

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

1 rank

Mitogen-activated protein kinase kinase kinase 12 : Homo sapiens

score: 4.006 on ChEMBL1908389 based on 5 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL3730276	0.703704	4.63	
MFP1	CHEMBL3715814	0.552632	12.00	
RDKit7	CHEMBL3728787	0.552040	130.00	
Pattern	CHEMBL3729398	0.824089	210.00	
AP_bits	CHEMBL3728787	0.596923	130.00	*
TT_bits	CHEMBL3728787	0.414634	130.00	
FP2	CHEMBL3729749	0.614213	137.00	
hybridization	CHEMBL3728787	0.674731	130.00	
substructure	CHEMBL3727745	1.000000	650.00	*
graph	CHEMBL3728787	0.800000	130.00	
pubchem	CHEMBL3730820	0.874286	220.00	*
cdk_maccs	CHEMBL3728787	0.851852	130.00	*
klekota_roth	CHEMBL3730148	0.682540	1360.00	*

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

based on 5 locally validated fgps ---> 365.364

["AP\_bits", "cdk\_maccs", "klekota\_roth", "substructure", "pubchem"]

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

1 rank

PI3-kinase p110-alpha subunit : Homo sapiens

score: 8.198 on ChEMBL4005 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL2017974	0.720000	30.0	*
MFP1	CHEMBL2017974	0.472222	30.0	
RDKit7	CHEMBL1258517	0.667313	8.0	
Pattern	CHEMBL1091596	0.866667	253.0	*
AP_bits	CHEMBL2017974	0.533898	30.0	*
TT_bits	CHEMBL1092394	0.493671	226.0	*
FP2	CHEMBL1258517	0.646707	8.0	*
hybridization	CHEMBL1258517	0.736196	8.0	*
substructure	CHEMBL1672330	0.923077	13.0	*
graph	CHEMBL1258517	0.789474	8.0	*
pubchem	CHEMBL2017974	0.877907	30.0	*
cdk_maccs	CHEMBL3736010	0.910714	220.0	*
klekota_roth	CHEMBL3601897	0.700000	2200.0	*

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

based on 11 locally validated fgps ---> 253.529

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

2 rank

Serine/threonine-protein kinase mTOR : Homo sapiens

score: 8.103 on ChEMBL2842 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL2017974	0.720000	4600.00	*
MFP1	CHEMBL2017974	0.472222	4600.00	
RDKit7	CHEMBL1258517	0.667313	0.42	
Pattern	CHEMBL1091596	0.866667	0.18	*
AP_bits	CHEMBL2017974	0.533898	4600.00	*
TT_bits	CHEMBL1092394	0.493671	0.89	*
FP2	CHEMBL1258517	0.646707	0.42	*
hybridization	CHEMBL1258517	0.736196	0.42	*
substructure	CHEMBL1684984	0.857143	1600.00	*
graph	CHEMBL1258517	0.789474	0.42	*
pubchem	CHEMBL2017974	0.877907	4600.00	*
cdk_maccs	CHEMBL586702	0.890909	350.00	*
klekota_roth	CHEMBL1092394	0.690141	0.89	*

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

based on 11 locally validated fgps ---> 1162.658

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

3 rank

PI3-kinase p110-beta subunit : Homo sapiens

score: 6.765 on ChEMBL3145 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL2017974	0.720000	166.0	*
MFP1	CHEMBL2017974	0.472222	166.0	
RDKit7	CHEMBL1258517	0.667313	24.0	
Pattern	CHEMBL1258517	0.820896	24.0	
AP_bits	CHEMBL2017974	0.533898	166.0	*
TT_bits	CHEMBL1258517	0.329670	24.0	
FP2	CHEMBL1258517	0.646707	24.0	*
hybridization	CHEMBL1258517	0.736196	24.0	*
substructure	CHEMBL1684984	0.857143	120.0	*
graph	CHEMBL1258517	0.789474	24.0	*
pubchem	CHEMBL2017974	0.877907	166.0	*
cdk_maccs	CHEMBL1911005	0.927273	41.0	*

