

MuSsel Prediction k_i:

1 rank

Cytochrome P450 19A1 : Homo sapiens

score: 10.442 on ChEMBL1978 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1627334		0.947368	100.0	*
MFP1	CHEMBL1627334		0.827586	100.0	*
RDKit7	CHEMBL3753034		0.712714	100.0	
Pattern	CHEMBL3752556		0.945518	100.0	*
AP_bits	CHEMBL3752556		0.637540	100.0	*
TT_bits	CHEMBL241993		0.769231	100.0	*
FP2	CHEMBL241993		0.727273	100.0	*
hybridization	CHEMBL3753034		0.881579	100.0	*
substructure	CHEMBL1627334		0.928571	100.0	*
graph	CHEMBL1627334		0.977273	100.0	*
pubchem	CHEMBL3752422		0.940678	100.0	*
cdk_maccs	CHEMBL1627334		0.947368	100.0	*
klekota_roth	CHEMBL1627334		0.911765	100.0	*

*** ki ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 97.735

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

2 rank

Steryl-sulfatase : Homo sapiens

score: 8.235 on ChEMBL3559 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1835544		0.850000	30.0	*
MFP1	CHEMBL1835544		0.540541	30.0	
RDKit7	CHEMBL482212		0.683849	250.0	
Pattern	CHEMBL482212		0.945111	250.0	*
AP_bits	CHEMBL1835544		0.554252	30.0	*
TT_bits	CHEMBL1945908		0.559524	23.0	*
FP2	CHEMBL1835544		0.670455	30.0	
hybridization	CHEMBL482212		0.873362	250.0	*
substructure	CHEMBL1835544		0.866667	30.0	*
graph	CHEMBL1835544		0.931818	30.0	*
pubchem	CHEMBL1835544		0.908333	30.0	*
cdk_maccs	CHEMBL1835544		0.948718	30.0	*
klekota_roth	CHEMBL1835544		0.797297	30.0	*

*** ki ACTIVITY *** value prediction

based on 10 locally validated fgps ---> 97.751

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

3 rank

Progesterone receptor : Bos taurus

score: 8.225 on ChEMBL1909044 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL135		0.789474	4247.0	*
MFP1	CHEMBL135		0.758621	4247.0	*
RDKit7	CHEMBL135		0.722429	4247.0	
Pattern	CHEMBL282575		0.919105	1253.0	*
AP_bits	CHEMBL135		0.558491	4247.0	*
TT_bits	CHEMBL135		0.742424	4247.0	*
FP2	CHEMBL135		0.675325	4247.0	
hybridization	CHEMBL135		0.905405	4247.0	*
substructure	CHEMBL135		0.857143	4247.0	
graph	CHEMBL1766		0.914894	11.0	*
pubchem	CHEMBL135		0.915254	4247.0	*
cdk_maccs	CHEMBL135		0.842105	4247.0	*

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    klekota_roth      CHEMBL135          0.878788      4247.0      *
    *** ki ACTIVITY *** value prediction
    based on 10 locally validated fgps ---> 2800.454
    ["TT_bits", "Pattern", "MFP1", "klekota_roth", "pubchem", "graph",
    "AP_bits", "FeatMFP1", "cdk_maccs", "hybridization"]

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4 rank

Glucocorticoid receptor : Homo sapiens

score: 8.225 on ChEMBL2034 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	18828.000	*
MFP1	CHEMBL135	0.758621	18828.000	*
RDKit7	CHEMBL135	0.722429	18828.000	
Pattern	CHEMBL282575	0.919105	2306.000	*
AP_bits	CHEMBL135	0.558491	18828.000	*
TT_bits	CHEMBL135	0.742424	18828.000	*
FP2	CHEMBL135	0.675325	18828.000	
hybridization	CHEMBL135	0.905405	18828.000	*
substructure	CHEMBL135	0.857143	18828.000	
graph	CHEMBL1766	0.914894	1.169	*
pubchem	CHEMBL135	0.915254	18828.000	*
cdk_maccs	CHEMBL135	0.842105	18828.000	*
klekota_roth	CHEMBL135	0.878788	18828.000	*

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    *** ki ACTIVITY *** value prediction
    based on 10 locally validated fgps ---> 13409.674
    ["TT_bits", "Pattern", "MFP1", "klekota_roth", "pubchem", "graph",
    "AP_bits", "FeatMFP1", "cdk_maccs", "hybridization"]

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5 rank

Androgen Receptor : Rattus norvegicus

score: 8.206 on ChEMBL3072 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	235.000	*
MFP1	CHEMBL135	0.758621	235.000	*
RDKit7	CHEMBL135	0.722429	235.000	
Pattern	CHEMBL282575	0.919105	6.981	*
AP_bits	CHEMBL135	0.558491	235.000	*
TT_bits	CHEMBL135	0.742424	235.000	*
FP2	CHEMBL135	0.675325	235.000	
hybridization	CHEMBL135	0.905405	235.000	*
substructure	CHEMBL135	0.857143	235.000	
graph	CHEMBL1200600	0.895833	857.000	*
pubchem	CHEMBL135	0.915254	235.000	*
cdk_maccs	CHEMBL135	0.842105	235.000	*
klekota_roth	CHEMBL135	0.878788	235.000	*

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    *** ki ACTIVITY *** value prediction
    based on 10 locally validated fgps ---> 1162.333
    ["TT_bits", "Pattern", "MFP1", "klekota_roth", "pubchem", "graph",
    "AP_bits", "FeatMFP1", "cdk_maccs", "hybridization"]

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6 rank

Corticosteroid binding globulin : Homo sapiens

score: 8.148 on ChEMBL2421 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	10000.00	*
MFP1	CHEMBL135	0.758621	10000.00	*
RDKit7	CHEMBL135	0.722429	10000.00	
Pattern	CHEMBL193482	0.861888	10000.00	*
AP_bits	CHEMBL135	0.558491	10000.00	*
TT_bits	CHEMBL135	0.742424	10000.00	*

FP2	CHEMBL135	0.675325	10000.00		
hybridization	CHEMBL135	0.905405	10000.00	*	
substructure	CHEMBL135	0.857143	10000.00		
graph	CHEMBL93948	0.895833	1584.89	*	
pubchem	CHEMBL135	0.915254	10000.00	*	
cdk_maccs	CHEMBL135	0.842105	10000.00	*	
klekota_roth	CHEMBL135	0.878788	10000.00	*	

*** ki ACTIVITY *** value prediction
 based on 10 locally validated fgps ---> 9158.489
 ["TT_bits", "Pattern", "MFP1", "klekota_roth", "pubchem", "graph",
 "AP_bits", "FeatMFP1", "cdk_maccs", "hybridization"]

7 rank

Estrogen receptor alpha : Homo sapiens

score: 7.336 on ChEMBL206 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1230314	0.789474	4.90	*	
MFP1	CHEMBL135	0.758621	0.16	*	
RDKit7	CHEMBL135	0.722429	0.16		
Pattern	CHEMBL282575	0.919105	18.00	*	
AP_bits	CHEMBL135	0.558491	0.16	*	
TT_bits	CHEMBL135	0.742424	0.16	*	
FP2	CHEMBL135	0.675325	0.16		
hybridization	CHEMBL135	0.905405	0.16	*	
substructure	CHEMBL135	0.857143	0.16		
graph	CHEMBL135	0.813953	0.16		
pubchem	CHEMBL135	0.915254	0.16	*	
cdk_maccs	CHEMBL135236	0.868421	8.00	*	
klekota_roth	CHEMBL135	0.878788	0.16	*	

*** ki ACTIVITY *** value prediction
 based on 9 locally validated fgps ---> 6.522
 ["TT_bits", "Pattern", "MFP1", "klekota_roth", "pubchem", "AP_bits",
 "FeatMFP1", "cdk_maccs", "hybridization"]

8 rank

Serotonin transporter : Homo sapiens

score: 7.310 on ChEMBL228 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	5714.0	*	
MFP1	CHEMBL135	0.758621	5714.0	*	
RDKit7	CHEMBL135	0.722429	5714.0		
Pattern	CHEMBL282575	0.919105	1951.0	*	
AP_bits	CHEMBL135	0.558491	5714.0	*	
TT_bits	CHEMBL135	0.742424	5714.0	*	
FP2	CHEMBL135	0.675325	5714.0		
hybridization	CHEMBL135	0.905405	5714.0	*	
substructure	CHEMBL135	0.857143	5714.0		
graph	CHEMBL135	0.813953	5714.0		
pubchem	CHEMBL135	0.915254	5714.0	*	
cdk_maccs	CHEMBL135	0.842105	5714.0	*	
klekota_roth	CHEMBL135	0.878788	5714.0	*	

*** ki ACTIVITY *** value prediction
 based on 9 locally validated fgps ---> 4730.993
 ["TT_bits", "Pattern", "MFP1", "klekota_roth", "pubchem", "AP_bits",
 "FeatMFP1", "cdk_maccs", "hybridization"]

