HitPickV2 results

Query Compound	Predicted/ Known Target	Protein Complex	Precision	Most Similar Compound	Tc	Occur
Propranolol	ABCB1		100	Propranolol	1.0	Known Target
Propranolol	ADRB1		100	Propranolol	1.0	Known Target
Propranolol	ADRB2	USP20,USP33: PolyUb-ADRB2 [endosome membrane]	100	Propranolol	1.0	Known Target
Propranolol	ADRB3		100	Propranolol	1.0	Known Target
Propranolol	CACNA1C	LTCC heteropentamer (open) [plasma membrane]	100	Propranolol	1.0	Known Target
Propranolol	CYP1A1		100	Propranolol	1.0	Known Target
Propranolol	CYP1A2		100	Propranolol	1.0	Known Target
Propranolol	CYP2C19		100	Propranolol	1.0	Known Target
Propranolol	CYP2D6		100	Propranolol	1.0	Known Target
Propranolol	CYP2J2		100	Propranolol	1.0	Known Target
Propranolol	CYP3A5		100	Propranolol	1.0	Known Target
Propranolol	CYP3A7-CYP3A51P		100	Propranolol	1.0	Known Target
Propranolol	DRD1		100	Propranolol	1.0	Known Target
Propranolol	DRD2		100	Propranolol	1.0	Known Target
Propranolol	HRH1		100	Propranolol	1.0	Known Target
Propranolol	HTR1A		100	Propranolol	1.0	Known Target
Propranolol	HTR1B		100	Propranolol	1.0	Known Target
Propranolol	HTR1D		100	Propranolol	1.0	Known Target
Propranolol	HTR2A		100	Propranolol	1.0	Known Target
Propranolol	HTR2B		100	Propranolol	1.0	Known Target
Propranolol	HTR2C		100	Propranolol	1.0	Known Target
Propranolol	HTR3A	2xHTR3A: 3xHTR3D [plasma membrane]	100	Propranolol	1.0	Known Target
Propranolol	HTR6		100	Propranolol	1.0	Known Target
Propranolol	KCNH2	Octamer of Voltage gated K+ channels [plasma membrane]	100	Propranolol	1.0	Known Target
Propranolol	ORM1		100	Propranolol	1.0	Known Target
Propranolol	SCN5A	SCNAs:SCNBs [plasma membrane]	100	Propranolol	1.0	Known Target
Propranolol	SIGMAR1		100	Propranolol	1.0	Known Target
Propranolol	SLC10A1		100	Propranolol	1.0	Known Target
Propranolol	SLC22A1		100	Propranolol	1.0	Known Target
Propranolol	SLC22A2		100	Propranolol	1.0	Known Target
Propranolol	SLC6A4		100	Propranolol	1.0	Known Target
Talinolol	EPHX2	PEX5S,L:Cargo protein [cytosol]	90.6	CHEMBL191968	0.586	8 compounds (3 unique scaffolds)Most

Query Compound	Predicted/ Known Target	Protein Complex	Precision	Most Similar Compound	Tc	Occur
						representative scaffolds: Ocurrence:6Ocurrence: 1Ocurrence:1
Talinolol	ADRB2	USP20,USP33: PolyUb-ADRB2 [endosome membrane]	84.6	CHEMBL13432	0. 56	4 compounds (4 unique scaffolds)Most representative scaffolds: Ocurrence:1Ocurrence: 1Ocurrence:1
Talinolol	ADRB1		81.3	CHEMBL182127	0. 618	7 compounds (7 unique scaffolds)Most representative scaffolds: Ocurrence:1Ocurrence: 1Ocurrence:1
Talinolol	ADRB3		79.6	CHEMBL182127	0. 618	5 compounds (5 unique scaffolds)Most representative scaffolds: Ocurrence:1Ocurrence: 1Ocurrence:1
Talinolol	CYP2D6		47.7	Practolol	0. 492	2 compound (1 unique scaffold)Compound scaffold:
Talinolol	EPHX1		43.6	CHEMBL1360431	0. 46	1 compound (1 unique scaffold)Compound scaffold:
Talinolol	CYP1A2		42.0	Practolol	0. 492	1 compound (1 unique scaffold)Compound scaffold:
Talinolol	CA12		41.5	CHEMBL2331759	0. 452	1 compound (1 unique scaffold)Compound scaffold:
Talinolol	CYP2C19		30.2	Practolol	0. 492	1 compound (1 unique scaffold)Compound scaffold:
Talinolol	CA9		28.7	CHEMBL2331759	0. 452	1 compound (1 unique scaffold)Compound scaffold:

