

MuSSEL Prediction k_i:

1 rank

p53-binding protein Mdm-2 : Homo sapiens

score: 6.243 on ChEMBL5023 based on 8 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL3355423	0.687500	1238.00	
MFP1	CHEMBL3355430	0.606557	0.16	*
RDKit7	CHEMBL3355430	0.917831	0.16	*
Pattern	CHEMBL3355430	0.794145	0.16	
AP_bits	CHEMBL3355430	0.447471	0.16	
TT_bits	CHEMBL3355430	0.671533	0.16	*
FP2	CHEMBL3355430	0.735426	0.16	*
hybridization	CHEMBL3355430	0.777305	0.16	*
substructure	CHEMBL3355430	0.777778	0.16	
graph	CHEMBL3355430	0.971429	0.16	*
pubchem	CHEMBL409889	0.841530	39.00	
cdk_maccs	CHEMBL3355421	0.891892	1.70	*
klekota_roth	CHEMBL3355430	0.670588	0.16	*

*** ki ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 162.342

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

MuSSEL Prediction IC₅₀:

1 rank

p53-binding protein Mdm-2 : Homo sapiens

score: 8.586 on ChEMBL5023 based on 11 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL3693968		0.733333	100.0	*
MFP1	ChEMBL3693972		0.612903	100.0	*
RDKit7	ChEMBL3355430		0.917831	4.4	*
Pattern	ChEMBL3693970		0.825922	100.0	
AP_bits	ChEMBL3703353		0.639013	80.1	*
TT_bits	ChEMBL3355430		0.671533	4.4	*
FP2	ChEMBL3693974		0.761062	100.0	*
hybridization	ChEMBL3693976		0.779167	100.0	*
substructure	ChEMBL3693969		0.791667	100.0	
graph	ChEMBL3355430		0.971429	4.4	*
pubchem	ChEMBL3693982		0.844920	100.0	*
cdk_maccs	ChEMBL3693982		0.931507	100.0	*
klekota_roth	ChEMBL3693983		0.723529	100.0	*

*** ic50 ACTIVITY *** value prediction

based on 11 locally validated fgps ---> 289.600

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

2 rank

Cholinesterase : Equus caballus

score: 5.506 on ChEMBL5763 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL3633479		0.516129	2650.0	
MFP1	ChEMBL3235943		0.356164	27120.0	
RDKit7	ChEMBL3235941		0.827957	11760.0	*
Pattern	ChEMBL3235948		0.874459	26300.0	*
AP_bits	ChEMBL2204447		0.587997	49.7	*
TT_bits	ChEMBL3235943		0.378531	27120.0	
FP2	ChEMBL3235952		0.583333	35860.0	
hybridization	ChEMBL2332534		0.676225	11740.0	*
substructure	ChEMBL3415565		0.680000	2377.0	
graph	ChEMBL2380672		0.814815	3130.0	*
pubchem	ChEMBL2380667		0.870968	9650.0	*
cdk_maccs	ChEMBL2332531		0.853333	9450.0	*
klekota_roth	ChEMBL2380672		0.549223	3130.0	

*** ic50 ACTIVITY *** value prediction

based on 7 locally validated fgps ---> 13259.989

["cdk_maccs", "Pattern", "AP_bits", "pubchem", "graph", "RDKit7", "hybridization"]

3 rank

Acetylcholinesterase : Homo sapiens

score: 5.442 on ChEMBL220 based on 7 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	ChEMBL1288823		0.529412	9860.00	
MFP1	ChEMBL1288825		0.347826	12200.00	
RDKit7	ChEMBL1288829		0.811321	4200.00	*
Pattern	ChEMBL3115036		0.855035	6140.00	*
AP_bits	ChEMBL575674		0.560129	5.96	*
TT_bits	ChEMBL1288825		0.357955	12200.00	
FP2	ChEMBL1288823		0.575875	9860.00	
hybridization	ChEMBL2332534		0.676225	13640.00	*
substructure	ChEMBL1288823		0.769231	9860.00	
graph	ChEMBL2380672		0.814815	29510.00	*
pubchem	ChEMBL2380667		0.870968	5810.00	*
cdk_maccs	ChEMBL2332531		0.853333	6960.00	*

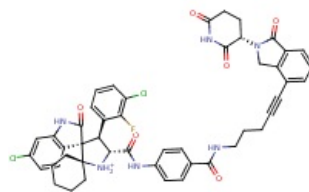
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klekota_roth CHEMBL2380672 0.549223 29510.00
  *** ic50 ACTIVITY *** value prediction
    based on 7 locally validated fgps ---> 11328.198
["cdk_maccs", "Pattern", "AP_bits", "pubchem", "graph", "RDKit7",
"hybridization"]
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SwissTargetPrediction 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
Microtubule-associated protein tau	P10636	MAPT	CHEMBL1293224	<div><div></div></div>	4 / 2	Unclassified
E3 ubiquitin-protein ligase Mdm2	Q00987	MDM2	CHEMBL5023	<div><div></div></div>	0 / 27	Nuclear other
Cholinesterase (<i>by homology</i>)	P06276	BCHE	CHEMBL1914	<div><div></div></div>	18 / 22	Enzyme
Acetylcholinesterase	P22303	ACHE	CHEMBL220	<div><div></div></div>	18 / 22	Enzyme
Muscleblind-like protein 1	Q9NR56	MBNL1	CHEMBL1293317	<div><div></div></div>	2 / 3	Unclassified
Muscleblind-like protein 2 (<i>by homology</i>)	Q5VZF2	MBNL2		<div><div></div></div>	2 / 3	Unclassified
Muscleblind-like protein 3 (<i>by homology</i>)	Q9NUK0	MBNL3		<div><div></div></div>	2 / 3	Unclassified
Calcitonin receptor (<i>by homology</i>)	P30988	CALCR	CHEMBL1832	<div><div></div></div>	20 / 8	Membrane receptor
Calcitonin gene-related peptide type 1 receptor	Q16602	CALCRL	CHEMBL3798	<div><div></div></div>	21 / 14	Membrane receptor
D(2) dopamine receptor	P14416	DRD2	CHEMBL217	<div><div></div></div>	44 / 34	Membrane receptor
D(4) dopamine receptor	P21917	DRD4	CHEMBL219	<div><div></div></div>	24 / 30	Membrane receptor
D(3) dopamine receptor	P35462	DRD3	CHEMBL234	<div><div></div></div>	33 / 30	Membrane receptor
Gastrin/cholecystokinin type B receptor	P32239	CCKBR	CHEMBL298	<div><div></div></div>	8 / 25	Membrane receptor
Cathepsin L1 light chain	P07711	CTSL1	CHEMBL3837	<div><div></div></div>	7 / 22	Cysteine Protease
Cathepsin S	P25774	CTSS	CHEMBL2954	<div><div></div></div>	7 / 22	Cysteine Protease

Polypharmacology Browser 2 not predicted