9 rank

Estrogen receptor beta : Homo sapiens

score: 7.308 on ChEMBL242 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
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FeatMFP1	CHEMBL1230314	0.789474	19.000	*
MFP1	CHEMBL135	0.758621	0.015	*
RDKit7	CHEMBL135	0.722429	0.015	
Pattern	CHEMBL1627464	0.891192	0.025	*
AP_bits	CHEMBL135	0.558491	0.015	*
TT_bits	CHEMBL135	0.742424	0.015	*
FP2	CHEMBL135	0.675325	0.015	
hybridization	CHEMBL135	0.905405	0.015	*
substructure	CHEMBL135	0.857143	0.015	
graph	CHEMBL135	0.813953	0.015	
pubchem	CHEMBL135	0.915254	0.015	*
cdk_maccs	CHEMBL135236	0.868421	24.000	*
klekota_roth	CHEMBL135	0.878788	0.015	*

*** ki ACTIVITY *** value prediction

based on 9 locally validated fgps ---> 7.811

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

10 rank

Dopamine transporter : Homo sapiens

score: 7.282 on CHEMBL238 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL135	0.789474	11847.0		*	
MFP1	CHEMBL135	0.758621	11847.0		*	
RDKit7	CHEMBL135	0.722429	11847.0			
Pattern	CHEMBL691	0.891192	444.0		*	
AP_bits	CHEMBL135	0.558491	11847.0		*	
TT_bits	CHEMBL135	0.742424	11847.0		*	
FP2	CHEMBL135	0.675325	11847.0			
hybridization	CHEMBL135	0.905405	11847.0		*	
substructure	CHEMBL135	0.857143	11847.0			
graph	CHEMBL135	0.813953	11847.0			
pubchem	CHEMBL135	0.915254	11847.0		*	
cdk_maccs	CHEMBL135	0.842105	11847.0		*	
klekota_roth	CHEMBL135	0.878788	11847.0		*	

*** ki ACTIVITY *** value prediction

based on 9 locally validated fgps ---> 9384.404

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

11 rank

Aldehyde oxidase : Homo sapiens

score: 7.282 on CHEMBL3257 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL135	0.789474	870.0		*	
MFP1	CHEMBL135	0.758621	870.0		*	
RDKit7	CHEMBL135	0.722429	870.0			
Pattern	CHEMBL691	0.891192	430.0		*	
AP_bits	CHEMBL135	0.558491	870.0		*	
TT_bits	CHEMBL135	0.742424	870.0		*	
FP2	CHEMBL135	0.675325	870.0			
hybridization	CHEMBL135	0.905405	870.0		*	
substructure	CHEMBL135	0.857143	870.0			
graph	CHEMBL135	0.813953	870.0			
pubchem	CHEMBL135	0.915254	870.0		*	
cdk_maccs	CHEMBL135	0.842105	870.0		*	
klekota_roth	CHEMBL135	0.878788	870.0		*	

*** ki ACTIVITY *** value prediction

based on 9 locally validated fgps ---> 774.977

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

12 rank

Solute carrier organic anion transporter family member 1A1 : Rattus
norvegicus

score: 7.274 on ChEMBL1781859 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL135		0.789474	4700.0	*	
MFP1	ChEMBL135		0.758621	4700.0	*	
RDKit7	ChEMBL135		0.722429	4700.0		
Pattern	ChEMBL1628111		0.882960	1100.0	*	
AP_bits	ChEMBL135		0.558491	4700.0	*	
TT_bits	ChEMBL135		0.742424	4700.0	*	
FP2	ChEMBL135		0.675325	4700.0		
hybridization	ChEMBL135		0.905405	4700.0	*	
substructure	ChEMBL135		0.857143	4700.0		
graph	ChEMBL135		0.813953	4700.0		
pubchem	ChEMBL135		0.915254	4700.0	*	
cdk_maccs	ChEMBL135		0.842105	4700.0	*	
klekota_roth	ChEMBL135		0.878788	4700.0	*	

*** ki ACTIVITY *** value prediction

based on 9 locally validated fgps ---> 5510.140

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

13 rank

Estrogen sulfotransferase : Sus scrofa

score: 5.857 on ChEMBL3811 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL1627683		0.842105	13600.0	*	
MFP1	ChEMBL1627683		0.857143	13600.0	*	
RDKit7	ChEMBL194749		0.634449	16300.0		
Pattern	ChEMBL1627977		0.826087	10200.0		
AP_bits	ChEMBL1627683		0.521898	13600.0		
TT_bits	ChEMBL1627683		0.742424	13600.0	*	
FP2	ChEMBL1627683		0.597561	13600.0		
hybridization	ChEMBL1627683		0.760331	13600.0	*	
substructure	ChEMBL1627683		0.857143	13600.0		
graph	ChEMBL1627977		0.977273	10200.0	*	
pubchem	ChEMBL1627977		0.771186	10200.0		
cdk_maccs	ChEMBL1627683		0.868421	13600.0	*	
klekota_roth	ChEMBL1627683		0.808824	13600.0	*	

*** ki ACTIVITY *** value prediction

based on 7 locally validated fgps ---> 12559.345

["TT_bits", "graph", "MFP1", "klekota_roth", "FeatMFP1", "hybridization",
"cdk_maccs"]

14 rank

Carbonic anhydrase II : Homo sapiens

score: 3.784 on ChEMBL205 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL2391082		0.625000	21800.0		
MFP1	ChEMBL220493		0.567568	13.0		
RDKit7	ChEMBL220493		0.670366	13.0		
Pattern	ChEMBL425287		0.876206	232.0	*	
AP_bits	ChEMBL220493		0.444444	13.0		
TT_bits	ChEMBL220493		0.608108	13.0	*	
FP2	ChEMBL220493		0.536082	13.0		
hybridization	ChEMBL220493		0.743590	13.0	*	

substructure	CHEMBL220493	0.733333	13.0	
graph	CHEMBL898	0.674419	9370.0	
pubchem	CHEMBL220493	0.856000	13.0	*
cdk_maccs	CHEMBL1946088	0.600000	380.0	
klekota_roth	CHEMBL220493	0.700000	13.0	*

*** ki ACTIVITY *** value prediction
 based on 5 locally validated fgps ---> 34.259
 ["Pattern", "klekota_roth", "TT_bits", "pubchem", "hybridization"]

15 rank

Carbonic anhydrase I : Homo sapiens

score: 3.773 on ChEMBL261 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL2391082		0.625000	760.0	
MFP1	CHEMBL220493		0.567568	15.0	
RDKit7	CHEMBL220493		0.670366	15.0	
Pattern	CHEMBL220493		0.865093	15.0	*
AP_bits	CHEMBL220493		0.444444	15.0	
TT_bits	CHEMBL220493		0.608108	15.0	*
FP2	CHEMBL220493		0.536082	15.0	
hybridization	CHEMBL220493		0.743590	15.0	*
substructure	CHEMBL220493		0.733333	15.0	
graph	CHEMBL898		0.674419	8450.0	
pubchem	CHEMBL220493		0.856000	15.0	*
cdk_maccs	CHEMBL1946088		0.600000	1040.0	
klekota_roth	CHEMBL220493		0.700000	15.0	*

*** ki ACTIVITY *** value prediction
 based on 5 locally validated fgps ---> 1197.155
 ["Pattern", "klekota_roth", "TT_bits", "pubchem", "hybridization"]

16 rank

Carbonic anhydrase IX : Homo sapiens

score: 3.773 on ChEMBL3594 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL2391082		0.625000	15700.0	
MFP1	CHEMBL220493		0.567568	32.0	
RDKit7	CHEMBL220493		0.670366	32.0	
Pattern	CHEMBL220493		0.865093	32.0	*
AP_bits	CHEMBL220493		0.444444	32.0	
TT_bits	CHEMBL220493		0.608108	32.0	*
FP2	CHEMBL220493		0.536082	32.0	
hybridization	CHEMBL220493		0.743590	32.0	*
substructure	CHEMBL220493		0.733333	32.0	
graph	CHEMBL1628004		0.561644	1725.0	
pubchem	CHEMBL220493		0.856000	32.0	*
cdk_maccs	CHEMBL2391082		0.551020	15700.0	
klekota_roth	CHEMBL220493		0.700000	32.0	*

*** ki ACTIVITY *** value prediction
 based on 5 locally validated fgps ---> 37.136
 ["Pattern", "klekota_roth", "TT_bits", "pubchem", "hybridization"]

17 rank

Norepinephrine transporter : Homo sapiens

score: 3.693 on ChEMBL222 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL691		0.636364	951.0	
MFP1	CHEMBL282575		0.583333	17087.0	
RDKit7	CHEMBL691		0.688940	951.0	
Pattern	CHEMBL282575		0.919105	17087.0	*
AP_bits	CHEMBL282575		0.538905	17087.0	*

TT_bits	CHEMBL282575	0.641026	17087.0	*
FP2	CHEMBL691	0.619048	951.0	
hybridization	CHEMBL691	0.816327	951.0	*
substructure	CHEMBL1601669	0.687500	1000.0	
graph	CHEMBL1200623	0.790698	2080.0	
pubchem	CHEMBL691	0.830645	951.0	
cdk_maccs	CHEMBL691	0.820513	951.0	
klekota_roth	CHEMBL691	0.777778	951.0	*