Propranolol

Predicted ligand-target interactions for your input compound

We predict **16** targets for your uploaded compound!

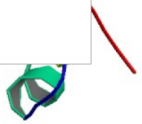
Please choose a protein from the list, to get detailed informations.

Predicted targets ordered by prediction score: Adrenergic receptor beta

- Adrenergic receptor beta
- Beta-2 adrenergic receptor
- Cytochrome P450 2D6
- Cytochrome P450 1A2
- X-box-binding protein 1
- Adrenergic receptor beta; ADRB1 & ADRB3
- Perilipin-5
- Perilipin-1
- Voltage-gated T-type calcium channel alpha-1H subunit
- Alpha-2c adrenergic receptor
- Serotonin 1a (5-HT1a) receptor
- Squalene synthetase
- Alpha adrenergic receptor (1a and 1d)
- Dopamine receptors; D2 & D4
- Cytochrome P450 2C19
- Adrenergic receptors; alpha-1 A & B

Name:	ADRB1
Recommended name:	Adrenergic receptor beta
Alternative Names:	• Beta-1 adrenoreceptor
Uniprot ID:	ADRB1_HUMAN
Synonyms:	ADRB1R, B1AR
Sequence length:	477
BindingDB:	P08588
Kegg:	hsa:153
Drug Bank:	DB01193
Chembl:	CHEMBL2094118
Prosite:	PS00237
Pfam:	PF00001
GeneID:	153
Ensembl:	ENST00000369295
Phosphosite:	P08588
RefSeq:	NP_000675.1
UniGene:	99913

ucture(s) available:



PDB-Name:	2LSQ
Sequence-Position:	199-215
Chain:	A
Method:	NMR
Resolution:	-

Talinolol

Predicted ligand-target interactions for your input compound

We predict **12** targets for your uploaded compound!

Please choose a protein from the list, to get detailed informations.

Predicted targets ordered by prediction score: Epoxide hydratase

- Epoxide hydratase
- Adrenergic receptor beta
- Adrenergic receptor beta; ADRB1 & ADRB3
- Carbonic anhydrase XII
- Nuclear factor NF-kappa-B complex
- Nuclear factor NF-kappa-B p65 subunit
- Carbonic anhydrases; II & IX
- Beta-2 adrenergic receptor
- Carbonic anhydrase I
- Cytochrome P450 2D6
- Cytochrome P450 2C19
- Carbonic anhydrase II

Name:	EPHX2
Recommended name:	Epoxide hydratase
Alternative Names:	• Epoxide hydratase • Soluble epoxide hydrolase
Uniprot ID:	HYES_HUMAN
Sequence length:	555
BindingDB:	P34913
Kegg:	hsa:2053
Drug Bank:	DB00675
Chembl:	CHEMBL2409
Pfam:	PF00561
GeneID:	2053
Ensembl:	ENST00000380476
Phosphosite:	P34913
RefSeq:	NP_001243411.1
UniGene:	212088

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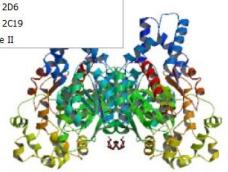
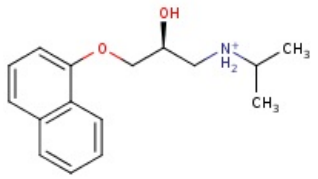


PDB-Name:	1S8O
Sequence-Position:	1-555
Chain:	A
Method:	X-ray
Resolution:	2.60

SwissTargetPrediction report:

