bits	ChEMBL1975121		1.000000	2511.89	*
TT_bits	ChEMBL1975121		1.000000	2511.89	*
FP2	ChEMBL1975121		1.000000	2511.89	*
hybridization	ChEMBL1975121		0.877451	2511.89	*
substructure	ChEMBL1969049		1.000000	3981.07	*
graph	ChEMBL1969049		0.829268	3981.07	*
pubchem	ChEMBL1970217		1.000000	1995.26	*
cdk_maccs	ChEMBL1975121		1.000000	2511.89	*
klekota_roth	ChEMBL1975121		1.000000	2511.89	*

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

based on 13 locally validated fgps ---> 2671.123

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

10 rank

Protein kinase N2 : Homo sapiens

score: 12.707 on ChEMBL3032 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL1975121		1.000000	79.43	*
MFP1	ChEMBL1975121		1.000000	79.43	*
RDKit7	ChEMBL1975121		1.000000	79.43	*
Pattern	ChEMBL1975121		1.000000	79.43	*
AP_bits	ChEMBL1975121		1.000000	79.43	*
TT_bits	ChEMBL1975121		1.000000	79.43	*
FP2	ChEMBL1975121		1.000000	79.43	*
hybridization	ChEMBL1975121		0.877451	79.43	*
substructure	ChEMBL1969049		1.000000	125.89	*
graph	ChEMBL1969049		0.829268	125.89	*
pubchem	ChEMBL1970217		1.000000	79.43	*
cdk_maccs	ChEMBL1975121		1.000000	79.43	*
klekota_roth	ChEMBL1975121		1.000000	79.43	*

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

based on 13 locally validated fgps ---> 280.648

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

11 rank

Cyclin-dependent kinase 1 : Homo sapiens

score: 12.707 on ChEMBL308 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL1975121		1.000000	3162.28	*
MFP1	ChEMBL1975121		1.000000	3162.28	*
RDKit7	ChEMBL1975121		1.000000	3162.28	*
Pattern	ChEMBL1975121		1.000000	3162.28	*
AP_bits	ChEMBL1975121		1.000000	3162.28	*
TT_bits	ChEMBL1975121		1.000000	3162.28	*

FP2	CHEMBL1975121	1.000000	3162.28	*
hybridization	CHEMBL1975121	0.877451	3162.28	*
substructure	CHEMBL1970217	1.000000	1584.89	*
graph	CHEMBL1970217	0.829268	1584.89	*
pubchem	CHEMBL1970217	1.000000	1584.89	*
cdk_maccs	CHEMBL1975121	1.000000	3162.28	*
klekota_roth	CHEMBL1975121	1.000000	3162.28	*

\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 13 locally validated fgps ---> 3099.333  
["TT\_bits", "substructure", "cdk\_maccs", "Pattern", "FP2", "MFP1",  
"klekota\_roth", "pubchem", "graph", "AP\_bits", "FeatMFP1", "RDKit7",  
"hybridization"]

12 rank  
Rho-associated protein kinase 1 : Homo sapiens  
score: 12.707 on ChEMBL3231 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1975121	1.000000	2.512	*	
MFP1	CHEMBL1975121	1.000000	2.512	*	
RDKit7	CHEMBL1975121	1.000000	2.512	*	
Pattern	CHEMBL1975121	1.000000	2.512	*	
AP_bits	CHEMBL1975121	1.000000	2.512	*	
TT_bits	CHEMBL1975121	1.000000	2.512	*	
FP2	CHEMBL1975121	1.000000	2.512	*	
hybridization	CHEMBL1975121	0.877451	2.512	*	
substructure	CHEMBL1969049	1.000000	25.120	*	
graph	CHEMBL1969049	0.829268	25.120	*	
pubchem	CHEMBL1970217	1.000000	19.950	*	
cdk_maccs	CHEMBL1975121	1.000000	2.512	*	
klekota_roth	CHEMBL1975121	1.000000	2.512	*	

\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 13 locally validated fgps ---> 14.191  
["TT\_bits", "substructure", "cdk\_maccs", "Pattern", "FP2", "MFP1",  
"klekota\_roth", "pubchem", "graph", "AP\_bits", "FeatMFP1", "RDKit7",  
"hybridization"]

13 rank  
Interleukin-1 receptor-associated kinase 1 : Homo sapiens  
score: 12.707 on ChEMBL3357 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1975121	1.000000	1000.00	*	
MFP1	CHEMBL1975121	1.000000	1000.00	*	
RDKit7	CHEMBL1975121	1.000000	1000.00	*	
Pattern	CHEMBL1975121	1.000000	1000.00	*	
AP_bits	CHEMBL1975121	1.000000	1000.00	*	
TT_bits	CHEMBL1975121	1.000000	1000.00	*	
FP2	CHEMBL1975121	1.000000	1000.00	*	
hybridization	CHEMBL1975121	0.877451	1000.00	*	
substructure	CHEMBL1970217	1.000000	630.96	*	
graph	CHEMBL1970217	0.829268	630.96	*	
pubchem	CHEMBL1970217	1.000000	630.96	*	
cdk_maccs	CHEMBL1975121	1.000000	1000.00	*	
klekota_roth	CHEMBL1975121	1.000000	1000.00	*	

\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 13 locally validated fgps ---> 1080.154  
["TT\_bits", "substructure", "cdk\_maccs", "Pattern", "FP2", "MFP1",  
"klekota\_roth", "pubchem", "graph", "AP\_bits", "FeatMFP1", "RDKit7",  
"hybridization"]

14 rank

Protein kinase C theta : Homo sapiens

score: 12.707 on ChEMBL3920 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1975121		1.000000	125.89	*	
MFP1	CHEMBL1975121		1.000000	125.89	*	
RDKit7	CHEMBL1975121		1.000000	125.89	*	
Pattern	CHEMBL1975121		1.000000	125.89	*	
AP_bits	CHEMBL1975121		1.000000	125.89	*	
TT_bits	CHEMBL1975121		1.000000	125.89	*	
FP2	CHEMBL1975121		1.000000	125.89	*	
hybridization	CHEMBL1975121		0.877451	125.89	*	
substructure	CHEMBL1975121		1.000000	125.89	*	
graph	CHEMBL1975121		0.829268	125.89	*	
pubchem	CHEMBL1975121		1.000000	125.89	*	
cdk_maccs	CHEMBL1975121		1.000000	125.89	*	
klekota_roth	CHEMBL1975121		1.000000	125.89	*	

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

based on 13 locally validated fgps ---> 259.806

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

15 rank

Cyclin-dependent kinase 5 : Homo sapiens

score: 12.707 on ChEMBL4036 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1975121		1.000000	3981.07	*	
MFP1	CHEMBL1975121		1.000000	3981.07	*	
RDKit7	CHEMBL1975121		1.000000	3981.07	*	
Pattern	CHEMBL1975121		1.000000	3981.07	*	
AP_bits	CHEMBL1975121		1.000000	3981.07	*	
TT_bits	CHEMBL1975121		1.000000	3981.07	*	
FP2	CHEMBL1975121		1.000000	3981.07	*	
hybridization	CHEMBL1975121		0.877451	3981.07	*	
substructure	CHEMBL1970217		1.000000	7943.28	*	
graph	CHEMBL1970217		0.829268	7943.28	*	
pubchem	CHEMBL1970217		1.000000	7943.28	*	
cdk_maccs	CHEMBL1975121		1.000000	3981.07	*	
klekota_roth	CHEMBL1975121		1.000000	3981.07	*	

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

based on 13 locally validated fgps ---> 5508.760

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

16 rank

MAP kinase ERK2 : Homo sapiens

score: 12.707 on ChEMBL4040 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1975121		1.000000	501.19	*	
MFP1	CHEMBL1975121		1.000000	501.19	*	
RDKit7	CHEMBL1975121		1.000000	501.19	*	
Pattern	CHEMBL1975121		1.000000	501.19	*	
AP_bits	CHEMBL1975121		1.000000	501.19	*	
TT_bits	CHEMBL1975121		1.000000	501.19	*	
FP2	CHEMBL1975121		1.000000	501.19	*	
hybridization	CHEMBL1975121		0.877451	501.19	*	
substructure	CHEMBL1969049		1.000000	630.96	*	
graph	CHEMBL1969049		0.829268	630.96	*	
pubchem	CHEMBL1970217		1.000000	251.19	*	

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        cdk_maccs  CHEMBL1975121          1.000000    501.19      *
        klekota_roth CHEMBL1975121          1.000000    501.19      *
        *** ki ACTIVITY *** value prediction
        based on 13 locally validated fgps ---> 655.112
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

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17 rank

cAMP-dependent protein kinase alpha-catalytic subunit : Homo sapiens  
score: 12.707 on ChEMBL4101 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1975121		1.000000	12.59		*
MFP1	CHEMBL1975121		1.000000	12.59		*
RDKit7	CHEMBL1975121		1.000000	12.59		*
Pattern	CHEMBL1975121		1.000000	12.59		*
AP_bits	CHEMBL1975121		1.000000	12.59		*
TT_bits	CHEMBL1975121		1.000000	12.59		*
FP2	CHEMBL1975121		1.000000	12.59		*
hybridization	CHEMBL1975121		0.877451	12.59		*
substructure	CHEMBL1969049		1.000000	79.43		*
graph	CHEMBL1969049		0.829268	79.43		*
pubchem	CHEMBL1970217		1.000000	25.12		*
cdk_maccs	CHEMBL1975121		1.000000	12.59		*
klekota_roth	CHEMBL1975121		1.000000	12.59		*