*** ki ACTIVITY *** value prediction
based on 5 locally validated fgps ---> 10631.626
["Pattern", "hybridization", "TT_bits", "klekota_roth", "AP_bits"]

18 rank

Adenosine A3 receptor : Homo sapiens

score: 3.693 on ChEMBL256 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL691		0.636364	18610.0	
MFP1	CHEMBL282575		0.583333	12312.0	
RDKit7	CHEMBL691		0.688940	18610.0	
Pattern	CHEMBL282575		0.919105	12312.0	*
AP_bits	CHEMBL282575		0.538905	12312.0	*
TT_bits	CHEMBL282575		0.641026	12312.0	*
FP2	CHEMBL691		0.619048	18610.0	
hybridization	CHEMBL691		0.816327	18610.0	*
substructure	CHEMBL691		0.687500	18610.0	
graph	CHEMBL691		0.767442	18610.0	
pubchem	CHEMBL691		0.830645	18610.0	
cdk_maccs	CHEMBL691		0.820513	18610.0	
klekota_roth	CHEMBL691		0.777778	18610.0	*

*** ki ACTIVITY *** value prediction
based on 5 locally validated fgps ---> 14831.580
["Pattern", "hybridization", "TT_bits", "klekota_roth", "AP_bits"]

19 rank

Serotonin 2b (5-HT2b) receptor : Homo sapiens

score: 3.627 on ChEMBL1833 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1405		0.590909	8676.0	
MFP1	CHEMBL282575		0.583333	7359.0	
RDKit7	CHEMBL282575		0.634737	7359.0	
Pattern	CHEMBL282575		0.919105	7359.0	*
AP_bits	CHEMBL282575		0.538905	7359.0	*
TT_bits	CHEMBL282575		0.641026	7359.0	*
FP2	CHEMBL1405		0.566265	8676.0	
hybridization	CHEMBL1405		0.775000	8676.0	*
substructure	CHEMBL1405		0.666667	8676.0	
graph	CHEMBL1405		0.767442	8676.0	
pubchem	CHEMBL1405		0.801587	8676.0	
cdk_maccs	CHEMBL282575		0.761905	7359.0	
klekota_roth	CHEMBL282575		0.753247	7359.0	*

*** ki ACTIVITY *** value prediction
based on 5 locally validated fgps ---> 7622.400
["Pattern", "hybridization", "TT_bits", "klekota_roth", "AP_bits"]

20 rank

Multidrug resistance-associated protein 1 : Homo sapiens

score: 3.202 on ChEMBL3004 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1697724		0.535714	22000.0	
MFP1	CHEMBL1628111		0.583333	380.0	

RDKit7	CHEMBL1628111	0.651366	380.0	
Pattern	CHEMBL1628111	0.882960	380.0	*
AP_bits	CHEMBL1628111	0.470238	380.0	
TT_bits	CHEMBL1628111	0.666667	380.0	*
FP2	CHEMBL1628111	0.525253	380.0	
hybridization	CHEMBL1628111	0.689420	380.0	
substructure	CHEMBL1628111	0.631579	380.0	
graph	CHEMBL1628111	0.564516	380.0	
pubchem	CHEMBL1628111	0.868852	380.0	*
cdk_maccs	CHEMBL2075011	0.607843	1400.0	
klekota_roth	CHEMBL1628111	0.783784	380.0	*

*** ki ACTIVITY *** value prediction

based on 4 locally validated fgps ---> 388.636

["Pattern", "klekota_roth", "TT_bits", "pubchem"]

21 rank

Alpha-2c adrenergic receptor : Homo sapiens

score: 2.852 on ChEMBL1916 based on 4 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL282575	0.541667	3582.0	
MFP1	CHEMBL282575	0.583333	3582.0	
RDKit7	CHEMBL282575	0.634737	3582.0	
Pattern	CHEMBL282575	0.919105	3582.0	*
AP_bits	CHEMBL282575	0.538905	3582.0	*
TT_bits	CHEMBL282575	0.641026	3582.0	*
FP2	CHEMBL282575	0.518868	3582.0	
hybridization	CHEMBL282575	0.681063	3582.0	
substructure	CHEMBL282575	0.666667	3582.0	
graph	CHEMBL282575	0.507246	3582.0	
pubchem	CHEMBL282575	0.746575	3582.0	
cdk_maccs	CHEMBL282575	0.761905	3582.0	
klekota_roth	CHEMBL282575	0.753247	3582.0	*

*** ki ACTIVITY *** value prediction

based on 4 locally validated fgps ---> 3582.000

["Pattern", "klekota_roth", "TT_bits", "AP_bits"]

MuSsel Prediction IC₅₀:

1 rank

Steryl-sulfatase : Homo sapiens

score: 10.910 on ChEMBL3559 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL1627410		0.850000	840.0	*
MFP1	ChEMBL135		0.758621	84000.0	*
RDKit7	ChEMBL1947227		0.751716	35.0	*
Pattern	ChEMBL482212		0.945111	220.0	*
AP_bits	ChEMBL1947227		0.571053	35.0	*
TT_bits	ChEMBL135		0.742424	84000.0	*
FP2	ChEMBL1947227		0.762500	35.0	*
hybridization	ChEMBL1627953		0.908297	120.0	*
substructure	ChEMBL270250		0.928571	62.0	*
graph	ChEMBL1823787		0.931818	126.0	*
pubchem	ChEMBL270250		0.932773	62.0	*
cdk_maccs	ChEMBL1627640		0.948718	130.0	*
klekota_roth	ChEMBL135		0.878788	84000.0	*

*** ic50 ACTIVITY *** value prediction

based on 13 locally validated fgps ---> 16832.382

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

2 rank

Tubulin beta chain : Bos taurus

score: 10.783 on ChEMBL3394 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL265926		0.947368	4800.0	*
MFP1	ChEMBL241993		0.733333	17000.0	*
RDKit7	ChEMBL241993		0.692575	17000.0	*
Pattern	ChEMBL1627838		0.903169	8600.0	*
AP_bits	ChEMBL1627439		0.618056	1100.0	*
TT_bits	ChEMBL1627439		0.787879	1100.0	*
FP2	ChEMBL241993		0.727273	17000.0	*
hybridization	ChEMBL1628145		0.945946	2400.0	*
substructure	ChEMBL389126		0.928571	4900.0	*
graph	ChEMBL1627436		0.813953	9400.0	*
pubchem	ChEMBL1627439		0.932773	1100.0	*
cdk_maccs	ChEMBL265926		0.897436	4800.0	*
klekota_roth	ChEMBL265926		0.855072	4800.0	*

*** ic50 ACTIVITY *** value prediction

based on 13 locally validated fgps ---> 7904.002

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

3 rank

Glucocorticoid receptor : Homo sapiens

score: 10.562 on ChEMBL2034 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL135		0.789474	41422.000	*
MFP1	ChEMBL135		0.758621	41422.000	*
RDKit7	ChEMBL135		0.722429	41422.000	*
Pattern	ChEMBL282575		0.919105	5074.000	*
AP_bits	ChEMBL135		0.558491	41422.000	*
TT_bits	ChEMBL135		0.742424	41422.000	*
FP2	ChEMBL135		0.675325	41422.000	*
hybridization	ChEMBL135		0.905405	41422.000	*
substructure	ChEMBL469944		0.928571	1.300	*
graph	ChEMBL1766		0.914894	2.573	*

```

pubchem      CHEMBL135      0.915254  41422.000      *
cdk_maccs    CHEMBL1256102  0.853659  15848.930      *
klekota_roth CHEMBL135      0.878788  41422.000      *
*** ic50 ACTIVITY *** value prediction
based on 13 locally validated fgps ---> 26907.660
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

```

4 rank

Androgen Receptor : Rattus norvegicus

score: 10.555 on CHEMBL3072 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL135		0.789474	353.00	*
MFP1	CHEMBL467987		0.785714	8511.38	*
RDKit7	CHEMBL135		0.722429	353.00	*
Pattern	CHEMBL282575		0.919105	10.00	*
AP_bits	CHEMBL467987		0.572993	8511.38	*
TT_bits	CHEMBL467987		0.757576	8511.38	*
FP2	CHEMBL135		0.675325	353.00	*
hybridization	CHEMBL135		0.905405	353.00	*
substructure	CHEMBL135		0.857143	353.00	*
graph	CHEMBL139841		0.933333	41200.00	*
pubchem	CHEMBL135		0.915254	353.00	*
cdk_maccs	CHEMBL135		0.842105	353.00	*
klekota_roth	CHEMBL135		0.878788	353.00	*

```

*** ic50 ACTIVITY *** value prediction
based on 13 locally validated fgps ---> 23995.105
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

