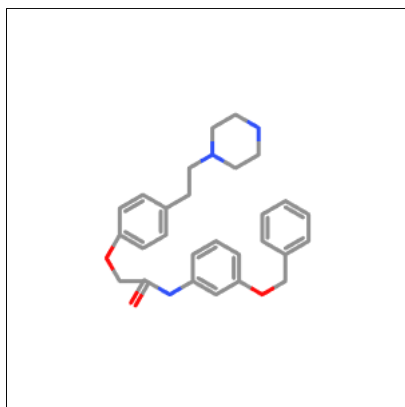
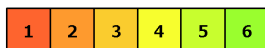


Oral toxicity prediction results for input compound



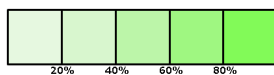
Predicted LD50: 600mg/kg

Predicted Toxicity Class: 4



Average similarity: 66.36%

Prediction accuracy: 68.07%



Name	User defined
Molweight	445.55
Number of hydrogen bond acceptors	6
Number of hydrogen bond donors	2
Number of atoms	33
Number of bonds	36
Number of rotatable bonds	11
Molecular refractivity	138.16
Topological Polar Surface Area	62.83
octanol/water partition coefficient(logP)	4.07

Toxicity Model Report

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Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	<u>Hepatotoxicity</u>	dili	Inactive	0.93
Organ toxicity	<u>Neurotoxicity</u>	neuro	Active	0.77
Organ toxicity	<u>Nephrotoxicity</u>	nephro	Active	0.62
Organ toxicity	<u>Respiratory toxicity</u>	respi	Active	0.86
Organ toxicity	<u>Cardiotoxicity</u>	cardio	Inactive	0.70
Toxicity end points	<u>Carcinogenicity</u>	carcino	Inactive	0.58
Toxicity end points	<u>Immunotoxicity</u>	immuno	Inactive	0.99
Toxicity end points	<u>Mutagenicity</u>	mutagen	Inactive	0.69
Toxicity end points	<u>Cytotoxicity</u>	cyto	Inactive	0.66
Toxicity end points	<u>BBB-barrier</u>	bbb	Active	0.70
Toxicity end points	<u>Ecotoxicity</u>	eco	Inactive	0.60
Toxicity end points	<u>Clinical toxicity</u>	clinical	Active	0.76
Toxicity end points	<u>Nutritional toxicity</u>	nutri	Inactive	0.62
Tox21-Nuclear receptor signalling pathways	<u>Aryl hydrocarbon Receptor (AhR)</u>	nr_ahr	Inactive	0.92
Tox21-Nuclear receptor signalling pathways	<u>Androgen Receptor (AR)</u>	nr_ar	Inactive	0.98
Tox21-Nuclear receptor signalling pathways	<u>Androgen Receptor Ligand Binding Domain (AR-LBD)</u>	nr_ar_lbd	Inactive	0.99
Tox21-Nuclear receptor signalling pathways	<u>Aromatase</u>	nr_aromatase	Inactive	0.97
Tox21-Nuclear receptor signalling pathways	<u>Estrogen Receptor Alpha (ER)</u>	nr_er	Inactive	0.91
Tox21-Nuclear receptor signalling pathways	<u>Estrogen Receptor Ligand Binding Domain (ER-LBD)</u>	nr_er_lbd	Inactive	0.98
Tox21-Nuclear receptor signalling pathways	<u>Peroxisome Proliferator Activated Receptor Gamma (PPAR-Gamma)</u>	nr_ppar_gamma	Inactive	1.0
Tox21-Stress response pathways	<u>Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE)</u>	sr_are	Inactive	0.97
Tox21-Stress response pathways	<u>Heat shock factor response element (HSE)</u>	sr_hse	Inactive	0.97
Tox21-Stress response pathways	<u>Mitochondrial Membrane Potential (MMP)</u>	sr_mmp	Inactive	0.93
Tox21-Stress response pathways	<u>Phosphoprotein (Tumor Suppressor), p53</u>	sr_p53	Inactive	0.92
Tox21-Stress response pathways	<u>ATPase family AAA domain-containing protein 5 (ATAD5)</u>	sr_atad5	Inactive	0.93
Molecular Initiating Events	<u>Thyroid hormone receptor alpha (THRα)</u>	mie_thr_alpha	Inactive	0.87
Molecular Initiating Events	<u>Thyroid hormone receptor beta (THRβ)</u>	mie_thr_beta	Inactive	0.79
Molecular Initiating Events	<u>Transthyretin (TTR)</u>	mie_ttr	Inactive	0.95
Molecular Initiating Events	<u>Ryanodine receptor (RyR)</u>	mie_ryr	Inactive	0.85
Molecular Initiating Events	<u>GABA receptor (GABAR)</u>	mie_gabar	Inactive	0.75
Molecular Initiating Events	<u>Glutamate N-methyl-D-aspartate receptor (NMDAR)</u>	mie_nmdar	Inactive	0.70
Molecular Initiating Events	<u>alpha-amino-3-hydroxy-5-methyl-4-isoxazolepropionate receptor (AMPA)</u>	mie_ampar	Inactive	1.0
Molecular Initiating Events	<u>Kainate receptor (KAR)</u>	mie_kar	Inactive	1.0
Molecular Initiating Events	<u>Achetylcholinesterase (AChE)</u>	mie_ache	Inactive	0.60
Molecular Initiating Events	<u>Constitutive androstane receptor (CAR)</u>	mie_car	Inactive	1.0
Molecular Initiating Events	<u>Pregnane X receptor (PXR)</u>	mie_pxr	Inactive	0.92

Classification	Target	Shorthand	Prediction	Probability
Molecular Initiating Events	NADH-quinone oxidoreductase (NADHOX)	mie_nadhox	Inactive	0.97
Molecular Initiating Events	Voltage-gated sodium channel (VGSC)	mie_vgsc	Active	0.77
Molecular Initiating Events	Na⁺/I⁻ symporter (NIS)	mie_nis	Inactive	0.94
Metabolism	Cytochrome CYP1A2	CYP1A2	Inactive	0.90
Metabolism	Cytochrome CYP2C19	CYP2C19	Inactive	0.87
Metabolism	Cytochrome CYP2C9	CYP2C9	Inactive	0.65
Metabolism	Cytochrome CYP2D6	CYP2D6	Active	0.63
Metabolism	Cytochrome CYP3A4	CYP3A4	Inactive	0.66
Metabolism	Cytochrome CYP2E1	CYP2E1	Inactive	0.99

Toxicity targets

Possible binding to toxicity targets is shown below. For more information on the targets, please click on the individual abbreviations.



AA2AR	ADRB2	ANDR	AOFA	CRFR1	DRD3	ESR1	ESR2	GCR	HRH1	NR1I2	OPRK	OPRM	PDE4D	PGH1	PRGR