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        *** ki ACTIVITY *** value prediction
        based on 13 locally validated fgps ---> 136.537
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

```

18 rank

Dual specificity protein kinase CLK4 : Homo sapiens  
score: 12.707 on ChEMBL4203 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1975121		1.000000	251.19		*
MFP1	CHEMBL1975121		1.000000	251.19		*
RDKit7	CHEMBL1975121		1.000000	251.19		*
Pattern	CHEMBL1975121		1.000000	251.19		*
AP_bits	CHEMBL1975121		1.000000	251.19		*
TT_bits	CHEMBL1975121		1.000000	251.19		*
FP2	CHEMBL1975121		1.000000	251.19		*
hybridization	CHEMBL1975121		0.877451	251.19		*
substructure	CHEMBL1969049		1.000000	1995.26		*
graph	CHEMBL1969049		0.829268	1995.26		*
pubchem	CHEMBL1970217		1.000000	794.33		*
cdk_maccs	CHEMBL1975121		1.000000	251.19		*
klekota_roth	CHEMBL1975121		1.000000	251.19		*

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        *** ki ACTIVITY *** value prediction
        based on 13 locally validated fgps ---> 705.105
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

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19 rank

Ribosomal protein S6 kinase alpha 5 : Homo sapiens  
score: 12.707 on ChEMBL4237 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1975121		1.000000	19.95		*
MFP1	CHEMBL1975121		1.000000	19.95		*

RDKit7	CHEMBL1975121	1.000000	19.95	*
Pattern	CHEMBL1975121	1.000000	19.95	*
AP_bits	CHEMBL1975121	1.000000	19.95	*
TT_bits	CHEMBL1975121	1.000000	19.95	*
FP2	CHEMBL1975121	1.000000	19.95	*
hybridization	CHEMBL1975121	0.877451	19.95	*
substructure	CHEMBL1969049	1.000000	1584.89	*
graph	CHEMBL1969049	0.829268	1584.89	*
pubchem	CHEMBL1970217	1.000000	199.53	*
cdk_maccs	CHEMBL1975121	1.000000	19.95	*
klekota_roth	CHEMBL1975121	1.000000	19.95	*

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

based on 13 locally validated fgps ---> 461.660

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

20 rank

cGMP-dependent protein kinase 1 beta : Homo sapiens

score: 12.707 on ChEMBL4273 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1975121	1.000000	7.943	*	
MFP1	CHEMBL1975121	1.000000	7.943	*	
RDKit7	CHEMBL1975121	1.000000	7.943	*	
Pattern	CHEMBL1975121	1.000000	7.943	*	
AP_bits	CHEMBL1975121	1.000000	7.943	*	
TT_bits	CHEMBL1975121	1.000000	7.943	*	
FP2	CHEMBL1975121	1.000000	7.943	*	
hybridization	CHEMBL1975121	0.877451	7.943	*	
substructure	CHEMBL1969049	1.000000	63.100	*	
graph	CHEMBL1969049	0.829268	63.100	*	
pubchem	CHEMBL1970217	1.000000	1000.000	*	
cdk_maccs	CHEMBL1975121	1.000000	7.943	*	
klekota_roth	CHEMBL1975121	1.000000	7.943	*	

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

based on 13 locally validated fgps ---> 216.852

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

21 rank

Ribosomal protein S6 kinase 1 : Homo sapiens

score: 12.707 on ChEMBL4501 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1975121	1.000000	630.96	*	
MFP1	CHEMBL1975121	1.000000	630.96	*	
RDKit7	CHEMBL1975121	1.000000	630.96	*	
Pattern	CHEMBL1975121	1.000000	630.96	*	
AP_bits	CHEMBL1975121	1.000000	630.96	*	
TT_bits	CHEMBL1975121	1.000000	630.96	*	
FP2	CHEMBL1975121	1.000000	630.96	*	
hybridization	CHEMBL1975121	0.877451	630.96	*	
substructure	CHEMBL1969049	1.000000	2511.89	*	
graph	CHEMBL1969049	0.829268	2511.89	*	
pubchem	CHEMBL1970217	1.000000	398.11	*	
cdk_maccs	CHEMBL1975121	1.000000	630.96	*	
klekota_roth	CHEMBL1975121	1.000000	630.96	*	

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

based on 13 locally validated fgps ---> 1349.714



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

22 rank

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

score: 12.707 on ChEMBL4516 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	ChEMBL1975121	1.000000	1258.93	*
MFP1	ChEMBL1975121	1.000000	1258.93	*
RDKit7	ChEMBL1975121	1.000000	1258.93	*
Pattern	ChEMBL1975121	1.000000	1258.93	*
AP_bits	ChEMBL1975121	1.000000	1258.93	*
TT_bits	ChEMBL1975121	1.000000	1258.93	*
FP2	ChEMBL1975121	1.000000	1258.93	*
hybridization	ChEMBL1975121	0.877451	1258.93	*
substructure	ChEMBL1969049	1.000000	1995.26	*
graph	ChEMBL1969049	0.829268	1995.26	*
pubchem	ChEMBL1970217	1.000000	1995.26	*
cdk_maccs	ChEMBL1975121	1.000000	1258.93	*
klekota_roth	ChEMBL1975121	1.000000	1258.93	*

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

based on 13 locally validated fgps ---> 1487.018

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

23 rank

Serine/threonine-protein kinase Chk1 : Homo sapiens

score: 12.707 on ChEMBL4630 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	ChEMBL1975121	1.000000	7943.28	*
MFP1	ChEMBL1975121	1.000000	7943.28	*
RDKit7	ChEMBL1975121	1.000000	7943.28	*
Pattern	ChEMBL1975121	1.000000	7943.28	*
AP_bits	ChEMBL1975121	1.000000	7943.28	*
TT_bits	ChEMBL1975121	1.000000	7943.28	*
FP2	ChEMBL1975121	1.000000	7943.28	*
hybridization	ChEMBL1975121	0.877451	7943.28	*
substructure	ChEMBL1970217	1.000000	5011.87	*
graph	ChEMBL1970217	0.829268	5011.87	*
pubchem	ChEMBL1970217	1.000000	5011.87	*
cdk_maccs	ChEMBL1975121	1.000000	7943.28	*
klekota_roth	ChEMBL1975121	1.000000	7943.28	*

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

based on 13 locally validated fgps ---> 6854.637

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

24 rank

Misshapen-like kinase 1 : Homo sapiens

score: 12.707 on ChEMBL5518 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	ChEMBL1975121	1.000000	7943.28	*
MFP1	ChEMBL1975121	1.000000	7943.28	*
RDKit7	ChEMBL1975121	1.000000	7943.28	*
Pattern	ChEMBL1975121	1.000000	7943.28	*
AP_bits	ChEMBL1975121	1.000000	7943.28	*
TT_bits	ChEMBL1975121	1.000000	7943.28	*

FP2	CHEMBL1975121	1.000000	7943.28	*
hybridization	CHEMBL1975121	0.877451	7943.28	*
substructure	CHEMBL1975121	1.000000	7943.28	*
graph	CHEMBL1975121	0.829268	7943.28	*
pubchem	CHEMBL1975121	1.000000	7943.28	*
cdk_maccs	CHEMBL1975121	1.000000	7943.28	*
klekota_roth	CHEMBL1975121	1.000000	7943.28	*

\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 13 locally validated fgps ---> 6813.416  
["TT\_bits", "substructure", "cdk\_maccs", "Pattern", "FP2", "MFP1",  
"klekota\_roth", "pubchem", "graph", "AP\_bits", "FeatMFP1", "RDKit7",  
"hybridization"]

25 rank  
Serine/threonine-protein kinase Sgk2 : Homo sapiens  
score: 12.707 on ChEMBL5794 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL1975121	1.000000	398.11	*
MFP1	CHEMBL1975121	1.000000	398.11	*
RDKit7	CHEMBL1975121	1.000000	398.11	*
Pattern	CHEMBL1975121	1.000000	398.11	*
AP_bits	CHEMBL1975121	1.000000	398.11	*
TT_bits	CHEMBL1975121	1.000000	398.11	*
FP2	CHEMBL1975121	1.000000	398.11	*
hybridization	CHEMBL1975121	0.877451	398.11	*
substructure	CHEMBL1969049	1.000000	316.23	*
graph	CHEMBL1969049	0.829268	316.23	*
pubchem	CHEMBL1970217	1.000000	199.53	*
cdk_maccs	CHEMBL1975121	1.000000	398.11	*
klekota_roth	CHEMBL1975121	1.000000	398.11	*

\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 13 locally validated fgps ---> 605.572  
["TT\_bits", "substructure", "cdk\_maccs", "Pattern", "FP2", "MFP1",  
"klekota\_roth", "pubchem", "graph", "AP\_bits", "FeatMFP1", "RDKit7",  
"hybridization"]

26 rank  
Serine/threonine-protein kinase PRKX : Homo sapiens  
score: 12.707 on ChEMBL5818 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL1975121	1.000000	39.81	*
MFP1	CHEMBL1975121	1.000000	39.81	*
RDKit7	CHEMBL1975121	1.000000	39.81	*
Pattern	CHEMBL1975121	1.000000	39.81	*
AP_bits	CHEMBL1975121	1.000000	39.81	*
TT_bits	CHEMBL1975121	1.000000	39.81	*
FP2	CHEMBL1975121	1.000000	39.81	*
hybridization	CHEMBL1975121	0.877451	39.81	*
substructure	CHEMBL1969049	1.000000	63.10	*
graph	CHEMBL1969049	0.829268	63.10	*
pubchem	CHEMBL1970217	1.000000	39.81	*
cdk_maccs	CHEMBL1975121	1.000000	39.81	*
klekota_roth	CHEMBL1975121	1.000000	39.81	*

\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 13 locally validated fgps ---> 154.267  
["TT\_bits", "substructure", "cdk\_maccs", "Pattern", "FP2", "MFP1",  
"klekota\_roth", "pubchem", "graph", "AP\_bits", "FeatMFP1", "RDKit7",  
"hybridization"]

27 rank

Serine/threonine-protein kinase Nek4 : Homo sapiens

score: 12.707 on ChEMBL5819 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1975121		1.000000	3162.28		*
MFP1	CHEMBL1975121		1.000000	3162.28		*
RDKit7	CHEMBL1975121		1.000000	3162.28		*
Pattern	CHEMBL1975121		1.000000	3162.28		*
AP_bits	CHEMBL1975121		1.000000	3162.28		*
TT_bits	CHEMBL1975121		1.000000	3162.28		*
FP2	CHEMBL1975121		1.000000	3162.28		*
hybridization	CHEMBL1975121		0.877451	3162.28		*
substructure	CHEMBL1970217		1.000000	5011.87		*
graph	CHEMBL1970217		0.829268	5011.87		*
pubchem	CHEMBL1970217		1.000000	5011.87		*
cdk_maccs	CHEMBL1975121		1.000000	3162.28		*
klekota_roth	CHEMBL1975121		1.000000	3162.28		*

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

based on 13 locally validated fgps ---> 3514.274

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

28 rank

Ribosomal protein S6 kinase alpha 3 : Homo sapiens

score: 11.841 on ChEMBL2345 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1969049		0.947368	3981.07		*
MFP1	CHEMBL1969049		0.892857	3981.07		*
RDKit7	CHEMBL1976240		0.896082	316.23		*
Pattern	CHEMBL1976240		0.978395	316.23		*
AP_bits	CHEMBL1969049		0.875536	3981.07		*
TT_bits	CHEMBL1976240		0.833333	316.23		*
FP2	CHEMBL1969049		0.922222	3981.07		*
hybridization	CHEMBL1970217		0.806306	398.11		*
substructure	CHEMBL1969049		1.000000	3981.07		*
graph	CHEMBL1969049		0.829268	3981.07		*
pubchem	CHEMBL1970217		1.000000	398.11		*
cdk_maccs	CHEMBL1969049		0.911765	3981.07		*
klekota_roth	CHEMBL1970217		0.947368	398.11		*

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

based on 13 locally validated fgps ---> 1703.729

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

29 rank

Serine/threonine-protein kinase AKT : Homo sapiens

score: 11.841 on ChEMBL4282 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1969049		0.947368	1995.26		*
MFP1	CHEMBL1969049		0.892857	1995.26		*
RDKit7	CHEMBL1976240		0.896082	199.53		*
Pattern	CHEMBL1976240		0.978395	199.53		*
AP_bits	CHEMBL1969049		0.875536	1995.26		*
TT_bits	CHEMBL1976240		0.833333	199.53		*
FP2	CHEMBL1969049		0.922222	1995.26		*
hybridization	CHEMBL1970217		0.806306	630.96		*
substructure	CHEMBL1969049		1.000000	1995.26		*
graph	CHEMBL1969049		0.829268	1995.26		*
pubchem	CHEMBL1970217		1.000000	630.96		*

```

        cdk_maccs  CHEMBL1969049          0.911765    1995.26      *
        klekota_roth CHEMBL1970217        0.947368     630.96      *
        *** ki ACTIVITY *** value prediction
        based on 13 locally validated fgps ---> 1020.087
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

```

30 rank

Serine/threonine-protein kinase AKT3 : Homo sapiens

score: 11.841 on ChEMBL4816 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1969049		0.947368	7943.28	*	
MFP1	CHEMBL1969049		0.892857	7943.28	*	
RDKit7	CHEMBL1976240		0.896082	630.96	*	
Pattern	CHEMBL1976240		0.978395	630.96	*	
AP_bits	CHEMBL1969049		0.875536	7943.28	*	
TT_bits	CHEMBL1976240		0.833333	630.96	*	
FP2	CHEMBL1969049		0.922222	7943.28	*	
hybridization	CHEMBL1970217		0.806306	1995.26	*	
substructure	CHEMBL1969049		1.000000	7943.28	*	
graph	CHEMBL1969049		0.829268	7943.28	*	
pubchem	CHEMBL1970217		1.000000	1995.26	*	
cdk_maccs	CHEMBL1969049		0.911765	7943.28	*	
klekota_roth	CHEMBL1970217		0.947368	1995.26	*	

```

        *** ki ACTIVITY *** value prediction
        based on 13 locally validated fgps ---> 4060.324
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

```

31 rank

Dual-specificity tyrosine-phosphorylation regulated kinase 1A : Homo sapiens

score: 11.773 on ChEMBL2292 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1970217		0.947368	2511.89	*	
MFP1	CHEMBL1970217		0.862069	2511.89	*	
RDKit7	CHEMBL1976240		0.896082	5011.87	*	
Pattern	CHEMBL1976240		0.978395	5011.87	*	
AP_bits	CHEMBL1970217		0.848739	2511.89	*	
TT_bits	CHEMBL1976240		0.833333	5011.87	*	
FP2	CHEMBL1970217		0.912088	2511.89	*	
hybridization	CHEMBL1970217		0.806306	2511.89	*	
substructure	CHEMBL1970217		1.000000	2511.89	*	
graph	CHEMBL1970217		0.829268	2511.89	*	
pubchem	CHEMBL1970217		1.000000	2511.89	*	
cdk_maccs	CHEMBL1970217		0.911765	2511.89	*	
klekota_roth	CHEMBL1970217		0.947368	2511.89	*	