```

5 rank

Estrogen receptor alpha : Homo sapiens

score: 10.539 on CHEMBL206 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL135		0.789474	0.41	*
MFP1	CHEMBL135		0.758621	0.41	*
RDKit7	CHEMBL135		0.722429	0.41	*
Pattern	CHEMBL282575		0.919105	65.00	*
AP_bits	CHEMBL135		0.558491	0.41	*
TT_bits	CHEMBL135		0.742424	0.41	*
FP2	CHEMBL135		0.675325	0.41	*
hybridization	CHEMBL135		0.905405	0.41	*
substructure	CHEMBL1628029		0.928571	193.00	*
graph	CHEMBL1257167		0.891304	15848.93	*
pubchem	CHEMBL135		0.915254	0.41	*
cdk_maccs	CHEMBL1256102		0.853659	15848.93	*
klekota_roth	CHEMBL135		0.878788	0.41	*

```

*** ic50 ACTIVITY *** value prediction
based on 13 locally validated fgps ---> 4983.664
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

```

6 rank

Estrogen receptor beta : Homo sapiens

score: 10.520 on CHEMBL242 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL135		0.789474	0.046	*

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
MFP1	CHEMBL135	0.758621	0.046	*
RDKit7	CHEMBL135	0.722429	0.046	*
Pattern	CHEMBL511812	0.900000	660.000	*
AP_bits	CHEMBL135	0.558491	0.046	*
TT_bits	CHEMBL135	0.742424	0.046	*
FP2	CHEMBL135	0.675325	0.046	*
hybridization	CHEMBL135	0.905405	0.046	*
substructure	CHEMBL1628029	0.928571	267.000	*
graph	CHEMBL1257167	0.891304	4045.760	*
pubchem	CHEMBL135	0.915254	0.046	*
cdk_maccs	CHEMBL1256102	0.853659	11857.690	*
klekota_roth	CHEMBL135	0.878788	0.046	*

*** ic50 ACTIVITY *** value prediction
based on 13 locally validated fgps ---> 1987.543
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

7 rank

Progesterone receptor : Bos taurus

score: 10.479 on CHEMBL1909044 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	32559.0	*
MFP1	CHEMBL135	0.758621	32559.0	*
RDKit7	CHEMBL135	0.722429	32559.0	*
Pattern	CHEMBL282575	0.919105	9608.0	*
AP_bits	CHEMBL135	0.558491	32559.0	*
TT_bits	CHEMBL135	0.742424	32559.0	*
FP2	CHEMBL135	0.675325	32559.0	*
hybridization	CHEMBL135	0.905405	32559.0	*
substructure	CHEMBL135	0.857143	32559.0	*
graph	CHEMBL1766	0.914894	84.0	*
pubchem	CHEMBL135	0.915254	32559.0	*
cdk_maccs	CHEMBL135	0.842105	32559.0	*
klekota_roth	CHEMBL135	0.878788	32559.0	*

*** ic50 ACTIVITY *** value prediction
based on 13 locally validated fgps ---> 19730.947
["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
"klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
"hybridization"]

8 rank

Androgen Receptor : Homo sapiens

score: 10.462 on CHEMBL1871 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	19.1	*
MFP1	CHEMBL135	0.758621	19.1	*
RDKit7	CHEMBL135	0.722429	19.1	*
Pattern	CHEMBL3421871	0.881864	300.0	*
AP_bits	CHEMBL135	0.558491	19.1	*
TT_bits	CHEMBL135	0.742424	19.1	*
FP2	CHEMBL135	0.675325	19.1	*
hybridization	CHEMBL135	0.905405	19.1	*
substructure	CHEMBL135	0.857143	19.1	*
graph	CHEMBL236699	0.934783	410.0	*
pubchem	CHEMBL135	0.915254	19.1	*
cdk_maccs	CHEMBL135	0.842105	19.1	*
klekota_roth	CHEMBL135	0.878788	19.1	*

*** ic50 ACTIVITY *** value prediction
based on 13 locally validated fgps ---> 319.119

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

9 rank

Serotonin transporter : Homo sapiens

score: 10.379 on ChEMBL228 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL135		0.789474	10755.0	*	
MFP1	ChEMBL135		0.758621	10755.0	*	
RDKit7	ChEMBL135		0.722429	10755.0	*	
Pattern	ChEMBL282575		0.919105	3672.0	*	
AP_bits	ChEMBL135		0.558491	10755.0	*	
TT_bits	ChEMBL135		0.742424	10755.0	*	
FP2	ChEMBL135		0.675325	10755.0	*	
hybridization	ChEMBL135		0.905405	10755.0	*	
substructure	ChEMBL135		0.857143	10755.0	*	
graph	ChEMBL135		0.813953	10755.0	*	
pubchem	ChEMBL135		0.915254	10755.0	*	
cdk_maccs	ChEMBL135		0.842105	10755.0	*	
klekota_roth	ChEMBL135		0.878788	10755.0	*	

*** ic50 ACTIVITY *** value prediction

based on 13 locally validated fgps ---> 8800.438

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

10 rank

Dopamine transporter : Homo sapiens

score: 10.351 on ChEMBL238 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL135		0.789474	14911.0	*	
MFP1	ChEMBL135		0.758621	14911.0	*	
RDKit7	ChEMBL135		0.722429	14911.0	*	
Pattern	ChEMBL691		0.891192	559.0	*	
AP_bits	ChEMBL135		0.558491	14911.0	*	
TT_bits	ChEMBL135		0.742424	14911.0	*	
FP2	ChEMBL135		0.675325	14911.0	*	
hybridization	ChEMBL135		0.905405	14911.0	*	
substructure	ChEMBL135		0.857143	14911.0	*	
graph	ChEMBL135		0.813953	14911.0	*	
pubchem	ChEMBL135		0.915254	14911.0	*	
cdk_maccs	ChEMBL135		0.842105	14911.0	*	
klekota_roth	ChEMBL135		0.878788	14911.0	*	

*** ic50 ACTIVITY *** value prediction

based on 13 locally validated fgps ---> 10703.291

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

11 rank

Aldehyde oxidase : Homo sapiens

score: 10.351 on ChEMBL3257 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	ChEMBL135		0.789474	80.0	*	
MFP1	ChEMBL135		0.758621	80.0	*	
RDKit7	ChEMBL135		0.722429	80.0	*	
Pattern	ChEMBL691		0.891192	570.0	*	
AP_bits	ChEMBL135		0.558491	80.0	*	
TT_bits	ChEMBL135		0.742424	80.0	*	

FP2	CHEMBL135	0.675325	80.0	*
hybridization	CHEMBL135	0.905405	80.0	*
substructure	CHEMBL135	0.857143	80.0	*
graph	CHEMBL135	0.813953	80.0	*
pubchem	CHEMBL135	0.915254	80.0	*
cdk_maccs	CHEMBL135	0.842105	80.0	*
klekota_roth	CHEMBL135	0.878788	80.0	*

*** ic50 ACTIVITY *** value prediction
 based on 13 locally validated fgps ---> 223.658
 ["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
 "klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
 "hybridization"]

12 rank

Arachidonate 15-lipoxygenase : *Oryctolagus cuniculus*

score: 10.351 on ChEMBL4358 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	11295.0	*
MFP1	CHEMBL135	0.758621	11295.0	*
RDKit7	CHEMBL135	0.722429	11295.0	*
Pattern	CHEMBL691	0.891192	5678.0	*
AP_bits	CHEMBL135	0.558491	11295.0	*
TT_bits	CHEMBL135	0.742424	11295.0	*
FP2	CHEMBL135	0.675325	11295.0	*
hybridization	CHEMBL135	0.905405	11295.0	*
substructure	CHEMBL135	0.857143	11295.0	*
graph	CHEMBL135	0.813953	11295.0	*
pubchem	CHEMBL135	0.915254	11295.0	*
cdk_maccs	CHEMBL135	0.842105	11295.0	*
klekota_roth	CHEMBL135	0.878788	11295.0	*

*** ic50 ACTIVITY *** value prediction
 based on 13 locally validated fgps ---> 9771.506
 ["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
 "klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
 "hybridization"]

13 rank

Estrogen-related receptor alpha : *Homo sapiens*

score: 10.317 on ChEMBL3429 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	3.6	*
MFP1	CHEMBL135	0.758621	3.6	*
RDKit7	CHEMBL135	0.722429	3.6	*
Pattern	CHEMBL2326071	0.857143	637.8	*
AP_bits	CHEMBL135	0.558491	3.6	*
TT_bits	CHEMBL135	0.742424	3.6	*
FP2	CHEMBL135	0.675325	3.6	*
hybridization	CHEMBL135	0.905405	3.6	*
substructure	CHEMBL135	0.857143	3.6	*
graph	CHEMBL135	0.813953	3.6	*
pubchem	CHEMBL135	0.915254	3.6	*
cdk_maccs	CHEMBL135	0.842105	3.6	*
klekota_roth	CHEMBL135	0.878788	3.6	*

*** ic50 ACTIVITY *** value prediction
 based on 13 locally validated fgps ---> 72.934
 ["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
 "klekota_roth", "pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7",
 "hybridization"]