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klekota_roth CHEMBL1258517          0.676056      24.0      *
*** ic50 ACTIVITY *** value prediction
based on 9 locally validated fgps ---> 73.466
["substructure", "AP_bits", "FP2", "klekota_roth", "pubchem", "graph",
"FeatMFP1", "cdk_maccs", "hybridization"]

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4 rank

PI3-kinase p110-gamma subunit : Homo sapiens

score: 6.738 on ChEMBL3267 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL2017974	0.720000	262.0	*
MFP1	CHEMBL2017974	0.472222	262.0	
RDKit7	CHEMBL1258517	0.667313	74.0	
Pattern	CHEMBL1258744	0.825806	33.0	
AP_bits	CHEMBL2017974	0.533898	262.0	*
TT_bits	CHEMBL1258634	0.351648	99.0	
FP2	CHEMBL1258517	0.646707	74.0	*
hybridization	CHEMBL1258517	0.736196	74.0	*
substructure	CHEMBL1684984	0.857143	36.0	*
graph	CHEMBL1258517	0.789474	74.0	*
pubchem	CHEMBL2017974	0.877907	262.0	*
cdk_maccs	CHEMBL586702	0.890909	5.0	*
klekota_roth	CHEMBL1258516	0.685714	150.0	*

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*** ic50 ACTIVITY *** value prediction
based on 9 locally validated fgps ---> 143.917
["substructure", "AP_bits", "FP2", "klekota_roth", "pubchem", "graph",
"FeatMFP1", "cdk_maccs", "hybridization"]

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5 rank

PI3-kinase p110-delta subunit : Homo sapiens

score: 6.728 on ChEMBL3130 based on 9 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL2017974	0.720000	116.0	*
MFP1	CHEMBL2017974	0.472222	116.0	
RDKit7	CHEMBL1258517	0.667313	77.0	
Pattern	CHEMBL1258517	0.820896	77.0	
AP_bits	CHEMBL2017974	0.533898	116.0	*
TT_bits	CHEMBL1258517	0.329670	77.0	
FP2	CHEMBL1258517	0.646707	77.0	*
hybridization	CHEMBL1258517	0.736196	77.0	*
substructure	CHEMBL1684984	0.857143	500.0	*
graph	CHEMBL1258517	0.789474	77.0	*
pubchem	CHEMBL2017974	0.877907	116.0	*
cdk_maccs	CHEMBL586702	0.890909	3.0	*
klekota_roth	CHEMBL1258517	0.676056	77.0	*

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*** ic50 ACTIVITY *** value prediction
based on 9 locally validated fgps ---> 105.529
["substructure", "AP_bits", "FP2", "klekota_roth", "pubchem", "graph",
"FeatMFP1", "cdk_maccs", "hybridization"]