```

        *** ki ACTIVITY *** value prediction
        based on 13 locally validated fgps ---> 3258.708
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

```

32 rank

Mitogen-activated protein kinase kinase kinase 4 : Homo sapiens

score: 11.773 on ChEMBL6166 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1970217		0.947368	2511.89	*	

MFP1	CHEMBL1970217	0.862069	2511.89	*
RDKit7	CHEMBL1976240	0.896082	1995.26	*
Pattern	CHEMBL1976240	0.978395	1995.26	*
AP_bits	CHEMBL1970217	0.848739	2511.89	*
TT_bits	CHEMBL1976240	0.833333	1995.26	*
FP2	CHEMBL1970217	0.912088	2511.89	*
hybridization	CHEMBL1970217	0.806306	2511.89	*
substructure	CHEMBL1970217	1.000000	2511.89	*
graph	CHEMBL1970217	0.829268	2511.89	*
pubchem	CHEMBL1970217	1.000000	2511.89	*
cdk_maccs	CHEMBL1970217	0.911765	2511.89	*
klekota_roth	CHEMBL1970217	0.947368	2511.89	*

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

based on 13 locally validated fgps ---> 3083.520

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

33 rank

Dual specificity protein kinase CLK2 : Homo sapiens

score: 11.614 on ChEMBL4225 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1970217		0.947368	3981.07		*
MFP1	CHEMBL1970217		0.862069	3981.07		*
RDKit7	CHEMBL1970217		0.863711	3981.07		*
Pattern	CHEMBL1970217		0.929619	3981.07		*
AP_bits	CHEMBL1970217		0.848739	3981.07		*
TT_bits	CHEMBL1970217		0.755556	3981.07		*
FP2	CHEMBL1970217		0.912088	3981.07		*
hybridization	CHEMBL1970217		0.806306	3981.07		*
substructure	CHEMBL1970217		1.000000	3981.07		*
graph	CHEMBL1970217		0.829268	3981.07		*
pubchem	CHEMBL1970217		1.000000	3981.07		*
cdk_maccs	CHEMBL1970217		0.911765	3981.07		*
klekota_roth	CHEMBL1970217		0.947368	3981.07		*

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

based on 13 locally validated fgps ---> 4095.601

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

34 rank

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

score: 10.576 on ChEMBL2185 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1984633		0.947368	3162.28		*
MFP1	CHEMBL1994724		0.827586	398.11		*
RDKit7	CHEMBL1976240		0.896082	6309.57		*
Pattern	CHEMBL1976240		0.978395	6309.57		*
AP_bits	CHEMBL1976240		0.772908	6309.57		*
TT_bits	CHEMBL1976240		0.833333	6309.57		*
FP2	CHEMBL1976240		0.892473	6309.57		*
hybridization	CHEMBL1976240		0.797357	6309.57		*
substructure	CHEMBL1994724		0.937500	398.11		*
graph	CHEMBL1976240		0.755556	6309.57		*
pubchem	CHEMBL1976240		0.983146	6309.57		*
cdk_maccs	CHEMBL1994724		0.837838	398.11		*
klekota_roth	CHEMBL1984633		0.871795	3162.28		*

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

based on 12 locally validated fgps ---> 3348.419

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

35 rank

Vascular endothelial growth factor receptor 3 : Homo sapiens

score: 10.260 on ChEMBL1955 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL2004934		0.857143	6309.57	*	
MFP1	ChEMBL2004934		0.862069	6309.57	*	
RDKit7	ChEMBL2004934		0.790977	6309.57	*	
Pattern	ChEMBL1999428		0.895899	501.19	*	
AP_bits	ChEMBL2004934		0.834025	6309.57	*	
TT_bits	ChEMBL2004934		0.777778	6309.57	*	
FP2	ChEMBL2004934		0.873684	6309.57	*	
hybridization	ChEMBL2004934		0.795556	6309.57	*	
substructure	ChEMBL2004934		0.937500	6309.57	*	
graph	ChEMBL2004934		0.723404	6309.57	*	
pubchem	ChEMBL2004934		0.983146	6309.57	*	
cdk_maccs	ChEMBL2004934		0.837838	6309.57	*	
klekota_roth	ChEMBL2004934		0.813953	6309.57	*	

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

based on 12 locally validated fgps ---> 4188.072

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

36 rank

Dual-specificity tyrosine-phosphorylation regulated kinase 3 : Homo sapiens

score: 9.666 on ChEMBL4575 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL1984633		0.947368	1995.26	*	
MFP1	ChEMBL1984633		0.774194	1995.26	*	
RDKit7	ChEMBL2007296		0.939286	794.33	*	
Pattern	ChEMBL2007296		0.969419	794.33	*	
AP_bits	ChEMBL2007296		0.722628	794.33	*	
TT_bits	ChEMBL2007296		0.857143	794.33	*	
FP2	ChEMBL2007296		0.922222	794.33	*	
hybridization	ChEMBL2007296		0.746888	794.33	*	
substructure	ChEMBL2007296		0.937500	794.33	*	
graph	ChEMBL2007296		0.739130	794.33	*	
pubchem	ChEMBL2007296		0.977654	794.33	*	
cdk_maccs	ChEMBL1984633		0.775000	1995.26	*	
klekota_roth	ChEMBL1984633		0.871795	1995.26	*	

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

based on 11 locally validated fgps ---> 948.221

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

37 rank

Serine/threonine-protein kinase Chk2 : Homo sapiens

score: 9.495 on ChEMBL2527 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL1976240		0.850000	398.11	*	
MFP1	ChEMBL1976240		0.766667	398.11	*	
RDKit7	ChEMBL1976240		0.896082	398.11	*	
Pattern	ChEMBL1976240		0.978395	398.11	*	
AP_bits	ChEMBL1976240		0.772908	398.11	*	
TT_bits	ChEMBL1976240		0.833333	398.11	*	

FP2	CHEMBL1976240	0.892473	398.11	*
hybridization	CHEMBL1976240	0.797357	398.11	*
substructure	CHEMBL1969264	0.875000	794.33	*
graph	CHEMBL1976240	0.755556	398.11	
pubchem	CHEMBL1976240	0.983146	398.11	*
cdk_maccs	CHEMBL1976240	0.731707	398.11	
klekota_roth	CHEMBL1976240	0.850000	398.11	*

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

based on 11 locally validated fgps ---> 450.893

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

38 rank

AMP-activated protein kinase, alpha-1 subunit : Homo sapiens

score: 9.495 on ChEMBL4045 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1976240		0.850000	251.19	*
MFP1	CHEMBL1976240		0.766667	251.19	*
RDKit7	CHEMBL1976240		0.896082	251.19	*
Pattern	CHEMBL1976240		0.978395	251.19	*
AP_bits	CHEMBL1976240		0.772908	251.19	*
TT_bits	CHEMBL1976240		0.833333	251.19	*
FP2	CHEMBL1976240		0.892473	251.19	*
hybridization	CHEMBL1976240		0.797357	251.19	*
substructure	CHEMBL1969264		0.875000	501.19	*
graph	CHEMBL1976240		0.755556	251.19	
pubchem	CHEMBL1976240		0.983146	251.19	*
cdk_maccs	CHEMBL1976240		0.731707	251.19	
klekota_roth	CHEMBL1976240		0.850000	251.19	*

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

based on 11 locally validated fgps ---> 326.755

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

39 rank

Casein kinase I alpha : Homo sapiens

score: 8.135 on ChEMBL2793 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1994724		0.900000	1584.89	*
MFP1	CHEMBL1994724		0.827586	1584.89	*
RDKit7	CHEMBL1990254		0.716753	5011.87	
Pattern	CHEMBL1990254		0.911950	5011.87	*
AP_bits	CHEMBL1994724		0.620690	1584.89	*
TT_bits	CHEMBL1994724		0.702128	1584.89	*
FP2	CHEMBL1990254		0.706522	5011.87	*
hybridization	CHEMBL1994724		0.640569	1584.89	
substructure	CHEMBL1994724		0.937500	1584.89	*
graph	CHEMBL1997275		0.698925	2511.89	
pubchem	CHEMBL1994724		0.880829	1584.89	*
cdk_maccs	CHEMBL1994724		0.837838	1584.89	*
klekota_roth	CHEMBL1994724		0.809524	1584.89	*

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

based on 10 locally validated fgps ---> 2453.148

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

40 rank

Macrophage colony stimulating factor receptor : Homo sapiens

score: 8.129 on ChEMBL1844 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
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Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1999428	0.833333	2511.89	*	
MFP1	CHEMBL1999428	0.800000	2511.89	*	
RDKit7	CHEMBL1999428	0.785171	2511.89	*	
Pattern	CHEMBL1999428	0.895899	2511.89	*	
AP_bits	CHEMBL1999428	0.768519	2511.89	*	
TT_bits	CHEMBL1999428	0.756098	2511.89	*	
FP2	CHEMBL1999428	0.783133	2511.89	*	
hybridization	CHEMBL1999428	0.651961	2511.89		
substructure	CHEMBL1999428	0.933333	2511.89	*	
graph	CHEMBL1999428	0.597561	2511.89		
pubchem	CHEMBL1991356	0.866667	2511.89	*	
cdk_maccs	CHEMBL1991356	0.731707	2511.89		
klekota_roth	CHEMBL1999428	0.707317	2511.89	*	

\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 10 locally validated fgps ---> 2486.892  
["TT\_bits", "substructure", "Pattern", "FP2", "MFP1", "klekota\_roth",  
"pubchem", "AP\_bits", "FeatMFP1", "RDKit7"]

41 rank

Serine/threonine-protein kinase c-TAK1 : Homo sapiens

score: 8.062 on ChEMBL5600 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1991188	0.857143	3162.28	*	
MFP1	CHEMBL1991188	0.750000	3162.28	*	
RDKit7	CHEMBL1990254	0.716753	5011.87		
Pattern	CHEMBL1990254	0.911950	5011.87	*	
AP_bits	CHEMBL1991188	0.680556	3162.28	*	
TT_bits	CHEMBL2006188	0.700000	5011.87	*	
FP2	CHEMBL1991188	0.790476	3162.28	*	
hybridization	CHEMBL1991188	0.728745	3162.28	*	
substructure	CHEMBL1991188	0.882353	3162.28	*	
graph	CHEMBL2006188	0.680000	5011.87		
pubchem	CHEMBL1991188	0.951087	3162.28	*	
cdk_maccs	CHEMBL1991188	0.756098	3162.28		
klekota_roth	CHEMBL1991188	0.809524	3162.28	*	

\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 10 locally validated fgps ---> 3883.412  
["TT\_bits", "substructure", "Pattern", "AP\_bits", "MFP1", "pubchem",  
"FP2", "FeatMFP1", "klekota\_roth", "hybridization"]

42 rank

Serine/threonine-protein kinase 2 : Homo sapiens

score: 7.984 on ChEMBL4202 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1991188	0.857143	6309.57	*	
MFP1	CHEMBL1991188	0.750000	6309.57	*	
RDKit7	CHEMBL1990254	0.716753	2511.89		
Pattern	CHEMBL1990254	0.911950	2511.89	*	
AP_bits	CHEMBL1991188	0.680556	6309.57	*	
TT_bits	CHEMBL1990254	0.622222	2511.89	*	
FP2	CHEMBL1991188	0.790476	6309.57	*	
hybridization	CHEMBL1991188	0.728745	6309.57	*	
substructure	CHEMBL1991188	0.882353	6309.57	*	
graph	CHEMBL1991188	0.644860	6309.57		
pubchem	CHEMBL1991188	0.951087	6309.57	*	
cdk_maccs	CHEMBL1991188	0.756098	6309.57		
klekota_roth	CHEMBL1991188	0.809524	6309.57	*	

\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 10 locally validated fgps ---> 4579.270



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

43 rank

Mitogen-activated protein kinase kinase kinase kinase 2 : Homo sapiens  
score: 7.984 on ChEMBL5330 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1991188		0.857143	6309.57		*
MFP1	CHEMBL1991188		0.750000	6309.57		*
RDKit7	CHEMBL1990254		0.716753	3981.07		
Pattern	CHEMBL1990254		0.911950	3981.07		*
AP_bits	CHEMBL1991188		0.680556	6309.57		*
TT_bits	CHEMBL1990254		0.622222	3981.07		*
FP2	CHEMBL1991188		0.790476	6309.57		*
hybridization	CHEMBL1991188		0.728745	6309.57		*
substructure	CHEMBL1991188		0.882353	6309.57		*
graph	CHEMBL1991188		0.644860	6309.57		
pubchem	CHEMBL1991188		0.951087	6309.57		*
cdk_maccs	CHEMBL1991188		0.756098	6309.57		
klekota_roth	CHEMBL1991188		0.809524	6309.57		*

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

based on 10 locally validated fgps ---> 4857.933

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

44 rank

Cell division protein kinase 8 : Homo sapiens  
score: 7.435 on ChEMBL5719 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1994724		0.900000	3162.28		*
MFP1	CHEMBL1994724		0.827586	3162.28		*
RDKit7	CHEMBL1986143		0.688633	2511.89		
Pattern	CHEMBL1986143		0.919003	2511.89		*
AP_bits	CHEMBL1994724		0.620690	3162.28		*
TT_bits	CHEMBL1994724		0.702128	3162.28		*
FP2	CHEMBL1986143		0.676768	2511.89		
hybridization	CHEMBL1994724		0.640569	3162.28		
substructure	CHEMBL1994724		0.937500	3162.28		*
graph	CHEMBL1997275		0.698925	251.19		
pubchem	CHEMBL1994724		0.880829	3162.28		*
cdk_maccs	CHEMBL1994724		0.837838	3162.28		*
klekota_roth	CHEMBL1994724		0.809524	3162.28		*

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

based on 9 locally validated fgps ---> 2940.331

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

45 rank

G protein-coupled receptor kinase 5 : Homo sapiens  
score: 7.397 on ChEMBL5678 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1994724		0.900000	1000.00		*
MFP1	CHEMBL1994724		0.827586	1000.00		*
RDKit7	CHEMBL1994724		0.554632	1000.00		
Pattern	CHEMBL2004159		0.875758	3981.07		*
AP_bits	CHEMBL2004159		0.625483	3981.07		*
TT_bits	CHEMBL1994724		0.702128	1000.00		*
FP2	CHEMBL1994724		0.640625	1000.00		
hybridization	CHEMBL1994724		0.640569	1000.00		
substructure	CHEMBL1994724		0.937500	1000.00		*

```

graph CHEMBL1986590 0.577778 3162.28
pubchem CHEMBL1994724 0.880829 1000.00 *
cdk_maccs CHEMBL1994724 0.837838 1000.00 *
klekota_roth CHEMBL1994724 0.809524 1000.00 *
*** ki ACTIVITY *** value prediction
based on 9 locally validated fgps ---> 1801.323
["TT_bits", "substructure", "Pattern", "MFP1", "pubchem", "AP_bits",
"FeatMFP1", "klekota_roth", "cdk_maccs"]

```

46 rank

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

score: 7.377 on CHEMBL4722 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1994724		0.900000	199.53	*	
MFP1	CHEMBL1994724		0.827586	199.53	*	
RDKit7	CHEMBL1994724		0.554632	199.53		
Pattern	CHEMBL1994724		0.860795	199.53	*	
AP_bits	CHEMBL1994724		0.620690	199.53	*	
TT_bits	CHEMBL1994724		0.702128	199.53	*	
FP2	CHEMBL1994724		0.640625	199.53		
hybridization	CHEMBL1994724		0.640569	199.53		
substructure	CHEMBL1994724		0.937500	199.53	*	
graph	CHEMBL1965845		0.583333	63.10		
pubchem	CHEMBL1994724		0.880829	199.53	*	
cdk_maccs	CHEMBL1994724		0.837838	199.53	*	
klekota_roth	CHEMBL1994724		0.809524	199.53	*	