14 rank

Estrogen-related receptor beta : Homo sapiens

score: 10.317 on ChEMBL3751 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	3.2	*
MFP1	CHEMBL135	0.758621	3.2	*
RDKit7	CHEMBL135	0.722429	3.2	*
Pattern	CHEMBL2326071	0.857143	565.9	*
AP_bits	CHEMBL135	0.558491	3.2	*
TT_bits	CHEMBL135	0.742424	3.2	*
FP2	CHEMBL135	0.675325	3.2	*
hybridization	CHEMBL135	0.905405	3.2	*
substructure	CHEMBL135	0.857143	3.2	*
graph	CHEMBL135	0.813953	3.2	*
pubchem	CHEMBL135	0.915254	3.2	*
cdk_maccs	CHEMBL135	0.842105	3.2	*
klekota_roth	CHEMBL135	0.878788	3.2	*

*** ic50 ACTIVITY *** value prediction

based on 13 locally validated fgps ---> 55.498

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

15 rank

Estradiol 17-beta-dehydrogenase 1 : Homo sapiens

score: 10.255 on ChEMBL3181 based on 13 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL270250	0.789474	790.0	*
MFP1	CHEMBL1627884	0.611111	4300.0	*
RDKit7	CHEMBL1627455	0.711165	1000.0	*
Pattern	CHEMBL270250	0.943860	790.0	*
AP_bits	CHEMBL1627453	0.552632	420.0	*
TT_bits	CHEMBL1627884	0.578947	4300.0	*
FP2	CHEMBL270250	0.666667	790.0	*
hybridization	CHEMBL270250	0.881579	790.0	*
substructure	CHEMBL270250	0.928571	790.0	*
graph	CHEMBL1627884	0.977273	4300.0	*
pubchem	CHEMBL270250	0.932773	790.0	*
cdk_maccs	CHEMBL1079595	0.800000	140.0	*
klekota_roth	CHEMBL1627884	0.880597	4300.0	*

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 1724.509

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

16 rank

Solute carrier family 22 member 2 : Rattus norvegicus

score: 9.459 on ChEMBL1770032 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	84800.0	*
MFP1	CHEMBL135	0.758621	84800.0	*
RDKit7	CHEMBL135	0.722429	84800.0	*
Pattern	CHEMBL135	0.831858	84800.0	*
AP_bits	CHEMBL135	0.558491	84800.0	*
TT_bits	CHEMBL135	0.742424	84800.0	*
FP2	CHEMBL135	0.675325	84800.0	*
hybridization	CHEMBL135	0.905405	84800.0	*
substructure	CHEMBL135	0.857143	84800.0	*
graph	CHEMBL135	0.813953	84800.0	*
pubchem	CHEMBL135	0.915254	84800.0	*
cdk_maccs	CHEMBL135	0.842105	84800.0	*

```

    klekota_roth CHEMBL135          0.878788    84800.0      *
    *** ic50 ACTIVITY *** value prediction
    based on 12 locally validated fgps ---> 81435.582
["TT_bits", "substructure", "cdk_maccs", "AP_bits", "MFP1",
"klekota_roth", "pubchem", "graph", "FP2", "FeatMFP1", "RDKit7",
"hybridization"]

```

17 rank

Voltage-gated L-type calcium channel alpha-1C subunit : Homo sapiens
score: 9.459 on CHEMBL1940 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	50000.0	*
MFP1	CHEMBL135	0.758621	50000.0	*
RDKit7	CHEMBL135	0.722429	50000.0	*
Pattern	CHEMBL135	0.831858	50000.0	
AP_bits	CHEMBL135	0.558491	50000.0	*
TT_bits	CHEMBL135	0.742424	50000.0	*
FP2	CHEMBL135	0.675325	50000.0	*
hybridization	CHEMBL135	0.905405	50000.0	*
substructure	CHEMBL135	0.857143	50000.0	*
graph	CHEMBL135	0.813953	50000.0	*
pubchem	CHEMBL135	0.915254	50000.0	*
cdk_maccs	CHEMBL135	0.842105	50000.0	*
klekota_roth	CHEMBL135	0.878788	50000.0	*

```

    *** ic50 ACTIVITY *** value prediction
    based on 12 locally validated fgps ---> 47918.083
["TT_bits", "substructure", "cdk_maccs", "AP_bits", "MFP1",
"klekota_roth", "pubchem", "graph", "FP2", "FeatMFP1", "RDKit7",
"hybridization"]

```

18 rank

Solute carrier family 22 member 3 : Homo sapiens

score: 9.459 on CHEMBL2073673 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	2880.0	*
MFP1	CHEMBL135	0.758621	2880.0	*
RDKit7	CHEMBL135	0.722429	2880.0	*
Pattern	CHEMBL135	0.831858	2880.0	
AP_bits	CHEMBL135	0.558491	2880.0	*
TT_bits	CHEMBL135	0.742424	2880.0	*
FP2	CHEMBL135	0.675325	2880.0	*
hybridization	CHEMBL135	0.905405	2880.0	*
substructure	CHEMBL135	0.857143	2880.0	*
graph	CHEMBL135	0.813953	2880.0	*
pubchem	CHEMBL135	0.915254	2880.0	*
cdk_maccs	CHEMBL135	0.842105	2880.0	*
klekota_roth	CHEMBL135	0.878788	2880.0	*

```

    *** ic50 ACTIVITY *** value prediction
    based on 12 locally validated fgps ---> 2880.000
["TT_bits", "substructure", "cdk_maccs", "AP_bits", "MFP1",
"klekota_roth", "pubchem", "graph", "FP2", "FeatMFP1", "RDKit7",
"hybridization"]

```

19 rank

Estrogen receptor alpha : Rattus norvegicus

score: 9.459 on CHEMBL2724 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	1.9	*
MFP1	CHEMBL135	0.758621	1.9	*
RDKit7	CHEMBL135	0.722429	1.9	*

Pattern	CHEMBL135	0.831858	1.9	
AP_bits	CHEMBL135	0.558491	1.9	*
TT_bits	CHEMBL135	0.742424	1.9	*
FP2	CHEMBL135	0.675325	1.9	*
hybridization	CHEMBL135	0.905405	1.9	*
substructure	CHEMBL135	0.857143	1.9	*
graph	CHEMBL135	0.813953	1.9	*
pubchem	CHEMBL135	0.915254	1.9	*
cdk_maccs	CHEMBL135	0.842105	1.9	*
klekota_roth	CHEMBL135	0.878788	1.9	*

*** ic50 ACTIVITY *** value prediction
based on 12 locally validated fgps ---> 2.190
["TT_bits", "substructure", "cdk_maccs", "AP_bits", "MFP1",
"klekota_roth", "pubchem", "graph", "FP2", "FeatMFP1", "RDKit7",
"hybridization"]

20 rank
Estrogen receptor beta : Rattus norvegicus
score: 9.459 on ChEMBL3021 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	1.7	*
MFP1	CHEMBL135	0.758621	1.7	*
RDKit7	CHEMBL135	0.722429	1.7	*
Pattern	CHEMBL135	0.831858	1.7	
AP_bits	CHEMBL135	0.558491	1.7	*
TT_bits	CHEMBL135	0.742424	1.7	*
FP2	CHEMBL135	0.675325	1.7	*
hybridization	CHEMBL135	0.905405	1.7	*
substructure	CHEMBL135	0.857143	1.7	*
graph	CHEMBL135	0.813953	1.7	*
pubchem	CHEMBL135	0.915254	1.7	*
cdk_maccs	CHEMBL135	0.842105	1.7	*
klekota_roth	CHEMBL135	0.878788	1.7	*

*** ic50 ACTIVITY *** value prediction
based on 12 locally validated fgps ---> 1.700
["TT_bits", "substructure", "cdk_maccs", "AP_bits", "MFP1",
"klekota_roth", "pubchem", "graph", "FP2", "FeatMFP1", "RDKit7",
"hybridization"]

21 rank
Testis-specific androgen-binding protein : Homo sapiens
score: 9.459 on ChEMBL3305 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL135	0.789474	50.0	*
MFP1	CHEMBL135	0.758621	50.0	*
RDKit7	CHEMBL135	0.722429	50.0	*
Pattern	CHEMBL135	0.831858	50.0	
AP_bits	CHEMBL135	0.558491	50.0	*
TT_bits	CHEMBL135	0.742424	50.0	*
FP2	CHEMBL135	0.675325	50.0	*
hybridization	CHEMBL135	0.905405	50.0	*
substructure	CHEMBL135	0.857143	50.0	*
graph	CHEMBL135	0.813953	50.0	*
pubchem	CHEMBL135	0.915254	50.0	*
cdk_maccs	CHEMBL135	0.842105	50.0	*
klekota_roth	CHEMBL135	0.878788	50.0	*

*** ic50 ACTIVITY *** value prediction
based on 12 locally validated fgps ---> 446.587

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

22 rank

Solute carrier family 22 member 1 : Homo sapiens

score: 9.459 on ChEMBL5685 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	ChEMBL135	0.789474	5730.0	*
MFP1	ChEMBL135	0.758621	5730.0	*
RDKit7	ChEMBL135	0.722429	5730.0	*
Pattern	ChEMBL135	0.831858	5730.0	
AP_bits	ChEMBL135	0.558491	5730.0	*
TT_bits	ChEMBL135	0.742424	5730.0	*
FP2	ChEMBL135	0.675325	5730.0	*
hybridization	ChEMBL135	0.905405	5730.0	*
substructure	ChEMBL135	0.857143	5730.0	*
graph	ChEMBL135	0.813953	5730.0	*
pubchem	ChEMBL135	0.915254	5730.0	*
cdk_maccs	ChEMBL135	0.842105	5730.0	*
klekota_roth	ChEMBL135	0.878788	5730.0	*