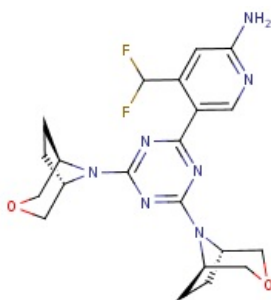
```

# SwissTargetPrediction report:

## Reference:

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

## Query Molecule



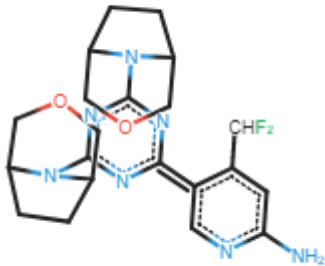
## Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform	O00329	PIK3CD	CHEMBL3130	<div><div></div></div>	95 / 129	Enzyme
Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform	P42336	PIK3CA	CHEMBL4005	<div><div></div></div>	95 / 129	Enzyme
Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit beta isoform	P42338	PIK3CB	CHEMBL3145	<div><div></div></div>	95 / 129	Enzyme
Serine/threonine-protein kinase mTOR	P42345	MTOR	CHEMBL2842	<div><div></div></div>	28 / 111	Enzyme
Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform	P48736	PIK3CG	CHEMBL3267	<div><div></div></div>	29 / 44	Enzyme
Cyclin-dependent kinase 1	P06493	CDK1	CHEMBL308	<div><div></div></div>	33 / 5	Ser_Thr Kinase
Cyclin-dependent kinase 4 ( <i>by homology</i> )	P11802	CDK4	CHEMBL331	<div><div></div></div>	33 / 5	Ser_Thr Kinase
Cyclin-dependent kinase 2	P24941	CDK2	CHEMBL301	<div><div></div></div>	33 / 5	Ser_Thr Kinase
Cyclin-dependent kinase 3 ( <i>by homology</i> )	Q00526	CDK3	CHEMBL4442	<div><div></div></div>	33 / 5	Ser_Thr Kinase
Cyclin-dependent kinase 6 ( <i>by homology</i> )	Q00534	CDK6	CHEMBL2508	<div><div></div></div>	33 / 5	Ser_Thr Kinase
Aurora kinase A	O14965	AURKA	CHEMBL4722	<div><div></div></div>	40 / 5	Ser_Thr Kinase
Aurora kinase B	Q96GD4	AURKB	CHEMBL2185	<div><div></div></div>	40 / 5	Ser_Thr Kinase
Aurora kinase C ( <i>by homology</i> )	Q9UQB9	AURKC	CHEMBL3935	<div><div></div></div>	40 / 5	Ser_Thr Kinase
Vascular endothelial growth factor receptor 1 ( <i>by homology</i> )	P17948	FLT1	CHEMBL1868	<div><div></div></div>	48 / 1	Tyr Kinase
Vascular endothelial growth factor receptor 3 ( <i>by homology</i> )	P35916	FLT4	CHEMBL1955	<div><div></div></div>	48 / 1	Tyr Kinase

# Polypharmacology Browser 2 Prediction:

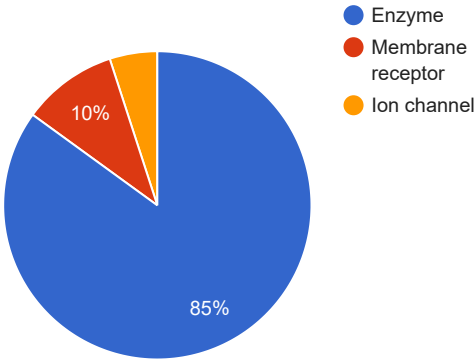
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL4005 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4005">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4005</a> )	PI3-kinase p110-alpha subunit	Show NN
2	CHEMBL2842 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2842">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2842</a> )	Serine/threonine-protein kinase mTOR	Show NN
3	CHEMBL3267 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3267">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3267</a> )	PI3-kinase p110-gamma subunit	Show NN
4	CHEMBL3130 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3130">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3130</a> )	PI3-kinase p110-delta subunit	Show NN
5	CHEMBL3145 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3145">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3145</a> )	PI3-kinase p110-beta subunit	Show NN
6	CHEMBL2148 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2148">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2148</a> )	Tyrosine-protein kinase JAK3	Show NN
7	CHEMBL1862 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1862">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1862</a> )	Tyrosine-protein kinase ABL	Show NN
8	CHEMBL2971 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2971">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2971</a> )	Tyrosine-protein kinase JAK2	Show NN
9	CHEMBL203 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL203">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL203</a> )	Epidermal growth factor receptor erbB1	Show NN
10	CHEMBL240 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL240">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL240</a> )	HERG	Show NN
11	CHEMBL1974 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1974">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1974</a> )	Tyrosine-protein kinase receptor FLT3	Show NN
12	CHEMBL2276 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2276">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2276</a> )	c-Jun N-terminal kinase 1	Show NN
13	CHEMBL253 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL253">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL253</a> )	Cannabinoid CB2 receptor	Show NN
14	CHEMBL4179 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4179">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4179</a> )	c-Jun N-terminal kinase 2	Show NN
15	CHEMBL2185 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2185">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2185</a> )	Serine/threonine-protein kinase Aurora-B	Show NN
16	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
17	CHEMBL218 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL218">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL218</a> )	Cannabinoid CB1 receptor	Show NN
18	CHEMBL2147 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2147">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2147</a> )	Serine/threonine-protein kinase PIM1	Show NN

19	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	<a href="#">Show NN</a>
20	CHEMBL1075104 ( <a href="https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1075104">https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1075104</a> )	Leucine-rich repeat serine/threonine-protein kinase 2	<a href="#">Show NN</a>