```

*** ki ACTIVITY *** value prediction
based on 9 locally validated fgps ---> 295.853
["TT_bits", "substructure", "Pattern", "MFP1", "pubchem", "AP_bits",
"FeatMFP1", "klekota_roth", "cdk_maccs"]

```

47 rank

Activin receptor type-1 : Homo sapiens

score: 7.377 on CHEMBL5903 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1994724		0.900000	2511.89	*	
MFP1	CHEMBL1994724		0.827586	2511.89	*	
RDKit7	CHEMBL1994724		0.554632	2511.89		
Pattern	CHEMBL1994724		0.860795	2511.89	*	
AP_bits	CHEMBL1994724		0.620690	2511.89	*	
TT_bits	CHEMBL1994724		0.702128	2511.89	*	
FP2	CHEMBL1994724		0.640625	2511.89		
hybridization	CHEMBL1994724		0.640569	2511.89		
substructure	CHEMBL1994724		0.937500	2511.89	*	
graph	CHEMBL1980329		0.563830	3162.28		
pubchem	CHEMBL1994724		0.880829	2511.89	*	
cdk_maccs	CHEMBL1994724		0.837838	2511.89	*	
klekota_roth	CHEMBL1994724		0.809524	2511.89	*	

```

*** ki ACTIVITY *** value prediction
based on 9 locally validated fgps ---> 2546.777
["TT_bits", "substructure", "Pattern", "MFP1", "pubchem", "AP_bits",
"FeatMFP1", "klekota_roth", "cdk_maccs"]

```

48 rank

LIM domain kinase 1 : Homo sapiens

score: 7.268 on CHEMBL3836 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1999428		0.833333	7943.28	*	
MFP1	CHEMBL1999428		0.800000	7943.28	*	
RDKit7	CHEMBL1999428		0.785171	7943.28	*	

Pattern	CHEMBL1996931	0.901493	3162.28	*
AP_bits	CHEMBL1999428	0.768519	7943.28	*
TT_bits	CHEMBL1999428	0.756098	7943.28	*
FP2	CHEMBL1999428	0.783133	7943.28	*
hybridization	CHEMBL1999428	0.651961	7943.28	
substructure	CHEMBL1999428	0.933333	7943.28	*
graph	CHEMBL1999428	0.597561	7943.28	
pubchem	CHEMBL1999428	0.817143	7943.28	
cdk_maccs	CHEMBL1999428	0.709677	7943.28	
klekota_roth	CHEMBL1999428	0.707317	7943.28	*

\*\*\* ki ACTIVITY \*\*\* value prediction  
 based on 9 locally validated fgps ---> 7266.786  
 ["TT\_bits", "substructure", "Pattern", "FP2", "MFP1", "klekota\_roth",  
 "AP\_bits", "FeatMFP1", "RDKit7"]

49 rank

Serine/threonine-protein kinase PLK3 : Homo sapiens

score: 7.267 on ChEMBL4897 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1999428	0.833333	1995.26	*	
MFP1	CHEMBL1999428	0.800000	1995.26	*	
RDKit7	CHEMBL1999428	0.785171	1995.26	*	
Pattern	CHEMBL1999428	0.895899	1995.26	*	
AP_bits	CHEMBL1999428	0.768519	1995.26	*	
TT_bits	CHEMBL1999428	0.756098	1995.26	*	
FP2	CHEMBL1999428	0.783133	1995.26	*	
hybridization	CHEMBL1999428	0.651961	1995.26		
substructure	CHEMBL2005375	0.937500	12.59	*	
graph	CHEMBL1999428	0.597561	1995.26		
pubchem	CHEMBL1999428	0.817143	1995.26		
cdk_maccs	CHEMBL1999428	0.709677	1995.26		
klekota_roth	CHEMBL1999428	0.707317	1995.26	*	

\*\*\* ki ACTIVITY \*\*\* value prediction  
 based on 9 locally validated fgps ---> 1884.866  
 ["TT\_bits", "substructure", "Pattern", "FP2", "MFP1", "klekota\_roth",  
 "AP\_bits", "FeatMFP1", "RDKit7"]

50 rank

Vascular endothelial growth factor receptor 1 : Homo sapiens

score: 7.263 on ChEMBL1868 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1999428	0.833333	158.49	*	
MFP1	CHEMBL1999428	0.800000	158.49	*	
RDKit7	CHEMBL1999428	0.785171	158.49	*	
Pattern	CHEMBL1999428	0.895899	158.49	*	
AP_bits	CHEMBL1999428	0.768519	158.49	*	
TT_bits	CHEMBL1999428	0.756098	158.49	*	
FP2	CHEMBL1999428	0.783133	158.49	*	
hybridization	CHEMBL1999428	0.651961	158.49		
substructure	CHEMBL1999428	0.933333	158.49	*	
graph	CHEMBL1999428	0.597561	158.49		
pubchem	CHEMBL1999428	0.817143	158.49		
cdk_maccs	CHEMBL1999428	0.709677	158.49		
klekota_roth	CHEMBL1999428	0.707317	158.49	*	

\*\*\* ki ACTIVITY \*\*\* value prediction  
 based on 9 locally validated fgps ---> 319.984  
 ["TT\_bits", "substructure", "Pattern", "FP2", "MFP1", "klekota\_roth",  
 "AP\_bits", "FeatMFP1", "RDKit7"]

51 rank

Tyrosine-protein kinase receptor FLT3 : Homo sapiens

score: 7.263 on ChEMBL1974 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1999428		0.833333	316.23		*
MFP1	CHEMBL1999428		0.800000	316.23		*
RDKit7	CHEMBL1999428		0.785171	316.23		*
Pattern	CHEMBL1999428		0.895899	316.23		*
AP_bits	CHEMBL1999428		0.768519	316.23		*
TT_bits	CHEMBL1999428		0.756098	316.23		*
FP2	CHEMBL1999428		0.783133	316.23		*
hybridization	CHEMBL1999428		0.651961	316.23		
substructure	CHEMBL1999428		0.933333	316.23		*
graph	CHEMBL1997275		0.698925	1584.89		
pubchem	CHEMBL1997275		0.842640	1584.89		
cdk_maccs	CHEMBL1982924		0.731707	398.11		
klekota_roth	CHEMBL1999428		0.707317	316.23		*

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

based on 9 locally validated fgps ---> 320.632

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

52 rank

Vascular endothelial growth factor receptor 2 : Homo sapiens

score: 7.263 on ChEMBL279 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1999428		0.833333	6309.57		*
MFP1	CHEMBL1999428		0.800000	6309.57		*
RDKit7	CHEMBL1999428		0.785171	6309.57		*
Pattern	CHEMBL1999428		0.895899	6309.57		*
AP_bits	CHEMBL1999428		0.768519	6309.57		*
TT_bits	CHEMBL1999428		0.756098	6309.57		*
FP2	CHEMBL1999428		0.783133	6309.57		*
hybridization	CHEMBL1999428		0.651961	6309.57		
substructure	CHEMBL1999428		0.933333	6309.57		*
graph	CHEMBL1997275		0.698925	2511.89		
pubchem	CHEMBL1997275		0.842640	2511.89		
cdk_maccs	CHEMBL1999428		0.709677	6309.57		
klekota_roth	CHEMBL1999428		0.707317	6309.57		*

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

based on 9 locally validated fgps ---> 6184.382

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

53 rank

Macrophage-stimulating protein receptor : Homo sapiens

score: 6.864 on ChEMBL2689 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL2003514		0.947368	398.11		*
MFP1	CHEMBL2003514		0.925926	398.11		*
RDKit7	CHEMBL2003514		0.575967	398.11		
Pattern	CHEMBL2003514		0.957576	398.11		*
AP_bits	CHEMBL2003514		0.804979	398.11		*
TT_bits	CHEMBL2003514		0.620000	398.11		*
FP2	CHEMBL2003514		0.640351	398.11		
hybridization	CHEMBL2003514		0.593625	398.11		
substructure	CHEMBL1984296		0.875000	3981.07		*
graph	CHEMBL1997275		0.698925	2511.89		
pubchem	CHEMBL1997275		0.842640	2511.89		
cdk_maccs	CHEMBL2003514		0.861111	398.11		*
klekota_roth	CHEMBL2003514		0.871795	398.11		*

\*\*\* ki ACTIVITY \*\*\* value prediction  
 based on 8 locally validated fgps ---> 622.045  
 ["TT\_bits", "substructure", "Pattern", "MFP1", "AP\_bits", "FeatMFP1",  
 "klekota\_roth", "cdk\_maccs"]

54 rank

Serine/threonine-protein kinase 17A : Homo sapiens

score: 6.301 on ChEMBL4525 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL1984633		0.947368	3162.28		*
MFP1	ChEMBL1984633		0.774194	3162.28		*
RDKit7	ChEMBL1990254		0.716753	1584.89		
Pattern	ChEMBL1990254		0.911950	1584.89		*
AP_bits	ChEMBL1990254		0.600000	1584.89		*
TT_bits	ChEMBL1990254		0.622222	1584.89		*
FP2	ChEMBL1990254		0.706522	1584.89		*
hybridization	ChEMBL1990254		0.605381	1584.89		
substructure	ChEMBL1978099		0.823529	1000.00		
graph	ChEMBL1965845		0.583333	1258.93		
pubchem	ChEMBL1991356		0.866667	630.96		*
cdk_maccs	ChEMBL1984633		0.775000	3162.28		
klekota_roth	ChEMBL1984633		0.871795	3162.28		*

\*\*\* ki ACTIVITY \*\*\* value prediction  
 based on 8 locally validated fgps ---> 2246.329  
 ["TT\_bits", "Pattern", "AP\_bits", "MFP1", "pubchem", "FP2", "FeatMFP1",  
 "klekota\_roth"]

55 rank

Serine/threonine-protein kinase PIM1 : Homo sapiens

score: 5.872 on ChEMBL2147 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL1990254		0.700000	3981.07		
MFP1	ChEMBL1997534		0.594595	3162.28		*
RDKit7	ChEMBL1990254		0.716753	3981.07		
Pattern	ChEMBL1990254		0.911950	3981.07		*
AP_bits	ChEMBL1990254		0.600000	3981.07		*
TT_bits	ChEMBL1990254		0.622222	3981.07		*
FP2	ChEMBL1990254		0.706522	3981.07		*
hybridization	ChEMBL1990254		0.605381	3981.07		
substructure	ChEMBL1997534		0.882353	3162.28		*
graph	ChEMBL272476		0.654762	4500.00		
pubchem	ChEMBL1991356		0.866667	501.19		*
cdk_maccs	ChEMBL1991356		0.731707	501.19		
klekota_roth	ChEMBL1997534		0.687500	3162.28		*

\*\*\* ki ACTIVITY \*\*\* value prediction  
 based on 8 locally validated fgps ---> 3289.999  
 ["TT\_bits", "substructure", "Pattern", "AP\_bits", "MFP1", "pubchem",  
 "FP2", "klekota\_roth"]

56 rank

Casein kinase I gamma 1 : Homo sapiens

score: 5.559 on ChEMBL2426 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL1984633		0.947368	5011.87		*
MFP1	ChEMBL1984633		0.774194	5011.87		*
RDKit7	ChEMBL1996931		0.517442	630.96		
Pattern	ChEMBL1996931		0.901493	630.96		*
AP_bits	ChEMBL1984633		0.557971	5011.87		*
TT_bits	ChEMBL1984633		0.568627	5011.87		*
FP2	ChEMBL1996931		0.556522	630.96		

```

hybridization CHEMBL1984633 0.472727 5011.87
substructure CHEMBL2005375 0.937500 1995.26 *
graph CHEMBL1996831 0.566265 1584.89
pubchem CHEMBL1982924 0.804762 1000.00
cdk_maccs CHEMBL1984633 0.775000 5011.87
klekota_roth CHEMBL1984633 0.871795 5011.87 *
*** ki ACTIVITY *** value prediction
based on 7 locally validated fgps ---> 3886.443
["TT_bits", "substructure", "Pattern", "MFP1", "AP_bits", "FeatMFP1",
"klekota_roth"]

```

57 rank

Protein kinase C nu : Homo sapiens

score: 5.060 on CHEMBL2595 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	2511.89	
MFP1	CHEMBL1997534		0.594595	794.33	*
RDKit7	CHEMBL1990254		0.716753	2511.89	
Pattern	CHEMBL1990254		0.911950	2511.89	*
AP_bits	CHEMBL1990254		0.600000	2511.89	*
TT_bits	CHEMBL1990254		0.622222	2511.89	*
FP2	CHEMBL1990254		0.706522	2511.89	*
hybridization	CHEMBL1990254		0.605381	2511.89	
substructure	CHEMBL2005375		0.937500	1995.26	*
graph	CHEMBL1997275		0.698925	794.33	
pubchem	CHEMBL1997275		0.842640	794.33	
cdk_maccs	CHEMBL1982924		0.731707	2511.89	
klekota_roth	CHEMBL1997534		0.687500	794.33	*