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 7986.176

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

23 rank

Glucose-6-phosphate 1-dehydrogenase : Homo sapiens

score: 8.592 on ChEMBL5347 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	ChEMBL1412489	0.789474	29100.0	*
MFP1	ChEMBL467987	0.785714	72500.0	*
RDKit7	ChEMBL467987	0.702768	72500.0	*
Pattern	ChEMBL1412489	0.874346	29100.0	*
AP_bits	ChEMBL467987	0.572993	72500.0	*
TT_bits	ChEMBL467987	0.757576	72500.0	*
FP2	ChEMBL467987	0.666667	72500.0	*
hybridization	ChEMBL467987	0.873913	72500.0	*
substructure	ChEMBL1412489	0.800000	29100.0	
graph	ChEMBL2057301	0.813953	4300.0	*
pubchem	ChEMBL1412489	0.887097	29100.0	*
cdk_maccs	ChEMBL1412489	0.780488	29100.0	
klekota_roth	ChEMBL467987	0.867647	72500.0	*

*** ic50 ACTIVITY *** value prediction

based on 11 locally validated fgps ---> 51686.893

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

24 rank

Glucose-6-phosphate dehydrogenase-6-phosphogluconolactonase : Plasmodium
berghei

score: 8.556 on ChEMBL1741212 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	ChEMBL1412489	0.789474	4020.0	*
MFP1	ChEMBL467987	0.785714	20900.0	*
RDKit7	ChEMBL467987	0.702768	20900.0	*
Pattern	ChEMBL1412489	0.874346	4020.0	*
AP_bits	ChEMBL467987	0.572993	20900.0	*
TT_bits	ChEMBL467987	0.757576	20900.0	*

	FP2	CHEMBL467987	0.666667	20900.0	*
hybridization	CHEMBL467987	0.873913	20900.0	*	
substructure	CHEMBL1736559	0.812500	35700.0		
graph	CHEMBL1412489	0.777778	4020.0	*	
pubchem	CHEMBL1412489	0.887097	4020.0	*	
cdk_maccs	CHEMBL1412489	0.780488	4020.0		
klekota_roth	CHEMBL467987	0.867647	20900.0	*	

*** ic50 ACTIVITY *** value prediction
 based on 11 locally validated fgps ---> 14726.341
 ["TT_bits", "Pattern", "FP2", "MFP1", "klekota_roth", "pubchem", "graph",
 "AP_bits", "FeatMFP1", "RDKit7", "hybridization"]

25 rank

M18 aspartyl aminopeptidase : Plasmodium falciparum 3D7

score: 7.575 on CHEMBL1293263 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1412489	0.789474	1220.0	*		
MFP1	CHEMBL1412489	0.700000	1220.0	*		
RDKit7	CHEMBL1412489	0.664062	1220.0			
Pattern	CHEMBL1412489	0.874346	1220.0	*		
AP_bits	CHEMBL1412489	0.569343	1220.0	*		
TT_bits	CHEMBL1412489	0.652778	1220.0	*		
FP2	CHEMBL1412489	0.654321	1220.0	*		
hybridization	CHEMBL1412489	0.841667	1220.0	*		
substructure	CHEMBL1412489	0.800000	1220.0			
graph	CHEMBL1412489	0.777778	1220.0	*		
pubchem	CHEMBL1412489	0.887097	1220.0	*		
cdk_maccs	CHEMBL1412489	0.780488	1220.0			
klekota_roth	CHEMBL1412489	0.828571	1220.0	*		

*** ic50 ACTIVITY *** value prediction
 based on 10 locally validated fgps ---> 1220.000
 ["TT_bits", "Pattern", "AP_bits", "MFP1", "pubchem", "graph", "FP2",
 "FeatMFP1", "klekota_roth", "hybridization"]

26 rank

Mannose-6-phosphate isomerase : Homo sapiens

score: 7.575 on CHEMBL2758 based on 10 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid	fg
FeatMFP1	CHEMBL1412489	0.789474	29007.0	*		
MFP1	CHEMBL1412489	0.700000	29007.0	*		
RDKit7	CHEMBL1412489	0.664062	29007.0			
Pattern	CHEMBL1412489	0.874346	29007.0	*		
AP_bits	CHEMBL1412489	0.569343	29007.0	*		
TT_bits	CHEMBL1412489	0.652778	29007.0	*		
FP2	CHEMBL1412489	0.654321	29007.0	*		
hybridization	CHEMBL1412489	0.841667	29007.0	*		
substructure	CHEMBL1412489	0.800000	29007.0			
graph	CHEMBL1412489	0.777778	29007.0	*		
pubchem	CHEMBL1412489	0.887097	29007.0	*		
cdk_maccs	CHEMBL1412489	0.780488	29007.0			
klekota_roth	CHEMBL1412489	0.828571	29007.0	*		

*** ic50 ACTIVITY *** value prediction
 based on 10 locally validated fgps ---> 29007.000
 ["TT_bits", "Pattern", "AP_bits", "MFP1", "pubchem", "graph", "FP2",
 "FeatMFP1", "klekota_roth", "hybridization"]

27 rank

Norepinephrine transporter : Homo sapiens

score: 7.407 on CHEMBL222 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	CHEMBL691	0.636364	959.0		
MFP1	CHEMBL282575	0.583333	17229.0		*
RDKit7	CHEMBL691	0.688940	959.0		*
Pattern	CHEMBL282575	0.919105	17229.0		*
AP_bits	CHEMBL282575	0.538905	17229.0		*
TT_bits	CHEMBL282575	0.641026	17229.0		*
FP2	CHEMBL691	0.619048	959.0		
hybridization	CHEMBL691	0.816327	959.0		*
substructure	CHEMBL3769872	0.733333	33.0		
graph	CHEMBL1200623	0.790698	2098.0		*
pubchem	CHEMBL691	0.830645	959.0		*
cdk_maccs	CHEMBL691	0.820513	959.0		*
klekota_roth	CHEMBL691	0.777778	959.0		*

*** ic50 ACTIVITY *** value prediction
based on 10 locally validated fgps ---> 7547.598
["TT_bits", "cdk_maccs", "Pattern", "MFP1", "klekota_roth", "pubchem",
"graph", "AP_bits", "RDKit7", "hybridization"]

28 rank

Adenosine A3 receptor : Homo sapiens

score: 6.617 on ChEMBL256 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL691	0.636364	32925.0		
MFP1	CHEMBL282575	0.583333	21780.0		*
RDKit7	CHEMBL691	0.688940	32925.0		*
Pattern	CHEMBL282575	0.919105	21780.0		*
AP_bits	CHEMBL282575	0.538905	21780.0		*
TT_bits	CHEMBL282575	0.641026	21780.0		*
FP2	CHEMBL691	0.619048	32925.0		
hybridization	CHEMBL691	0.816327	32925.0		*
substructure	CHEMBL691	0.687500	32925.0		
graph	CHEMBL691	0.767442	32925.0		
pubchem	CHEMBL691	0.830645	32925.0		*
cdk_maccs	CHEMBL691	0.820513	32925.0		*
klekota_roth	CHEMBL691	0.777778	32925.0		*

*** ic50 ACTIVITY *** value prediction
based on 9 locally validated fgps ---> 27997.013
["TT_bits", "cdk_maccs", "Pattern", "MFP1", "klekota_roth", "pubchem",
"AP_bits", "RDKit7", "hybridization"]

29 rank

Nuclear receptor subfamily 1 group I member 3 : Homo sapiens

score: 6.144 on ChEMBL5503 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL691	0.636364	3000.0		
MFP1	CHEMBL691	0.527778	3000.0		*
RDKit7	CHEMBL691	0.688940	3000.0		*
Pattern	CHEMBL691	0.891192	3000.0		*
AP_bits	CHEMBL691	0.465574	3000.0		
TT_bits	CHEMBL691	0.487805	3000.0		
FP2	CHEMBL691	0.619048	3000.0		
hybridization	CHEMBL691	0.816327	3000.0		*
substructure	CHEMBL2311171	0.714286	1200.0		
graph	CHEMBL2311171	0.790698	1200.0		*
pubchem	CHEMBL691	0.830645	3000.0		*
cdk_maccs	CHEMBL691	0.820513	3000.0		*
klekota_roth	CHEMBL691	0.777778	3000.0		*

*** ic50 ACTIVITY *** value prediction
based on 8 locally validated fgps ---> 2674.102

["cdk_maccs", "Pattern", "MFP1", "klekota_roth", "pubchem", "graph", "RDKit7", "hybridization"]