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

Query Molecule



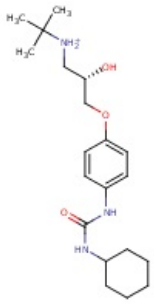
Frequency of Target Class

Target	Uniprot ID	Gene code	ChEMBL ID	Probability	# sim. cmpds (3D / 2D)	Target Class
Beta-2 adrenergic receptor	P07550	ADRB2	CHEMBL210		452 / 217	Membrane receptor
Beta-1 adrenergic receptor	P08588	ADRB1	CHEMBL213		450 / 210	Membrane receptor
Beta-3 adrenergic receptor	P13945	ADRB3	CHEMBL246		433 / 199	Membrane receptor
Sodium-dependent noradrenaline transporter *(by homology)*	P23975	SLC6A2	CHEMBL222		413 / 83	Transporter
5-hydroxytryptamine receptor 1D *(by homology)*	P28221	HTR1D	CHEMBL1983		37 / 14	Membrane receptor
5-hydroxytryptamine receptor 1B *(by homology)*	P28222	HTR1B	CHEMBL1898		170 / 68	Membrane receptor
5-hydroxytryptamine receptor 2A	P28223	HTR2A	CHEMBL224		115 / 18	Membrane receptor
5-hydroxytryptamine receptor 2C	P28335	HTR2C	CHEMBL225		82 / 14	Membrane receptor
Sodium-dependent serotonin transporter	P31645	SLC6A4	CHEMBL228		445 / 87	Transporter
5-hydroxytryptamine receptor 2B	P41595	HTR2B	CHEMBL1833		82 / 14	Membrane receptor
Sodium- and chloride-dependent glycine transporter 1 *(by homology)*	P48067	SLC6A9	CHEMBL2337		330 / 80	Transporter
5-hydroxytryptamine receptor 6	P50406	HTR6	CHEMBL3371		42 / 5	Membrane receptor
Sodium-dependent dopamine transporter *(by homology)*	Q01959	SLC6A3	CHEMBL238		413 / 83	Transporter
Sigma non-opioid intracellular receptor 1	Q99720	SIGMAR1	CHEMBL287		81 / 52	Membrane receptor
Sodium-dependent proline transporter *(by homology)*	Q99884	SLC6A7			330 / 80	Transporter

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
Lipid-phosphate phosphatase	P34913	EPHX2	CHEMBL2409		59 / 314	Serine Protease
Neuropeptide Y receptor type 5	Q15761	NPY5R	CHEMBL4561		26 / 32	Membrane receptor
D(2) dopamine receptor	P14416	DRD2	CHEMBL217		124 / 87	Membrane receptor
Beta-2 adrenergic receptor	P07550	ADRB2	CHEMBL210		301 / 134	Membrane receptor
Beta-1 adrenergic receptor	P08588	ADRB1	CHEMBL213		306 / 122	Membrane receptor
Beta-3 adrenergic receptor *(by homology)*	P13945	ADRB3	CHEMBL246		301 / 120	Membrane receptor
Acyl-CoA desaturase	O00767	SCD	CHEMBL5555		15 / 16	Enzyme
Stearoyl-CoA desaturase 5 *(by homology)*	Q86SK9	SCD5	CHEMBL1275210		15 / 16	Enzyme
Muscleblind-like protein 1	Q9NR56	MBNL1	CHEMBL1293317		112 / 34	Unclassified
Muscleblind-like protein 2 *(by homology)*	Q5VZF2	MBNL2			112 / 34	Unclassified
Muscleblind-like protein 3 *(by homology)*	Q9NUK0	MBNL3			112 / 34	Unclassified
C-C chemokine receptor type 1	P32246	CCR1	CHEMBL2413		130 / 124	Membrane receptor
C-C chemokine receptor type 2 *(by homology)*	P41597	CCR2	CHEMBL4015		130 / 124	Membrane receptor
C-C chemokine receptor type 3	P51677	CCR3	CHEMBL3473		130 / 124	Membrane receptor
C-C chemokine receptor type 5 *(by homology)*	P51681	CCR5	CHEMBL274		130 / 124	Membrane receptor