```

*** ki ACTIVITY *** value prediction
based on 7 locally validated fgps ---> 1864.173
["TT_bits", "substructure", "Pattern", "AP_bits", "MFP1", "FP2",
"klekota_roth"]

```

58 rank

CaM kinase II delta : Homo sapiens

score: 5.060 on CHEMBL2801 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	2511.89	
MFP1	CHEMBL1997534		0.594595	5011.87	*
RDKit7	CHEMBL1990254		0.716753	2511.89	
Pattern	CHEMBL1990254		0.911950	2511.89	*
AP_bits	CHEMBL1990254		0.600000	2511.89	*
TT_bits	CHEMBL1990254		0.622222	2511.89	*
FP2	CHEMBL1990254		0.706522	2511.89	*
hybridization	CHEMBL1990254		0.605381	2511.89	
substructure	CHEMBL2005375		0.937500	5011.87	*
graph	CHEMBL2002649		0.581197	1584.89	
pubchem	CHEMBL1982924		0.804762	1258.93	
cdk_maccs	CHEMBL1982924		0.731707	1258.93	
klekota_roth	CHEMBL1997534		0.687500	5011.87	*

```

*** ki ACTIVITY *** value prediction
based on 7 locally validated fgps ---> 3583.310
["TT_bits", "substructure", "Pattern", "AP_bits", "MFP1", "FP2",
"klekota_roth"]

```

59 rank

CaM kinase II gamma : Homo sapiens

score: 5.060 on CHEMBL3829 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	3162.28	

MFP1	CHEMBL1997534	0.594595	5011.87	*
RDKit7	CHEMBL1990254	0.716753	3162.28	
Pattern	CHEMBL1990254	0.911950	3162.28	*
AP_bits	CHEMBL1990254	0.600000	3162.28	*
TT_bits	CHEMBL1990254	0.622222	3162.28	*
FP2	CHEMBL1990254	0.706522	3162.28	*
hybridization	CHEMBL1990254	0.605381	3162.28	
substructure	CHEMBL2005375	0.937500	2511.89	*
graph	CHEMBL1965845	0.583333	5011.87	
pubchem	CHEMBL1982924	0.804762	630.96	
cdk_maccs	CHEMBL1982924	0.731707	630.96	
klekota_roth	CHEMBL1997534	0.687500	5011.87	*

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

based on 7 locally validated fgps ---> 3770.980

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

60 rank

Serine/threonine-protein kinase D2 : Homo sapiens

score: 5.060 on ChEMBL4900 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254	0.700000	1258.93		
MFP1	CHEMBL1997534	0.594595	398.11		*
RDKit7	CHEMBL1990254	0.716753	1258.93		
Pattern	CHEMBL1990254	0.911950	1258.93		*
AP_bits	CHEMBL1990254	0.600000	1258.93		*
TT_bits	CHEMBL1990254	0.622222	1258.93		*
FP2	CHEMBL1990254	0.706522	1258.93		*
hybridization	CHEMBL1990254	0.605381	1258.93		
substructure	CHEMBL2005375	0.937500	5011.87		*
graph	CHEMBL1965845	0.583333	501.19		
pubchem	CHEMBL1982924	0.804762	1995.26		
cdk_maccs	CHEMBL1982924	0.731707	1995.26		
klekota_roth	CHEMBL1997534	0.687500	398.11		*

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

based on 7 locally validated fgps ---> 1229.548

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

61 rank

Mitogen-activated protein kinase kinase kinase kinase 5 : Homo sapiens

score: 5.022 on ChEMBL4852 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254	0.700000	2511.89		
MFP1	CHEMBL1997534	0.594595	316.23		*
RDKit7	CHEMBL1990254	0.716753	2511.89		
Pattern	CHEMBL1990254	0.911950	2511.89		*
AP_bits	CHEMBL1990254	0.600000	2511.89		*
TT_bits	CHEMBL1990254	0.622222	2511.89		*
FP2	CHEMBL1977135	0.722892	7943.28		*
hybridization	CHEMBL1977135	0.627451	7943.28		
substructure	CHEMBL1997534	0.882353	316.23		*
graph	CHEMBL1977135	0.597561	7943.28		
pubchem	CHEMBL1982924	0.804762	2511.89		
cdk_maccs	CHEMBL1982924	0.731707	2511.89		
klekota_roth	CHEMBL1997534	0.687500	316.23		*

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

based on 7 locally validated fgps ---> 2494.818

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

62 rank

CaM kinase II beta : Homo sapiens

score: 5.005 on ChEMBL4121 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	7943.28	
MFP1	CHEMBL1997534		0.594595	3162.28	*
RDKit7	CHEMBL1990254		0.716753	7943.28	
Pattern	CHEMBL1990254		0.911950	7943.28	*
AP_bits	CHEMBL1990254		0.600000	7943.28	*
TT_bits	CHEMBL1990254		0.622222	7943.28	*
FP2	CHEMBL1990254		0.706522	7943.28	*
hybridization	CHEMBL1990254		0.605381	7943.28	
substructure	CHEMBL1997534		0.882353	3162.28	*
graph	CHEMBL1965845		0.583333	7943.28	
pubchem	CHEMBL1982924		0.804762	1584.89	
cdk_maccs	CHEMBL1982924		0.731707	1584.89	
klekota_roth	CHEMBL1997534		0.687500	3162.28	*

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

based on 7 locally validated fgps ---> 5782.081

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

63 rank

MAP kinase signal-integrating kinase 2 : Homo sapiens

score: 4.590 on ChEMBL4204 based on 6 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	3981.07	
MFP1	CHEMBL1990254		0.566667	3981.07	
RDKit7	CHEMBL1990254		0.716753	3981.07	
Pattern	CHEMBL1990254		0.911950	3981.07	*
AP_bits	CHEMBL1990254		0.600000	3981.07	*
TT_bits	CHEMBL1990254		0.622222	3981.07	*
FP2	CHEMBL1990254		0.706522	3981.07	*
hybridization	CHEMBL1990254		0.605381	3981.07	
substructure	CHEMBL3632744		0.882353	18.00	*
graph	CHEMBL1965845		0.583333	630.96	
pubchem	CHEMBL1991356		0.866667	3981.07	*
cdk_maccs	CHEMBL1982924		0.731707	1584.89	
klekota_roth	CHEMBL1990254		0.595238	3981.07	

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

based on 6 locally validated fgps ---> 3320.558

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

64 rank

Casein kinase I delta : Homo sapiens

score: 4.582 on ChEMBL2828 based on 6 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	1000.00	
MFP1	CHEMBL1990254		0.566667	1000.00	
RDKit7	CHEMBL1990254		0.716753	1000.00	
Pattern	CHEMBL1990254		0.911950	1000.00	*
AP_bits	CHEMBL1990254		0.600000	1000.00	*
TT_bits	CHEMBL1990254		0.622222	1000.00	*
FP2	CHEMBL1990254		0.706522	1000.00	*
hybridization	CHEMBL1990254		0.605381	1000.00	
substructure	CHEMBL1969264		0.875000	1258.93	*
graph	CHEMBL2002649		0.581197	3162.28	
pubchem	CHEMBL1991356		0.866667	158.49	*
cdk_maccs	CHEMBL1982924		0.731707	3981.07	



