

MuSsel Prediction IC₅₀:

1 rank

Transient receptor potential cation channel subfamily V member 4 : Homo sapiens

score: 9.515 on ChEMBL3119 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3218112		0.863636	12.9	*
MFP1	CHEMBL3218118		0.756098	3.8	*
RDKit7	CHEMBL3218118		0.764706	3.8	*
Pattern	CHEMBL3218118		0.886756	3.8	*
AP_bits	CHEMBL3218118		0.621134	3.8	*
TT_bits	CHEMBL3218118		0.605634	3.8	*
FP2	CHEMBL3218118		0.833333	3.8	*
hybridization	CHEMBL3218118		0.720207	3.8	*
substructure	CHEMBL3218116		0.894737	3.4	*
graph	CHEMBL3218118		0.683258	3.8	*
pubchem	CHEMBL3218112		0.918750	12.9	*
cdk_maccs	CHEMBL3218116		0.875000	3.4	*
klekota_roth	CHEMBL3218118		0.775281	3.8	*

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 8.257

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

2 rank

Transient receptor potential cation channel subfamily M member 8 : Homo sapiens

score: 9.508 on ChEMBL1075319 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3218114		0.863636	4800.0	*
MFP1	CHEMBL3218118		0.756098	9580.0	*
RDKit7	CHEMBL3218118		0.764706	9580.0	*
Pattern	CHEMBL3218118		0.886756	9580.0	*
AP_bits	CHEMBL3218118		0.621134	9580.0	*
TT_bits	CHEMBL3218118		0.605634	9580.0	*
FP2	CHEMBL3218118		0.833333	9580.0	*
hybridization	CHEMBL3218118		0.720207	9580.0	*
substructure	CHEMBL3218118		0.894737	9580.0	*
graph	CHEMBL3218118		0.683258	9580.0	*
pubchem	CHEMBL3218118		0.911950	9580.0	*
cdk_maccs	CHEMBL3218118		0.875000	9580.0	*
klekota_roth	CHEMBL3218118		0.775281	9580.0	*

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 8262.064

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

3 rank

HERG : Homo sapiens

score: 9.508 on ChEMBL240 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto	Similarity	activity	Valid fg
FeatMFP1	CHEMBL3218118		0.863636	9670.0	*
MFP1	CHEMBL3218118		0.756098	9670.0	*
RDKit7	CHEMBL3218118		0.764706	9670.0	*
Pattern	CHEMBL3218118		0.886756	9670.0	*
AP_bits	CHEMBL3218118		0.621134	9670.0	*
TT_bits	CHEMBL3218118		0.605634	9670.0	*
FP2	CHEMBL3218118		0.833333	9670.0	*
hybridization	CHEMBL3218118		0.720207	9670.0	*

substructure	CHEMBL3218118	0.894737	9670.0	*
graph	CHEMBL3218118	0.683258	9670.0	
pubchem	CHEMBL3218118	0.911950	9670.0	*
cdk_maccs	CHEMBL3218118	0.875000	9670.0	*
klekota_roth	CHEMBL3218118	0.775281	9670.0	*

*** ic50 ACTIVITY *** value prediction
 based on 12 locally validated fgps ---> 9670.000
 ["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
 "klekota_roth", "pubchem", "AP_bits", "FeatMFP1", "RDKit7",
 "hybridization"]

4 rank

Transient receptor potential cation channel subfamily V member 4 : Rattus norvegicus

score: 9.508 on ChEMBL2775 based on 12 fingerprints

Fingerprint type	Ligand	Tanimoto Similarity	activity	Valid fg
FeatMFP1	CHEMBL3218114	0.863636	1150.0	*
MFP1	CHEMBL3218118	0.756098	34.1	*
RDKit7	CHEMBL3218118	0.764706	34.1	*
Pattern	CHEMBL3218118	0.886756	34.1	*
AP_bits	CHEMBL3218118	0.621134	34.1	*
TT_bits	CHEMBL3218118	0.605634	34.1	*
FP2	CHEMBL3218118	0.833333	34.1	*
hybridization	CHEMBL3218118	0.720207	34.1	*
substructure	CHEMBL3218118	0.894737	34.1	*
graph	CHEMBL3218118	0.683258	34.1	
pubchem	CHEMBL3218118	0.911950	34.1	*
cdk_maccs	CHEMBL3218118	0.875000	34.1	*
klekota_roth	CHEMBL3218118	0.775281	34.1	*

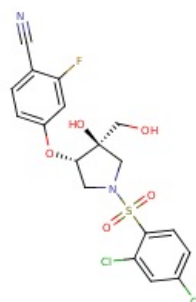
*** ic50 ACTIVITY *** value prediction
 based on 12 locally validated fgps ---> 341.775
 ["TT_bits", "substructure", "cdk_maccs", "Pattern", "FP2", "MFP1",
 "klekota_roth", "pubchem", "AP_bits", "FeatMFP1", "RDKit7",
 "hybridization"]

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
5-hydroxytryptamine receptor 1A	P08908	HTR1A	CHEMBL214	<div><div></div></div>	26 / 31	Membrane receptor
5-hydroxytryptamine receptor 1B (by homology)	P28222	HTR1B	CHEMBL1898	<div><div></div></div>	29 / 32	Membrane receptor
Potassium voltage-gated channel subfamily H member 2	Q12809	KCNH2	CHEMBL240	<div><div></div></div>	23 / 10	Ion channel
Potassium voltage-gated channel subfamily H member 6 (by homology)	Q9H252	KCNH6		<div><div></div></div>	23 / 10	Ion channel
Potassium voltage-gated channel subfamily H member 7 (by homology)	Q9NS40	KCNH7		<div><div></div></div>	23 / 10	Ion channel
22 kDa interstitial collagenase (by homology)	P03956	MMP1	CHEMBL332	<div><div></div></div>	135 / 79	Metallo Protease
Stromelysin-1	P08254	MMP3	CHEMBL283	<div><div></div></div>	135 / 79	Metallo Protease
Macrophage metalloelastase (by homology)	P39900	MMP12	CHEMBL4393	<div><div></div></div>	126 / 79	Metallo Protease
Collagenase 3	P45452	MMP13	CHEMBL280	<div><div></div></div>	126 / 79	Metallo Protease
Stromelysin-2 (by homology)	P09238	MMP10	CHEMBL4270	<div><div></div></div>	135 / 79	Metallo Protease
Matrix metalloproteinase-27 (by homology)	Q9H306	MMP27		<div><div></div></div>	135 / 79	Metallo Protease
Androgen receptor	P10275	AR	CHEMBL1871	<div><div></div></div>	33 / 1	Transcription Factor
5-hydroxytryptamine receptor 7	P34969	HTR7	CHEMBL3155	<div><div></div></div>	2 / 36	Membrane receptor
Microtubule-associated protein tau	P10636	MAPT	CHEMBL1293224	<div><div></div></div>	105 / 1	Unclassified
PEX	P08253	MMP2	CHEMBL333	<div><div></div></div>	71 / 55	Metallo Protease

Polypharmacology Browser 2 not predicted