30 rank

UDP-glucuronosyltransferase 1-1 : Homo sapiens

score: 5.353 on ChEMBL1287617 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL691	0.636364	21000.0	
MFP1	CHEMBL691	0.527778	21000.0	*
RDKit7	CHEMBL691	0.688940	21000.0	*
Pattern	CHEMBL691	0.891192	21000.0	*
AP_bits	CHEMBL691	0.465574	21000.0	
TT_bits	CHEMBL691	0.487805	21000.0	
FP2	CHEMBL691	0.619048	21000.0	
hybridization	CHEMBL691	0.816327	21000.0	*
substructure	CHEMBL691	0.687500	21000.0	
graph	CHEMBL691	0.767442	21000.0	
pubchem	CHEMBL691	0.830645	21000.0	*
cdk_maccs	CHEMBL691	0.820513	21000.0	*
klekota_roth	CHEMBL691	0.777778	21000.0	*

*** ic50 ACTIVITY *** value prediction

based on 7 locally validated fgps ---> 21000.000

["Pattern", "MFP1", "pubchem", "klekota_roth", "hybridization", "RDKit7", "cdk_maccs"]

31 rank

Solute carrier family 22 member 2 : Homo sapiens

score: 5.353 on ChEMBL1743122 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL691	0.636364	2200.0	
MFP1	CHEMBL691	0.527778	2200.0	*
RDKit7	CHEMBL691	0.688940	2200.0	*
Pattern	CHEMBL691	0.891192	2200.0	*
AP_bits	CHEMBL691	0.465574	2200.0	
TT_bits	CHEMBL691	0.487805	2200.0	
FP2	CHEMBL691	0.619048	2200.0	
hybridization	CHEMBL691	0.816327	2200.0	*
substructure	CHEMBL691	0.687500	2200.0	
graph	CHEMBL103	0.767442	26700.0	
pubchem	CHEMBL691	0.830645	2200.0	*
cdk_maccs	CHEMBL691	0.820513	2200.0	*
klekota_roth	CHEMBL691	0.777778	2200.0	*

*** ic50 ACTIVITY *** value prediction

based on 7 locally validated fgps ---> 2200.000

["Pattern", "MFP1", "pubchem", "klekota_roth", "hybridization", "RDKit7", "cdk_maccs"]

32 rank

Multidrug and toxin extrusion protein 1 : Homo sapiens

score: 5.353 on ChEMBL1743126 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL691	0.636364	21100.0	
MFP1	CHEMBL691	0.527778	21100.0	*
RDKit7	CHEMBL691	0.688940	21100.0	*
Pattern	CHEMBL691	0.891192	21100.0	*
AP_bits	CHEMBL691	0.465574	21100.0	
TT_bits	CHEMBL691	0.487805	21100.0	
FP2	CHEMBL691	0.619048	21100.0	
hybridization	CHEMBL691	0.816327	21100.0	*
substructure	CHEMBL691	0.687500	21100.0	

```

graph CHEMBL691 0.767442 21100.0
pubchem CHEMBL691 0.830645 21100.0 *
cdk_maccs CHEMBL691 0.820513 21100.0 *
klekota_roth CHEMBL691 0.777778 21100.0 *
*** ic50 ACTIVITY *** value prediction
based on 7 locally validated fgps ---> 21100.000
["Pattern", "MFP1", "pubchem", "klekota_roth", "hybridization", "RDKit7",
"cdk_maccs"]

```

33 rank

Multidrug and toxin extrusion protein 2 : Homo sapiens

score: 5.353 on CHEMBL1743127 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL691	0.636364	20200.0	
MFP1	CHEMBL691	0.527778	20200.0	*
RDKit7	CHEMBL691	0.688940	20200.0	*
Pattern	CHEMBL691	0.891192	20200.0	*
AP_bits	CHEMBL691	0.465574	20200.0	
TT_bits	CHEMBL691	0.487805	20200.0	
FP2	CHEMBL691	0.619048	20200.0	
hybridization	CHEMBL691	0.816327	20200.0	*
substructure	CHEMBL691	0.687500	20200.0	
graph	CHEMBL691	0.767442	20200.0	
pubchem	CHEMBL691	0.830645	20200.0	*
cdk_maccs	CHEMBL691	0.820513	20200.0	*
klekota_roth	CHEMBL691	0.777778	20200.0	*

```

*** ic50 ACTIVITY *** value prediction
based on 7 locally validated fgps ---> 20200.000
["Pattern", "MFP1", "pubchem", "klekota_roth", "hybridization", "RDKit7",
"cdk_maccs"]

```

34 rank

Mu opioid receptor : Homo sapiens

score: 5.353 on CHEMBL233 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL691	0.636364	26769.0	
MFP1	CHEMBL691	0.527778	26769.0	*
RDKit7	CHEMBL691	0.688940	26769.0	*
Pattern	CHEMBL691	0.891192	26769.0	*
AP_bits	CHEMBL691	0.465574	26769.0	
TT_bits	CHEMBL691	0.487805	26769.0	
FP2	CHEMBL691	0.619048	26769.0	
hybridization	CHEMBL691	0.816327	26769.0	*
substructure	CHEMBL691	0.687500	26769.0	
graph	CHEMBL691	0.767442	26769.0	
pubchem	CHEMBL691	0.830645	26769.0	*
cdk_maccs	CHEMBL691	0.820513	26769.0	*
klekota_roth	CHEMBL691	0.777778	26769.0	*

```

*** ic50 ACTIVITY *** value prediction
based on 7 locally validated fgps ---> 26769.000
["Pattern", "MFP1", "pubchem", "klekota_roth", "hybridization", "RDKit7",
"cdk_maccs"]

```

35 rank

Kappa opioid receptor : Homo sapiens

score: 5.353 on CHEMBL237 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL68354	0.640000	3.8	
MFP1	CHEMBL691	0.527778	25894.0	*
RDKit7	CHEMBL691	0.688940	25894.0	*

Pattern	CHEMBL691	0.891192	25894.0	*
AP_bits	CHEMBL691	0.465574	25894.0	
TT_bits	CHEMBL691	0.487805	25894.0	
FP2	CHEMBL691	0.619048	25894.0	
hybridization	CHEMBL691	0.816327	25894.0	*
substructure	CHEMBL691	0.687500	25894.0	
graph	CHEMBL691	0.767442	25894.0	
pubchem	CHEMBL691	0.830645	25894.0	*
cdk_maccs	CHEMBL691	0.820513	25894.0	*
klekota_roth	CHEMBL691	0.777778	25894.0	*

*** ic50 ACTIVITY *** value prediction
 based on 7 locally validated fgps ---> 25894.000
 ["Pattern", "MFP1", "pubchem", "klekota_roth", "hybridization", "RDKit7",
 "cdk_maccs"]

36 rank

Adenosine A2a receptor : Homo sapiens

score: 5.353 on ChEMBL251 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL691	0.636364	20931.0	
MFP1	CHEMBL691	0.527778	20931.0	*
RDKit7	CHEMBL691	0.688940	20931.0	*
Pattern	CHEMBL691	0.891192	20931.0	*
AP_bits	CHEMBL691	0.465574	20931.0	
TT_bits	CHEMBL691	0.487805	20931.0	
FP2	CHEMBL691	0.619048	20931.0	
hybridization	CHEMBL691	0.816327	20931.0	*
substructure	CHEMBL691	0.687500	20931.0	
graph	CHEMBL691	0.767442	20931.0	
pubchem	CHEMBL691	0.830645	20931.0	*
cdk_maccs	CHEMBL691	0.820513	20931.0	*
klekota_roth	CHEMBL691	0.777778	20931.0	*

*** ic50 ACTIVITY *** value prediction
 based on 7 locally validated fgps ---> 20931.000
 ["Pattern", "MFP1", "pubchem", "klekota_roth", "hybridization", "RDKit7",
 "cdk_maccs"]

37 rank

Serotonin 4 (5-HT4) receptor : Cavia porcellus

score: 5.353 on ChEMBL5017 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL691	0.636364	7953.0	
MFP1	CHEMBL691	0.527778	7953.0	*
RDKit7	CHEMBL691	0.688940	7953.0	*
Pattern	CHEMBL691	0.891192	7953.0	*
AP_bits	CHEMBL691	0.465574	7953.0	
TT_bits	CHEMBL691	0.487805	7953.0	
FP2	CHEMBL691	0.619048	7953.0	
hybridization	CHEMBL691	0.816327	7953.0	*
substructure	CHEMBL691	0.687500	7953.0	
graph	CHEMBL691	0.767442	7953.0	
pubchem	CHEMBL691	0.830645	7953.0	*
cdk_maccs	CHEMBL691	0.820513	7953.0	*
klekota_roth	CHEMBL691	0.777778	7953.0	*

*** ic50 ACTIVITY *** value prediction
 based on 7 locally validated fgps ---> 7953.000
 ["Pattern", "MFP1", "pubchem", "klekota_roth", "hybridization", "RDKit7",
 "cdk_maccs"]