```

klekota_roth CHEMBL1990254          0.595238    1000.00
*** ki ACTIVITY *** value prediction
based on 6 locally validated fgps ---> 1129.748
["TT_bits", "substructure", "Pattern", "AP_bits", "pubchem", "FP2"]

```

65 rank

Cytochrome P450 3A4 : Homo sapiens

score: 3.876 on ChEMBL340 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3338848		0.695652	5600.0	
MFP1	CHEMBL2152014		0.593750	540.0	*
RDKit7	CHEMBL3338848		0.334451	5600.0	
Pattern	CHEMBL1743350		0.829851	2600.0	
AP_bits	CHEMBL2152010		0.530534	3100.0	*
TT_bits	CHEMBL2152014		0.354839	540.0	
FP2	CHEMBL2152014		0.488189	540.0	
hybridization	CHEMBL3338848		0.433702	5600.0	
substructure	CHEMBL3338848		1.000000	5600.0	*
graph	CHEMBL2152010		0.727273	3100.0	
pubchem	CHEMBL2152014		0.869110	540.0	*
cdk_maccs	CHEMBL2152010		0.882353	3100.0	*
klekota_roth	CHEMBL2152014		0.307692	540.0	

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

based on 5 locally validated fgps ---> 4783.422

["AP\_bits", "cdk\_maccs", "MFP1", "substructure", "pubchem"]

66 rank

Neurokinin 3 receptor : Homo sapiens

score: 3.739 on ChEMBL4429 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL2113673		0.772727	1.80	*
MFP1	CHEMBL297736		0.625000	57.00	*
RDKit7	CHEMBL1277075		0.462779	158.49	
Pattern	CHEMBL51352		0.754386	355.00	
AP_bits	CHEMBL50291		0.550314	666.00	*
TT_bits	CHEMBL1277075		0.385965	158.49	
FP2	CHEMBL51120		0.567797	870.00	
hybridization	CHEMBL10295		0.630522	1144.00	
substructure	CHEMBL10536		0.933333	295.00	*
graph	CHEMBL10079		0.730337	13.80	
pubchem	CHEMBL50742		0.826531	919.00	
cdk_maccs	CHEMBL53699		0.857143	1671.00	*
klekota_roth	CHEMBL274763		0.480769	251.19	

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

based on 5 locally validated fgps ---> 752.461

["FeatMFP1", "AP\_bits", "MFP1", "substructure", "cdk\_maccs"]

67 rank

BR serine/threonine-protein kinase 1 : Homo sapiens

score: 3.719 on ChEMBL5650 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	398.11	
MFP1	CHEMBL1974288		0.586207	5011.87	
RDKit7	CHEMBL1990254		0.716753	398.11	
Pattern	CHEMBL1974288		0.912500	5011.87	*
AP_bits	CHEMBL1990254		0.600000	398.11	*
TT_bits	CHEMBL1974288		0.622222	5011.87	*
FP2	CHEMBL1974288		0.709677	5011.87	*
hybridization	CHEMBL1990254		0.605381	398.11	
substructure	CHEMBL1982924		0.875000	6309.57	*

graph	CHEMBL1965845	0.583333	1584.89
pubchem	CHEMBL1974288	0.824176	5011.87
cdk_maccs	CHEMBL1982924	0.731707	6309.57
klekota_roth	CHEMBL1990254	0.595238	398.11

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

based on 5 locally validated fgps ---> 3789.103

["Pattern", "FP2", "TT\_bits", "substructure", "AP\_bits"]

68 rank

Casein kinase I gamma 2 : Homo sapiens

score: 3.716 on ChEMBL2543 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	2511.89	
MFP1	CHEMBL1990254		0.566667	2511.89	
RDKit7	CHEMBL1990254		0.716753	2511.89	
Pattern	CHEMBL1990254		0.911950	2511.89	*
AP_bits	CHEMBL1990254		0.600000	2511.89	*
TT_bits	CHEMBL1990254		0.622222	2511.89	*
FP2	CHEMBL1990254		0.706522	2511.89	*
hybridization	CHEMBL1990254		0.605381	2511.89	
substructure	CHEMBL1982924		0.875000	6309.57	*
graph	CHEMBL2007064		0.567010	6309.57	
pubchem	CHEMBL1982924		0.804762	6309.57	
cdk_maccs	CHEMBL1982924		0.731707	6309.57	
klekota_roth	CHEMBL1990254		0.595238	2511.89	

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

based on 5 locally validated fgps ---> 3271.426

["Pattern", "FP2", "TT\_bits", "substructure", "AP\_bits"]

69 rank

Cyclin-dependent kinase 9 : Homo sapiens

score: 3.716 on ChEMBL3116 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	158.49	
MFP1	CHEMBL1990254		0.566667	158.49	
RDKit7	CHEMBL1990254		0.716753	158.49	
Pattern	CHEMBL1990254		0.911950	158.49	*
AP_bits	CHEMBL1990254		0.600000	158.49	*
TT_bits	CHEMBL1990254		0.622222	158.49	*
FP2	CHEMBL1990254		0.706522	158.49	*
hybridization	CHEMBL1990254		0.605381	158.49	
substructure	CHEMBL1984296		0.875000	398.11	*
graph	CHEMBL2002649		0.581197	501.19	
pubchem	CHEMBL1990254		0.802260	158.49	
cdk_maccs	CHEMBL2002649		0.613636	501.19	
klekota_roth	CHEMBL1990254		0.595238	158.49	

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

based on 5 locally validated fgps ---> 206.414

["Pattern", "FP2", "TT\_bits", "substructure", "AP\_bits"]

70 rank

Interleukin-1 receptor-associated kinase 4 : Homo sapiens

score: 3.716 on ChEMBL3778 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	10000.00	
MFP1	CHEMBL1990254		0.566667	10000.00	
RDKit7	CHEMBL1990254		0.716753	10000.00	
Pattern	CHEMBL1990254		0.911950	10000.00	*
AP_bits	CHEMBL1990254		0.600000	10000.00	*
TT_bits	CHEMBL1990254		0.622222	10000.00	*

FP2	CHEMBL1990254	0.706522	10000.00	*
hybridization	CHEMBL1990254	0.605381	10000.00	
substructure	CHEMBL1982924	0.875000	2511.89	*
graph	CHEMBL1965845	0.583333	794.33	
pubchem	CHEMBL1982924	0.804762	2511.89	
cdk_maccs	CHEMBL1982924	0.731707	2511.89	
klekota_roth	CHEMBL1990254	0.595238	10000.00	

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

based on 5 locally validated fgps ---> 8409.678

["Pattern", "FP2", "TT\_bits", "substructure", "AP\_bits"]

71 rank

MAP/microtubule affinity-regulating kinase 2 : Homo sapiens

score: 3.716 on ChEMBL3831 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254	0.700000	6309.57		
MFP1	CHEMBL1990254	0.566667	6309.57		
RDKit7	CHEMBL1990254	0.716753	6309.57		
Pattern	CHEMBL1990254	0.911950	6309.57		*
AP_bits	CHEMBL1990254	0.600000	6309.57		*
TT_bits	CHEMBL1990254	0.622222	6309.57		*
FP2	CHEMBL1990254	0.706522	6309.57		*
hybridization	CHEMBL1990254	0.605381	6309.57		
substructure	CHEMBL1982924	0.875000	1258.93		*
graph	CHEMBL1965845	0.583333	794.33		
pubchem	CHEMBL1982924	0.804762	1258.93		
cdk_maccs	CHEMBL1982924	0.731707	1258.93		
klekota_roth	CHEMBL1990254	0.595238	6309.57		

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

based on 5 locally validated fgps ---> 5332.038

["Pattern", "FP2", "TT\_bits", "substructure", "AP\_bits"]

72 rank

Dual specificity tyrosine-phosphorylation-regulated kinase 1B : Homo sapiens

score: 3.716 on ChEMBL5543 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254	0.700000	1584.89		
MFP1	CHEMBL1990254	0.566667	1584.89		
RDKit7	CHEMBL1990254	0.716753	1584.89		
Pattern	CHEMBL1990254	0.911950	1584.89		*
AP_bits	CHEMBL1990254	0.600000	1584.89		*
TT_bits	CHEMBL1990254	0.622222	1584.89		*
FP2	CHEMBL1990254	0.706522	1584.89		*
hybridization	CHEMBL1990254	0.605381	1584.89		
substructure	CHEMBL1984296	0.875000	1000.00		*
graph	CHEMBL1968394	0.609756	19952.62		
pubchem	CHEMBL1990254	0.802260	1584.89		
cdk_maccs	CHEMBL269538	0.648649	166.00		
klekota_roth	CHEMBL1990254	0.595238	1584.89		

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

based on 5 locally validated fgps ---> 1467.912

["Pattern", "FP2", "TT\_bits", "substructure", "AP\_bits"]

73 rank

Serine/threonine-protein kinase PAK 4 : Homo sapiens

score: 3.701 on ChEMBL4482 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1974288	0.666667	2511.89		
MFP1	CHEMBL1974288	0.586207	2511.89		

RDKit7	CHEMBL1974288	0.712821	2511.89	
Pattern	CHEMBL1974288	0.912500	2511.89	*
AP_bits	CHEMBL1974288	0.582031	2511.89	*
TT_bits	CHEMBL1974288	0.622222	2511.89	*
FP2	CHEMBL1974288	0.709677	2511.89	*
hybridization	CHEMBL1974288	0.587719	2511.89	
substructure	CHEMBL1984296	0.875000	3981.07	*
graph	CHEMBL1974288	0.556818	2511.89	
pubchem	CHEMBL1974288	0.824176	2511.89	
cdk_maccs	CHEMBL1984296	0.609756	3981.07	
klekota_roth	CHEMBL1974288	0.530612	2511.89	

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

based on 5 locally validated fgps ---> 2805.726

["Pattern", "FP2", "TT\_bits", "substructure", "AP\_bits"]

74 rank

Serotonin 1a (5-HT1a) receptor : Rattus norvegicus

score: 3.479 on ChEMBL273 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL104593	0.652174	0.360		
MFP1	CHEMBL147483	0.500000	27.000		
RDKit7	CHEMBL294747	0.455335	3.162		
Pattern	CHEMBL156845	0.885886	432.000		*
AP_bits	CHEMBL72981	0.422343	1258.930		
TT_bits	CHEMBL309021	0.392857	19952.620		
FP2	CHEMBL294747	0.568966	3.162		
hybridization	CHEMBL1161083	0.463343	2.600		
substructure	CHEMBL2112905	0.882353	58.600		*
graph	CHEMBL315684	0.831325	2.800		*
pubchem	CHEMBL309021	0.878947	19952.620		*
cdk_maccs	CHEMBL2112774	0.591837	17.000		
klekota_roth	CHEMBL2112384	0.459016	4300.000		

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

based on 4 locally validated fgps ---> 2746.154

["Pattern", "pubchem", "substructure", "graph"]

75 rank

MAP kinase p38 delta : Homo sapiens

score: 2.844 on ChEMBL2939 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254	0.700000	794.33		
MFP1	CHEMBL1974288	0.586207	5011.87		
RDKit7	CHEMBL1990254	0.716753	794.33		
Pattern	CHEMBL1974288	0.912500	5011.87		*
AP_bits	CHEMBL1990254	0.600000	794.33		*
TT_bits	CHEMBL1974288	0.622222	5011.87		*
FP2	CHEMBL1974288	0.709677	5011.87		*
hybridization	CHEMBL1990254	0.605381	794.33		
substructure	CHEMBL1991078	0.823529	501.19		
graph	CHEMBL1990254	0.563218	794.33		
pubchem	CHEMBL1974288	0.824176	5011.87		
cdk_maccs	CHEMBL1997759	0.625000	251.19		
klekota_roth	CHEMBL1990254	0.595238	794.33		

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

based on 4 locally validated fgps ---> 2896.420

["Pattern", "FP2", "TT\_bits", "AP\_bits"]

76 rank

MAP kinase-activated protein kinase 2 : Homo sapiens

score: 2.841 on ChEMBL2208 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	794.33	
MFP1	CHEMBL1990254		0.566667	794.33	
RDKit7	CHEMBL1990254		0.716753	794.33	
Pattern	CHEMBL1990254		0.911950	794.33	*
AP_bits	CHEMBL1990254		0.600000	794.33	*
TT_bits	CHEMBL1990254		0.622222	794.33	*
FP2	CHEMBL1990254		0.706522	794.33	*
hybridization	CHEMBL1990254		0.605381	794.33	
substructure	CHEMBL1987009		0.823529	6309.57	
graph	CHEMBL235658		0.613636	330.00	
pubchem	CHEMBL1990254		0.802260	794.33	
cdk_maccs	CHEMBL1982506		0.617021	3981.07	
klekota_roth	CHEMBL1990254		0.595238	794.33	

\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 4 locally validated fgps ---> 794.330  
["Pattern", "FP2", "TT\_bits", "AP\_bits"]

77 rank

Serine/threonine-protein kinase PAK 1 : Homo sapiens

score: 2.841 on ChEMBL4600 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	6309.57	
MFP1	CHEMBL1990254		0.566667	6309.57	
RDKit7	CHEMBL1990254		0.716753	6309.57	
Pattern	CHEMBL1990254		0.911950	6309.57	*
AP_bits	CHEMBL1990254		0.600000	6309.57	*
TT_bits	CHEMBL1990254		0.622222	6309.57	*
FP2	CHEMBL1990254		0.706522	6309.57	*
hybridization	CHEMBL1990254		0.605381	6309.57	
substructure	CHEMBL1999931		0.764706	3981.07	
graph	CHEMBL1990254		0.563218	6309.57	
pubchem	CHEMBL1990254		0.802260	6309.57	
cdk_maccs	CHEMBL1967302		0.583333	7943.28	
klekota_roth	CHEMBL1990254		0.595238	6309.57	

\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 4 locally validated fgps ---> 6309.570  
["Pattern", "FP2", "TT\_bits", "AP\_bits"]

78 rank

MAP kinase p38 gamma : Homo sapiens

score: 2.841 on ChEMBL4674 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1990254		0.700000	3162.28	
MFP1	CHEMBL1990254		0.566667	3162.28	
RDKit7	CHEMBL1990254		0.716753	3162.28	
Pattern	CHEMBL1990254		0.911950	3162.28	*
AP_bits	CHEMBL1990254		0.600000	3162.28	*
TT_bits	CHEMBL1990254		0.622222	3162.28	*
FP2	CHEMBL1990254		0.706522	3162.28	*
hybridization	CHEMBL1990254		0.605381	3162.28	
substructure	CHEMBL1978099		0.823529	3162.28	
graph	CHEMBL1990254		0.563218	3162.28	
pubchem	CHEMBL1990254		0.802260	3162.28	
cdk_maccs	CHEMBL116070		0.613636	5011.87	
klekota_roth	CHEMBL1990254		0.595238	3162.28	

\*\*\* ki ACTIVITY \*\*\* value prediction  
based on 4 locally validated fgps ---> 3162.280  
["Pattern", "FP2", "TT\_bits", "AP\_bits"]



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

1 rank

Rho-associated protein kinase 2 : Homo sapiens

score: 8.799 on ChEMBL2973 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL3578250		0.947368	0.51	*
MFP1	ChEMBL3578250		0.727273	0.51	*
RDKit7	ChEMBL3578250		0.595696	0.51	
Pattern	ChEMBL597321		0.889231	5000.00	*
AP_bits	ChEMBL3578250		0.714815	0.51	*
TT_bits	ChEMBL3578250		0.589286	0.51	*
FP2	ChEMBL1923167		0.708738	2.00	*
hybridization	ChEMBL3578253		0.647619	1.16	*
substructure	ChEMBL3578250		1.000000	0.51	*
graph	ChEMBL3578253		0.788462	1.16	*
pubchem	ChEMBL3578250		0.935829	0.51	*
cdk_maccs	ChEMBL3578250		0.769231	0.51	
klekota_roth	ChEMBL3578253		0.850000	1.16	*

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

based on 11 locally validated fgps ---> 233.845

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

2 rank

MAP kinase p38 alpha : Homo sapiens

score: 7.489 on ChEMBL260 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL197753		0.695652	130.0	*
MFP1	ChEMBL2059876		0.545455	22000.0	*
RDKit7	ChEMBL517671		0.590258	23.0	
Pattern	ChEMBL1796293		0.884146	600.0	*
AP_bits	ChEMBL186802		0.529595	140.0	*
TT_bits	ChEMBL158477		0.436364	420.0	
FP2	ChEMBL517671		0.656566	23.0	*
hybridization	ChEMBL517671		0.680000	23.0	*
substructure	ChEMBL184555		1.000000	70.0	*
graph	ChEMBL517671		0.817073	23.0	*
pubchem	ChEMBL492266		0.880829	0.6	*
cdk_maccs	ChEMBL1427458		0.800000	4700.0	*
klekota_roth	ChEMBL252535		0.583333	2.2	

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

based on 9 locally validated fgps ---> 4528.984

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

3 rank

Rho-associated protein kinase 1 : Homo sapiens

score: 7.466 on ChEMBL3231 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL3218282		0.772727	30.0	*
MFP1	ChEMBL3218282		0.696970	30.0	*
RDKit7	ChEMBL1923173		0.547750	2.0	
Pattern	ChEMBL598336		0.854396	4300.0	*
AP_bits	ChEMBL1923173		0.652330	2.0	*
TT_bits	ChEMBL3218282		0.518519	30.0	*
FP2	ChEMBL1923167		0.708738	11.0	*
hybridization	ChEMBL1923167		0.644689	11.0	*
substructure	ChEMBL1923163		0.937500	1200.0	*
graph	ChEMBL1923052		0.670000	1900.0	
pubchem	ChEMBL598336		0.875000	4300.0	*
cdk_maccs	ChEMBL1923167		0.697674	11.0	

```

    klekota_roth CHEMBL1923181          0.804878      6.0      *
    *** ic50 ACTIVITY *** value prediction
    based on 10 locally validated fgps ---> 1103.528
    ["TT_bits", "substructure", "Pattern", "AP_bits", "MFP1", "pubchem",
    "FP2", "FeatMFP1", "klekota_roth", "hybridization"]

```

4 rank

Acetyl-CoA carboxylase 2 : Homo sapiens

score: 7.156 on ChEMBL4829 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3690672		0.800000	530.0	*
MFP1	CHEMBL576037		0.714286	373.0	*
RDKit7	CHEMBL568145		0.524862	609.0	
Pattern	CHEMBL576037		0.913174	373.0	*
AP_bits	CHEMBL567936		0.461300	33.0	
TT_bits	CHEMBL576037		0.595745	373.0	*
FP2	CHEMBL565418		0.628866	113.0	
hybridization	CHEMBL3690674		0.478261	2700.0	
substructure	CHEMBL3659849		0.882353	530.0	*
graph	CHEMBL3698542		0.770115	3400.0	*
pubchem	CHEMBL3690650		0.897297	930.0	*
cdk_maccs	CHEMBL585491		0.909091	32.0	*
klekota_roth	CHEMBL576037		0.673469	373.0	*

```

    *** ic50 ACTIVITY *** value prediction
    based on 9 locally validated fgps ---> 705.977
    ["TT_bits", "substructure", "Pattern", "MFP1", "pubchem", "graph",
    "FeatMFP1", "klekota_roth", "cdk_maccs"]

```

5 rank

Matrix metalloproteinase 13 : Homo sapiens

score: 6.703 on ChEMBL280 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1796289		0.684211	39810.72	*
MFP1	CHEMBL605201		0.551724	1350.00	*
RDKit7	CHEMBL1796289		0.531876	39810.72	
Pattern	CHEMBL1796282		0.940439	50118.72	*
AP_bits	CHEMBL1796289		0.510373	39810.72	*
TT_bits	CHEMBL1796289		0.468085	39810.72	
FP2	CHEMBL1796289		0.686047	39810.72	*
hybridization	CHEMBL605201		0.715640	1350.00	*
substructure	CHEMBL511942		0.933333	72.00	*
graph	CHEMBL596494		0.700000	77.00	
pubchem	CHEMBL1427458		0.875000	10000.00	*
cdk_maccs	CHEMBL1796287		0.806452	25118.86	*
klekota_roth	CHEMBL1796281		0.510638	25118.86	

