

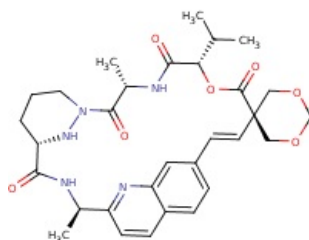
MuSSel not predicted

SwissTargetPrediction report:

Reference:

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

Query Molecule



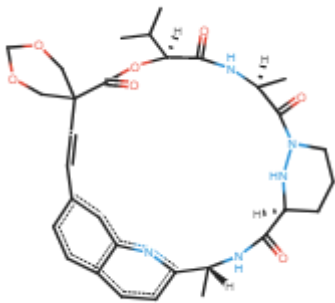
Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
Caspase-3 subunit p12	P42574	CASP3	CHEMBL2334	<div><div></div></div>	70 / 1	Cysteine Protease
Caspase-7 subunit p20 (by homology)	P55210	CASP7	CHEMBL3468	<div><div></div></div>	70 / 1	Cysteine Protease
Caspase-6 subunit p18 (by homology)	P55212	CASP6	CHEMBL3308	<div><div></div></div>	70 / 1	Cysteine Protease
Caspase-1 subunit p20	P29466	CASP1	CHEMBL4801	<div><div></div></div>	95 / 12	Cysteine Protease
Caspase-8 subunit p18	Q14790	CASP8	CHEMBL3776	<div><div></div></div>	64 / 6	Cysteine Protease
Caspase-4 (by homology)	P49662	CASP4	CHEMBL2226	<div><div></div></div>	95 / 12	Cysteine Protease
Caspase-5 subunit p10 (by homology)	P51878	CASP5	CHEMBL3131	<div><div></div></div>	95 / 12	Cysteine Protease
Inactive caspase-12 (by homology)	Q6UXS9	CASP12		<div><div></div></div>	95 / 12	Cysteine Protease
Cathepsin L2 (by homology)	O60911	CTSL2	CHEMBL3272	<div><div></div></div>	222 / 8	Cysteine Protease
Cathepsin L1 light chain	P07711	CTSL1	CHEMBL3837	<div><div></div></div>	222 / 8	Cysteine Protease
Cathepsin S	P25774	CTSS	CHEMBL2954	<div><div></div></div>	221 / 8	Cysteine Protease
Cathepsin K	P43235	CTSK	CHEMBL268	<div><div></div></div>	221 / 8	Cysteine Protease
Cathepsin B	P07858	CTSB	CHEMBL4072	<div><div></div></div>	53 / 1	Cysteine Protease
Microtubule-associated protein tau	P10636	MAPT	CHEMBL1293224	<div><div></div></div>	665 / 1	Unclassified
Renin	P00797	REN	CHEMBL286	<div><div></div></div>	360 / 57	Aspartic Protease

Polypharmacology Browser 2 Prediction:

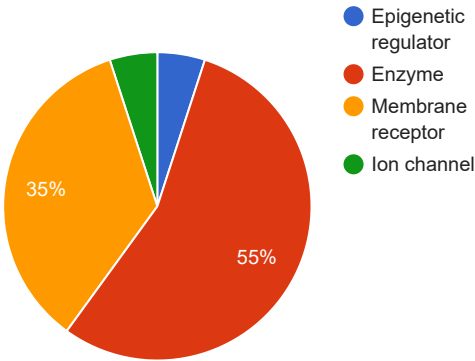
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



Rank	ChEMBL ID	Common name	Nearest neighbours
1	CHEMBL240 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL240)	HERG	Show NN
2	CHEMBL214 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL214)	Serotonin 1a (5-HT1a) receptor	Show NN
3	CHEMBL4822 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4822)	Beta-secretase 1	Show NN
4	CHEMBL268 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL268)	Cathepsin K	Show NN
5	CHEMBL274 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL274)	C-C chemokine receptor type 5	Show NN
6	CHEMBL340 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL340)	Cytochrome P450 3A4	Show NN
7	CHEMBL253 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL253)	Cannabinoid CB2 receptor	Show NN
8	CHEMBL325 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL325)	Histone deacetylase 1	Show NN
9	CHEMBL4072 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4072)	Cathepsin B	Show NN
10	CHEMBL2954 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2954)	Cathepsin S	Show NN
11	CHEMBL3105 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3105)	Poly [ADP-ribose] polymerase-1	Show NN
12	CHEMBL4409 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4409)	Phosphodiesterase 10A	Show NN
13	CHEMBL260 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL260)	MAP kinase p38 alpha	Show NN
14	CHEMBL262 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL262)	Glycogen synthase kinase-3 beta	Show NN
15	CHEMBL4005 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4005)	PI3-kinase p110-alpha subunit	Show NN
16	CHEMBL3837 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3837)	Cathepsin L	Show NN
17	CHEMBL344 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL344)	Melanin-concentrating hormone receptor 1	Show NN
18	CHEMBL273 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL273)	Serotonin 1a (5-HT1a) receptor	Show NN

19	CHEMBL3996 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3996)	Oxytocin receptor	Show NN
20	CHEMBL233 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL233)	Mu opioid receptor	Show NN