38 rank

Tubulin : Bos taurus

score: 5.303 on ChEMBL2111464 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1627442		0.652174	660.0	
MFP1	CHEMBL299613		0.687500	1400.0	*
RDKit7	CHEMBL299613		0.669318	1400.0	
Pattern	CHEMBL1627442		0.885563	660.0	*
AP_bits	CHEMBL299613		0.553265	1400.0	*
TT_bits	CHEMBL299613		0.735294	1400.0	*
FP2	CHEMBL299613		0.597701	1400.0	
hybridization	CHEMBL299613		0.755639	1400.0	*
substructure	CHEMBL1627442		0.866667	660.0	*
graph	CHEMBL299613		0.614035	1400.0	
pubchem	CHEMBL299613		0.785185	1400.0	
cdk_maccs	CHEMBL299613		0.744186	1400.0	
klekota_roth	CHEMBL299613		0.819444	1400.0	*

*** ic50 ACTIVITY *** value prediction

based on 7 locally validated fgps ---> 1070.962

["TT_bits", "substructure", "Pattern", "MFP1", "AP_bits", "klekota_roth", "hybridization"]

39 rank

Cytochrome P450 3A4 : Homo sapiens

score: 5.240 on ChEMBL340 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL410242		0.625000	1500.0	
MFP1	CHEMBL410242		0.512195	1500.0	
RDKit7	CHEMBL410242		0.644468	1500.0	
Pattern	CHEMBL410242		0.910596	1500.0	*
AP_bits	CHEMBL410242		0.539945	1500.0	*
TT_bits	CHEMBL410242		0.511628	1500.0	*
FP2	CHEMBL410242		0.557895	1500.0	
hybridization	CHEMBL410242		0.825397	1500.0	*
substructure	CHEMBL410242		0.722222	1500.0	
graph	CHEMBL1451		0.895833	49100.0	*
pubchem	CHEMBL469227		0.834711	2770.0	*
cdk_maccs	CHEMBL539168		0.711111	3364.0	
klekota_roth	CHEMBL410242		0.721519	1500.0	*

*** ic50 ACTIVITY *** value prediction

based on 7 locally validated fgps ---> 6546.329

["TT_bits", "Pattern", "AP_bits", "pubchem", "graph", "klekota_roth", "hybridization"]

40 rank

Multidrug resistance-associated protein 4 : Homo sapiens

score: 4.945 on ChEMBL1743128 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL1697724		0.535714	30000.0	
MFP1	CHEMBL3349339		0.583333	50000.0	*
RDKit7	CHEMBL3349339		0.651366	50000.0	
Pattern	CHEMBL3349339		0.882960	50000.0	*
AP_bits	CHEMBL3349339		0.470238	50000.0	*
TT_bits	CHEMBL3349339		0.666667	50000.0	*
FP2	CHEMBL3349339		0.525253	50000.0	
hybridization	CHEMBL3349339		0.689420	50000.0	*
substructure	CHEMBL3349339		0.631579	50000.0	
graph	CHEMBL3349339		0.564516	50000.0	
pubchem	CHEMBL3349339		0.868852	50000.0	*
cdk_maccs	CHEMBL2074591		0.627451	80000.0	
klekota_roth	CHEMBL3349339		0.783784	50000.0	*

*** ic50 ACTIVITY *** value prediction
 based on 7 locally validated fgps ---> 39849.623
 ["TT_bits", "Pattern", "MFP1", "pubchem", "AP_bits", "klekota_roth",
 "hybridization"]

41 rank

Protein-tyrosine phosphatase 2C : Homo sapiens

score: 4.881 on ChEMBL3864 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL461415		0.555556	2270.0	
MFP1	ChEMBL1642763		0.526316	19900.0	*
RDKit7	ChEMBL1642763		0.662971	19900.0	
Pattern	ChEMBL1642763		0.881443	19900.0	*
AP_bits	ChEMBL518627		0.475000	3910.0	*
TT_bits	ChEMBL1642763		0.600000	19900.0	*
FP2	ChEMBL1642763		0.576087	19900.0	
hybridization	ChEMBL1642763		0.742647	19900.0	*
substructure	ChEMBL1642763		0.578947	19900.0	
graph	ChEMBL230006		0.727273	9600.0	
pubchem	ChEMBL1642763		0.856000	19900.0	*
cdk_maccs	ChEMBL461199		0.704545	6400.0	
klekota_roth	ChEMBL1642763		0.800000	19900.0	*

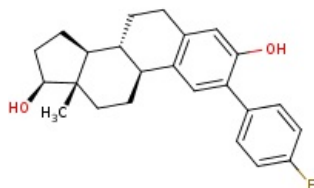
*** ic50 ACTIVITY *** value prediction
 based on 7 locally validated fgps ---> 16500.755
 ["TT_bits", "Pattern", "MFP1", "pubchem", "AP_bits", "klekota_roth",
 "hybridization"]

SwissTargetPrediction report:

Reference:

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

Query Molecule



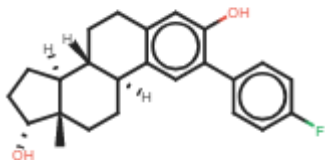
Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
cDNA FLJ16289 fis, clone OCBBF2009920, highly similar to TUBULIN BETA-3 CHAIN (by homology)	A8K854	TUBB3		<div><div></div></div>	3 / 12	Structural
Uncharacterized protein (by homology)	I3L2F9			<div><div></div></div>	3 / 12	Structural
Tubulin beta-4A chain (by homology)	P04350	TUBB4A	CHEMBL3838	<div><div></div></div>	3 / 12	Structural
Tubulin beta chain (by homology)	P07437	TUBB	CHEMBL5444	<div><div></div></div>	3 / 12	Structural
Tubulin beta-4B chain (by homology)	P68371	TUBB4B	CHEMBL1848	<div><div></div></div>	3 / 12	Structural
Melanocyte-stimulating hormone receptor (by homology)	Q01726	MC1R	CHEMBL3795	<div><div></div></div>	9 / 12	Membrane receptor
Tubulin beta-3 chain (by homology)	Q13509	TUBB3	CHEMBL2597	<div><div></div></div>	3 / 12	Structural
Tubulin beta-2A chain (by homology)	Q13885	TUBB2A		<div><div></div></div>	3 / 12	Structural
Tubulin beta-6 chain (by homology)	Q9BUF5	TUBB6		<div><div></div></div>	3 / 12	Structural
Tubulin beta-2B chain (by homology)	Q9BVA1	TUBB2B		<div><div></div></div>	3 / 12	Structural
Steryl-sulfatase	P08842	STS	CHEMBL3559	<div><div></div></div>	10 / 56	Enzyme
Arylsulfatase D (by homology)	P51689	ARSD		<div><div></div></div>	10 / 56	Enzyme
Arylsulfatase E (by homology)	P51690	ARSE		<div><div></div></div>	10 / 56	Enzyme
Arylsulfatase F (by homology)	P54793	ARSF		<div><div></div></div>	10 / 56	Enzyme
Arylsulfatase H (by homology)	Q5FYA8	ARSH		<div><div></div></div>	10 / 56	Enzyme

Polypharmacology Browser 2 Prediction:

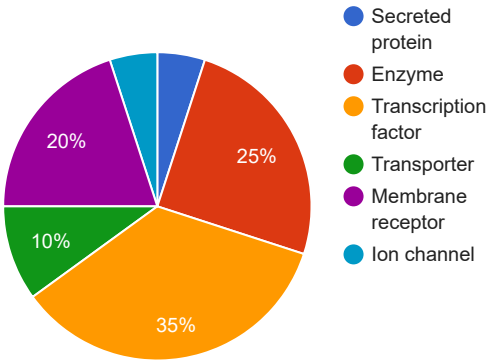
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL206 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL206)	Estrogen receptor alpha	Show NN
2	CHEMBL242 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL242)	Estrogen receptor beta	Show NN
3	CHEMBL3559 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3559)	Steryl-sulfatase	Show NN
4	CHEMBL3181 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3181)	Estradiol 17-beta-dehydrogenase 1	Show NN
5	CHEMBL3305 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3305)	Testis-specific androgen-binding protein	Show NN
6	CHEMBL228 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL228)	Serotonin transporter	Show NN
7	CHEMBL1871 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1871)	Androgen Receptor	Show NN
8	CHEMBL1978 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1978)	Cytochrome P450 19A1	Show NN
9	CHEMBL2034 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2034)	Glucocorticoid receptor	Show NN
10	CHEMBL208 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL208)	Progesterone receptor	Show NN
11	CHEMBL3072 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3072)	Androgen Receptor	Show NN
12	CHEMBL1994 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1994)	Mineralocorticoid receptor	Show NN
13	CHEMBL340 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL340)	Cytochrome P450 3A4	Show NN
14	CHEMBL1781859 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1781859)	Solute carrier organic anion transporter family member 1A1	Show NN
15	CHEMBL3602 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3602)	Sigma opioid receptor	Show NN
16	CHEMBL339 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL339)	Dopamine D2 receptor	Show NN
17	CHEMBL224 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL224)	Serotonin 2a (5-HT2a) receptor	Show NN

18	CHEMBL217 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL217)	Dopamine D2 receptor	Show NN
19	CHEMBL205 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL205)	Carbonic anhydrase II	Show NN
20	CHEMBL240 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL240)	HERG	Show NN