```

    *** ic50 ACTIVITY *** value prediction
    based on 9 locally validated fgps ---> 18351.504
    ["substructure", "Pattern", "AP_bits", "MFP1", "pubchem", "FP2",
    "FeatMFP1", "cdk_maccs", "hybridization"]

```

6 rank

Platelet activating factor receptor : Homo sapiens

score: 6.602 on ChEMBL250 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL432324		0.809524	50.0	*
MFP1	CHEMBL51238		0.718750	20.0	*
RDKit7	CHEMBL412441		0.533632	280.0	
Pattern	CHEMBL51238		0.936937	20.0	*
AP_bits	CHEMBL299760		0.457227	50.0	
TT_bits	CHEMBL51238		0.551020	20.0	*



FP2	CHEMBL412441	0.620690	280.0	
hybridization	CHEMBL299856	0.448387	30.0	
substructure	CHEMBL432324	0.937500	50.0	*
graph	CHEMBL99294	0.816092	1.0	*
pubchem	CHEMBL51238	0.994286	20.0	*
cdk_maccs	CHEMBL53014	0.837838	10.0	*
klekota_roth	CHEMBL51238	0.524590	20.0	

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 8 locally validated fgps ---> 52.564  
 ["TT\_bits", "substructure", "Pattern", "MFP1", "pubchem", "graph",  
 "FeatMFP1", "cdk\_maccs"]

7 rank

Cytochrome P450 3A4 : Homo sapiens

score: 6.586 on CHEMBL340 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL271622		0.714286	33000.0		*
MFP1	CHEMBL1951443		0.655172	130.0		*
RDKit7	CHEMBL598336		0.486150	4000.0		
Pattern	CHEMBL1796293		0.884146	1000.0		*
AP_bits	CHEMBL1951330		0.537415	200.0		*
TT_bits	CHEMBL1951443		0.540000	130.0		*
FP2	CHEMBL598336		0.642202	4000.0		*
hybridization	CHEMBL10188		0.578947	4000.0		
substructure	CHEMBL271326		0.937500	34000.0		*
graph	CHEMBL1650646		0.684783	2050.0		
pubchem	CHEMBL1427458		0.875000	1000.0		*
cdk_maccs	CHEMBL1427458		0.800000	1000.0		*
klekota_roth	CHEMBL2017287		0.510204	2000.0		

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 8 locally validated fgps ---> 6704.417  
 ["TT\_bits", "substructure", "Pattern", "AP\_bits", "MFP1", "pubchem",  
 "FP2", "FeatMFP1"]

8 rank

Cytochrome P450 11B1 : Homo sapiens

score: 6.164 on CHEMBL1908 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL502823		0.750000	41557.0		*
MFP1	CHEMBL438802		0.607143	10505.0		*
RDKit7	CHEMBL3421782		0.575472	1150.0		
Pattern	CHEMBL3421782		0.934132	1150.0		*
AP_bits	CHEMBL500393		0.504167	151.0		*
TT_bits	CHEMBL1173259		0.416667	3100.0		
FP2	CHEMBL3421782		0.723810	1150.0		*
hybridization	CHEMBL176098		0.406844	206.0		
substructure	CHEMBL3421634		0.875000	1207.0		*
graph	CHEMBL1765226		0.758621	128.0		
pubchem	CHEMBL3421781		0.912568	594.0		*
cdk_maccs	CHEMBL502823		0.857143	41557.0		*
klekota_roth	CHEMBL3286405		0.461538	2300.0		

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 8 locally validated fgps ---> 9019.047  
 ["substructure", "Pattern", "AP\_bits", "MFP1", "pubchem", "FP2",  
 "FeatMFP1", "cdk\_maccs"]

9 rank

Cytochrome P450 11B2 : Homo sapiens

score: 6.164 on CHEMBL2722 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
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FeatMFP1	CHEMBL502823	0.750000	94.0	*
MFP1	CHEMBL438802	0.607143	72.0	*
RDKit7	CHEMBL3421782	0.575472	816.0	
Pattern	CHEMBL3421782	0.934132	816.0	*
AP_bits	CHEMBL500393	0.504167	4.8	*
TT_bits	CHEMBL1173259	0.416667	3450.0	
FP2	CHEMBL3421782	0.723810	816.0	*
hybridization	CHEMBL175979	0.411067	22.0	
substructure	CHEMBL3421634	0.875000	756.0	*
graph	CHEMBL1765226	0.758621	2.4	
pubchem	CHEMBL3421781	0.912568	299.0	*
cdk_maccs	CHEMBL502823	0.857143	94.0	*
klekota_roth	CHEMBL3286405	0.461538	5.0	

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 8 locally validated fgps ---> 352.011  
 ["substructure", "Pattern", "AP\_bits", "MFP1", "pubchem", "FP2",  
 "FeatMFP1", "cdk\_maccs"]

10 rank

Gamma-secretase : Homo sapiens

score: 5.520 on ChEMBL2094135 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL2415087	0.666667	158.0		
MFP1	CHEMBL3086721	0.625000	150.0		*
RDKit7	CHEMBL3087026	0.549142	2120.0		
Pattern	CHEMBL3087026	0.876106	2120.0		*
AP_bits	CHEMBL3086738	0.616935	6000.0		*
TT_bits	CHEMBL2018334	0.431034	2600.0		
FP2	CHEMBL3087026	0.576577	2120.0		
hybridization	CHEMBL3792849	0.528455	95000.0		
substructure	CHEMBL2415087	0.937500	158.0		*
graph	CHEMBL3086721	0.674699	150.0		
pubchem	CHEMBL3086721	0.857143	150.0		*
cdk_maccs	CHEMBL3086721	0.911765	150.0		*
klekota_roth	CHEMBL2018334	0.695652	2600.0		*

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 7 locally validated fgps ---> 1832.581  
 ["substructure", "Pattern", "MFP1", "pubchem", "AP\_bits", "klekota\_roth",  
 "cdk\_maccs"]

11 rank

Sentrin-specific protease 7 : Homo sapiens

score: 5.479 on ChEMBL1741213 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1387142	0.636364	4980.0		
MFP1	CHEMBL1475973	0.571429	5270.0		*
RDKit7	CHEMBL1573380	0.392744	5620.0		
Pattern	CHEMBL1475973	0.879880	5270.0		*
AP_bits	CHEMBL1387142	0.592742	4980.0		*
TT_bits	CHEMBL1578879	0.479167	2680.0		
FP2	CHEMBL1573380	0.567010	5620.0		
hybridization	CHEMBL1319034	0.484496	6130.0		
substructure	CHEMBL1507938	0.933333	3980.0		*
graph	CHEMBL1578879	0.780488	2680.0		*
pubchem	CHEMBL1387142	0.892473	4980.0		*
cdk_maccs	CHEMBL1387142	0.828571	4980.0		*
klekota_roth	CHEMBL1469986	0.454545	18400.0		

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 7 locally validated fgps ---> 4170.557

["substructure", "Pattern", "AP\_bits", "MFP1", "pubchem", "graph",  
"cdk\_maccs"]

12 rank

Caspase-3 : Homo sapiens

score: 5.479 on ChEMBL2334 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL1387142		0.636364	17500.0	
MFP1	ChEMBL1475973		0.571429	30300.0	*
RDKit7	ChEMBL1573380		0.392744	21800.0	
Pattern	ChEMBL1475973		0.879880	30300.0	*
AP_bits	ChEMBL1387142		0.592742	17500.0	*
TT_bits	ChEMBL1578879		0.479167	5560.0	
FP2	ChEMBL1573380		0.567010	21800.0	
hybridization	ChEMBL205983		0.584000	4630.0	
substructure	ChEMBL1507938		0.933333	15600.0	*
graph	ChEMBL1578879		0.780488	5560.0	*
pubchem	ChEMBL1387142		0.892473	17500.0	*
cdk_maccs	ChEMBL1387142		0.828571	17500.0	*
klekota_roth	ChEMBL2391777		0.471698	85.0	

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

based on 7 locally validated fgps ---> 14761.051

["substructure", "Pattern", "AP\_bits", "MFP1", "pubchem", "graph",  
"cdk\_maccs"]

13 rank

Poly [ADP-ribose] polymerase-1 : Homo sapiens

score: 5.467 on ChEMBL3105 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL480233		0.714286	62000.0	*
MFP1	ChEMBL123978		0.500000	17000.0	
RDKit7	ChEMBL3105430		0.412162	820.0	
Pattern	ChEMBL480710		0.894895	18.0	*
AP_bits	ChEMBL501290		0.481356	4533.0	*
TT_bits	ChEMBL480233		0.396226	62000.0	
FP2	ChEMBL480233		0.514019	62000.0	
hybridization	ChEMBL594596		0.516432	540.0	
substructure	ChEMBL3589258		0.866667	43000.0	*
graph	ChEMBL294995		0.809524	184.0	*
pubchem	ChEMBL480233		0.842932	62000.0	*
cdk_maccs	ChEMBL480233		0.857143	62000.0	*
klekota_roth	ChEMBL3827329		0.444444	2404.0	

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

based on 7 locally validated fgps ---> 24685.036

["substructure", "Pattern", "AP\_bits", "pubchem", "graph", "FeatMFP1",  
"cdk\_maccs"]

14 rank

Luciferase : Luciola lateralis

score: 5.325 on ChEMBL3701 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL467971		0.750000	310.0	*
MFP1	ChEMBL467971		0.586207	310.0	*
RDKit7	ChEMBL467971		0.409731	310.0	
Pattern	ChEMBL467971		0.852410	310.0	*
AP_bits	ChEMBL467971		0.496124	310.0	*
TT_bits	ChEMBL467971		0.384615	310.0	
FP2	ChEMBL467971		0.460938	310.0	
hybridization	ChEMBL467971		0.295547	310.0	
substructure	ChEMBL405914		0.937500	610.0	*

graph	CHEMBL467971	0.567308	310.0	
pubchem	CHEMBL467971	0.869110	310.0	*
cdk_maccs	CHEMBL467971	0.833333	310.0	*
klekota_roth	CHEMBL467971	0.372093	310.0	

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 7 locally validated fgps ---> 755.039  
 ["substructure", "Pattern", "MFP1", "pubchem", "AP\_bits", "FeatMFP1",  
 "cdk\_maccs"]

15 rank

Vascular endothelial growth factor receptor 2 : Homo sapiens

score: 5.314 on ChEMBL279 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL269871	0.727273	1.2880	*
MFP1	CHEMBL408211	0.606061	5.0000	*
RDKit7	CHEMBL271271	0.481956	16000.0000	
Pattern	CHEMBL427725	0.866667	200.0000	*
AP_bits	CHEMBL518652	0.517460	110.0000	*
TT_bits	CHEMBL526639	0.403846	500.0000	
FP2	CHEMBL270342	0.558824	0.4467	
hybridization	CHEMBL184223	0.619926	21.0000	
substructure	CHEMBL269871	0.937500	1.2880	*
graph	CHEMBL452812	0.656250	13000.0000	
pubchem	CHEMBL245745	0.830918	5.0000	*
cdk_maccs	CHEMBL272252	0.828571	1.2000	*
klekota_roth	CHEMBL271271	0.500000	16000.0000	

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 7 locally validated fgps ---> 1281.064  
 ["substructure", "Pattern", "MFP1", "pubchem", "AP\_bits", "FeatMFP1",  
 "cdk\_maccs"]

16 rank

HERG : Homo sapiens

score: 5.299 on ChEMBL240 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL1671897	0.727273	10000.00	*
MFP1	CHEMBL1779014	0.514286	18800.00	
RDKit7	CHEMBL1671897	0.437204	10000.00	
Pattern	CHEMBL1779014	0.911504	18800.00	*
AP_bits	CHEMBL3185736	0.470383	12400.00	*
TT_bits	CHEMBL2069407	0.370968	2511.89	
FP2	CHEMBL271801	0.594340	363.08	
hybridization	CHEMBL3099899	0.630435	6950.00	*
substructure	CHEMBL1671897	0.875000	10000.00	*
graph	CHEMBL1671885	0.772727	100.00	*
pubchem	CHEMBL1671897	0.912088	10000.00	*
cdk_maccs	CHEMBL1779014	0.714286	18800.00	
klekota_roth	CHEMBL2069416	0.444444	3981.07	

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
 based on 7 locally validated fgps ---> 12025.348  
 ["substructure", "Pattern", "AP\_bits", "pubchem", "graph", "FeatMFP1",  
 "hybridization"]

17 rank

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

score: 5.290 on ChEMBL2185 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL269871	0.727273	46.00	*
MFP1	CHEMBL408211	0.606061	190.00	*
RDKit7	CHEMBL3343058	0.362220	18100.00	

Pattern	CHEMBL3343044	0.848901	5910.00	*
AP_bits	CHEMBL382590	0.493976	1250.00	*
TT_bits	CHEMBL3680499	0.424242	0.94	
FP2	CHEMBL408211	0.542857	190.00	
hybridization	CHEMBL452812	0.498246	4900.00	
substructure	CHEMBL269871	0.937500	46.00	*
graph	CHEMBL388956	0.715789	2140.00	
pubchem	CHEMBL3670416	0.847716	8.20	*
cdk_maccs	CHEMBL272252	0.828571	130.00	*
klekota_roth	CHEMBL408211	0.473684	190.00	

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
based on 7 locally validated fgps ---> 2157.602  
["substructure", "Pattern", "MFP1", "pubchem", "AP\_bits", "FeatMFP1",  
"cdk\_maccs"]

18 rank

Mitochondrial import inner membrane translocase subunit TIM10 :  
Saccharomyces cerevisiae S288c

score: 5.240 on CHEMBL1741194 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1467168	0.600000	17200.0		
MFP1	CHEMBL1389690	0.592593	24400.0		*
RDKit7	CHEMBL438729	0.547382	47300.0		
Pattern	CHEMBL1475973	0.879880	27300.0		*
AP_bits	CHEMBL1475973	0.496479	27300.0		*
TT_bits	CHEMBL1398317	0.361702	3420.0		
FP2	CHEMBL438729	0.633929	47300.0		*
hybridization	CHEMBL1363382	0.536765	2890.0		
substructure	CHEMBL1482509	1.000000	22800.0		*
graph	CHEMBL1336269	0.780488	6800.0		*
pubchem	CHEMBL1482509	0.856410	22800.0		*
cdk_maccs	CHEMBL1389690	0.727273	24400.0		
klekota_roth	CHEMBL1389690	0.431818	24400.0		

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
based on 7 locally validated fgps ---> 22781.988  
["substructure", "Pattern", "AP\_bits", "MFP1", "pubchem", "graph", "FP2"]

19 rank

Acetyl-CoA carboxylase 1 : Homo sapiens

score: 5.197 on CHEMBL3351 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL566681	0.727273	415.0		*
MFP1	CHEMBL585885	0.642857	41.0		*
RDKit7	CHEMBL568145	0.524862	36.0		
Pattern	CHEMBL567934	0.896450	81.0		*
AP_bits	CHEMBL567936	0.461300	17.0		
TT_bits	CHEMBL568145	0.543860	36.0		*
FP2	CHEMBL565418	0.628866	35.0		
hybridization	CHEMBL566024	0.435737	35.0		
substructure	CHEMBL1630706	0.812500	14600.0		
graph	CHEMBL566025	0.600000	2770.0		
pubchem	CHEMBL566862	0.885870	69.0		*
cdk_maccs	CHEMBL585491	0.909091	49.0		*
klekota_roth	CHEMBL585491	0.591837	49.0		*

\*\*\* ic50 ACTIVITY \*\*\* value prediction  
based on 7 locally validated fgps ---> 1602.694  
["TT\_bits", "Pattern", "MFP1", "pubchem", "klekota\_roth", "FeatMFP1",  
"cdk\_maccs"]

20 rank

Epidermal growth factor receptor erbB1 : Homo sapiens  
score: 5.195 on ChEMBL203 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL143968	0.619048	1100.00	
MFP1	CHEMBL3753836	0.531250	131.09	*
RDKit7	CHEMBL143160	0.559006	5400.00	
Pattern	CHEMBL142831	0.846154	10000.00	*
AP_bits	CHEMBL186802	0.529595	5600.00	*
TT_bits	CHEMBL55979	0.415094	400.00	
FP2	CHEMBL143160	0.677778	5400.00	*
hybridization	CHEMBL143160	0.608491	5400.00	
substructure	CHEMBL186747	1.000000	3200.00	*
graph	CHEMBL2336357	0.780488	9050.00	*
pubchem	CHEMBL148514	0.830000	30500.00	*
cdk_maccs	CHEMBL2336357	0.705882	9050.00	
klekota_roth	CHEMBL3758278	0.450980	2.00	

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

based on 6 locally validated fgps ---> 12761.728

["substructure", "Pattern", "AP\_bits", "MFP1", "graph", "FP2"]

21 rank

Signal transducer and activator of transcription 3 : Homo sapiens  
score: 5.180 on ChEMBL4026 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL1530735	0.636364	2106.0	
MFP1	CHEMBL1447188	0.545455	16420.0	*
RDKit7	CHEMBL1478316	0.396197	2157.0	
Pattern	CHEMBL1427458	0.883281	5360.0	*
AP_bits	CHEMBL1353939	0.500000	1298.0	*
TT_bits	CHEMBL1478316	0.478261	2157.0	
FP2	CHEMBL1427458	0.638298	5360.0	*
hybridization	CHEMBL3133457	0.517606	52000.0	
substructure	CHEMBL1530735	0.937500	2106.0	*
graph	CHEMBL3133461	0.738636	33300.0	
pubchem	CHEMBL1427458	0.875000	5360.0	*
cdk_maccs	CHEMBL1427458	0.800000	5360.0	*
klekota_roth	CHEMBL1339432	0.362069	3832.0	

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

based on 6 locally validated fgps ---> 6426.275

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

22 rank

Vanilloid receptor : Homo sapiens

score: 5.174 on ChEMBL4794 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL214274	0.625000	62.0	
MFP1	CHEMBL483866	0.629630	147.0	*
RDKit7	CHEMBL3769572	0.468333	7110.0	
Pattern	CHEMBL249943	0.855114	680.0	*
AP_bits	CHEMBL483866	0.567227	147.0	*
TT_bits	CHEMBL483866	0.510638	147.0	*
FP2	CHEMBL400880	0.622807	370.0	
hybridization	CHEMBL3769572	0.491379	7110.0	
substructure	CHEMBL215015	0.933333	2585.0	*
graph	CHEMBL195257	0.780488	140.0	*
pubchem	CHEMBL215439	0.897297	974.0	*
cdk_maccs	CHEMBL483866	0.735294	147.0	
klekota_roth	CHEMBL231392	0.530612	749.0	

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

based on 7 locally validated fgps ---> 1011.643

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

23 rank

Estradiol 17-beta-dehydrogenase 2 : Homo sapiens

score: 5.129 on ChEMBL2789 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL3289858	0.666667	621.0	
MFP1	CHEMBL3645224	0.607143	601.0	*
RDKit7	CHEMBL1915937	0.645161	265.0	
Pattern	CHEMBL1915936	0.903323	594.0	*
AP_bits	CHEMBL1915937	0.538732	265.0	*
TT_bits	CHEMBL3645223	0.416667	1760.0	
FP2	CHEMBL1915935	0.744186	494.0	*
hybridization	CHEMBL1915937	0.693694	265.0	*
substructure	CHEMBL2324690	0.764706	58.0	
graph	CHEMBL1915935	0.829268	494.0	*
pubchem	CHEMBL1097417	0.823204	2970.0	
cdk_maccs	CHEMBL1097417	0.812500	2970.0	*
klekota_roth	CHEMBL1915935	0.431373	494.0	

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

based on 7 locally validated fgps ---> 875.823

["Pattern", "AP\_bits", "MFP1", "graph", "FP2", "cdk\_maccs",  
"hybridization"]

24 rank

Cytochrome P450 2C9 : Homo sapiens

score: 5.020 on ChEMBL3397 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL271622	0.714286	39000.0	*
MFP1	CHEMBL598336	0.562500	16000.0	*
RDKit7	CHEMBL598336	0.486150	16000.0	
Pattern	CHEMBL560537	0.855799	30000.0	*
AP_bits	CHEMBL2332097	0.488294	600.0	*
TT_bits	CHEMBL485968	0.388889	3000.0	
FP2	CHEMBL598336	0.642202	16000.0	*
hybridization	CHEMBL10188	0.578947	2000.0	
substructure	CHEMBL2348850	0.882353	16000.0	*
graph	CHEMBL1650646	0.684783	224.0	
pubchem	CHEMBL598336	0.875000	16000.0	*
cdk_maccs	CHEMBL3822473	0.756757	5030.0	
klekota_roth	CHEMBL2017287	0.510204	1300.0	

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

based on 7 locally validated fgps ---> 15476.314

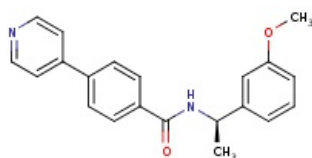
["substructure", "Pattern", "AP\_bits", "MFP1", "pubchem", "FP2",  
"FeatMFP1"]

# 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

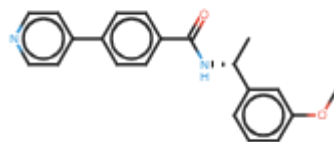
Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
Corticosteroid 11-beta-dehydrogenase isozyme 2	P80365	HSD11B2	CHEMBL3746	<div><div></div></div>	39 / 16	Enzyme
Rho-associated protein kinase 2	O75116	ROCK2	CHEMBL2973	<div><div></div></div>	159 / 41	Ser_Thr Kinase
Rho-associated protein kinase 1	Q13464	ROCK1	CHEMBL3231	<div><div></div></div>	159 / 41	Ser_Thr Kinase
Estradiol 17-beta-dehydrogenase 2	P37059	HSD17B2	CHEMBL2789	<div><div></div></div>	13 / 16	Enzyme
Epidermal growth factor receptor	P00533	EGFR	CHEMBL203	<div><div></div></div>	156 / 10	Tyr Kinase
Receptor tyrosine-protein kinase erbB-2	P04626	ERBB2	CHEMBL1824	<div><div></div></div>	156 / 9	Tyr Kinase
Receptor tyrosine-protein kinase erbB-3 (by homology)	P21860	ERBB3	CHEMBL5838	<div><div></div></div>	156 / 9	Tyr Kinase
ERBB4 intracellular domain (by homology)	Q15303	ERBB4	CHEMBL3009	<div><div></div></div>	156 / 9	Tyr Kinase
Mitogen-activated protein kinase 11 (by homology)	Q15759	MAPK11	CHEMBL3961	<div><div></div></div>	435 / 48	Ser_Thr Kinase
Mitogen-activated protein kinase 14	Q16539	MAPK14	CHEMBL260	<div><div></div></div>	435 / 48	Ser_Thr Kinase
Muscleblind-like protein 1	Q9NR56	MBNL1	CHEMBL1293317	<div><div></div></div>	709 / 67	Unclassified
Muscleblind-like protein 2 (by homology)	Q5VZF2	MBNL2		<div><div></div></div>	709 / 67	Unclassified
Muscleblind-like protein 3 (by homology)	Q9NUK0	MBNL3		<div><div></div></div>	709 / 67	Unclassified
Mitogen-activated protein kinase 8 (by homology)	P45983	MAPK8	CHEMBL2276	<div><div></div></div>	425 / 48	Ser_Thr Kinase
Mitogen-activated protein kinase 9 (by homology)	P45984	MAPK9	CHEMBL4179	<div><div></div></div>	425 / 48	Ser_Thr Kinase



## Polypharmacology Browser 2 Prediction:

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

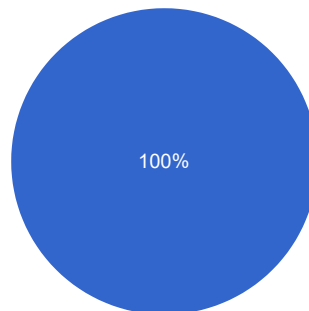
Save Table



Query molecule

Target class overview

● Enzyme



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL3231 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3231">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3231</a> )	Rho-associated protein kinase 1	Show NN
2	CHEMBL262 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL262">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL262</a> )	Glycogen synthase kinase-3 beta	Show NN
3	CHEMBL4101 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4101">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4101</a> )	cAMP-dependent protein kinase alpha-catalytic subunit	Show NN
4	CHEMBL2850 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2850">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2850</a> )	Glycogen synthase kinase-3 alpha	Show NN
5	CHEMBL4203 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4203">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4203</a> )	Dual specificity protein kinase CLK4	Show NN
6	CHEMBL2973 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2973">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2973</a> )	Rho-associated protein kinase 2	Show NN
7	CHEMBL5818 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL5818">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL5818</a> )	Serine/threonine-protein kinase PRKX	Show NN
8	CHEMBL3032 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3032">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3032</a> )	Protein kinase N2	Show NN
9	CHEMBL4273 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4273">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4273</a> )	cGMP-dependent protein kinase 1 beta	Show NN
10	CHEMBL4040 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4040">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4040</a> )	MAP kinase ERK2	Show NN
11	CHEMBL5794 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL5794">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL5794</a> )	Serine/threonine-protein kinase Sgk2	Show NN
12	CHEMBL4501 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4501">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4501</a> )	Ribosomal protein S6 kinase 1	Show NN
13	CHEMBL2996 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2996">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2996</a> )	Protein kinase C delta	Show NN

14	CHEMBL301 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL301">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL301</a> )	Cyclin-dependent kinase 2	Show NN
15	CHEMBL2896 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2896">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2896</a> )	cGMP-dependent protein kinase 2	Show NN
16	CHEMBL4516 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4516">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4516</a> )	Serine/threonine-protein kinase MRCK-A	Show NN
17	CHEMBL2345 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2345">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2345</a> )	Ribosomal protein S6 kinase alpha 3	Show NN
18	CHEMBL4282 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4282">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4282</a> )	Serine/threonine-protein kinase AKT	Show NN
19	CHEMBL2938 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2938">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2938</a> )	Protein kinase C gamma	Show NN
20	CHEMBL6166 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL6166">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL6166</a> )	Mitogen-activated protein kinase kinase kinase kinase 4	Show NN