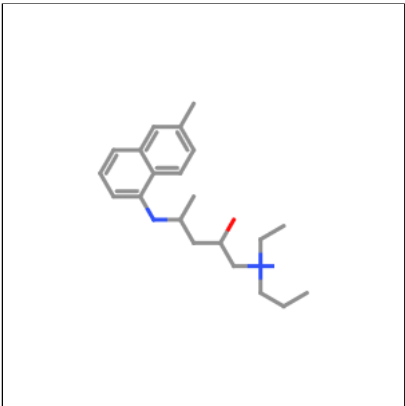


Oral toxicity prediction results for input compound



Predicted LD50: 1200mg/kg

Predicted Toxicity Class: 4

1

2

3

4

5

6

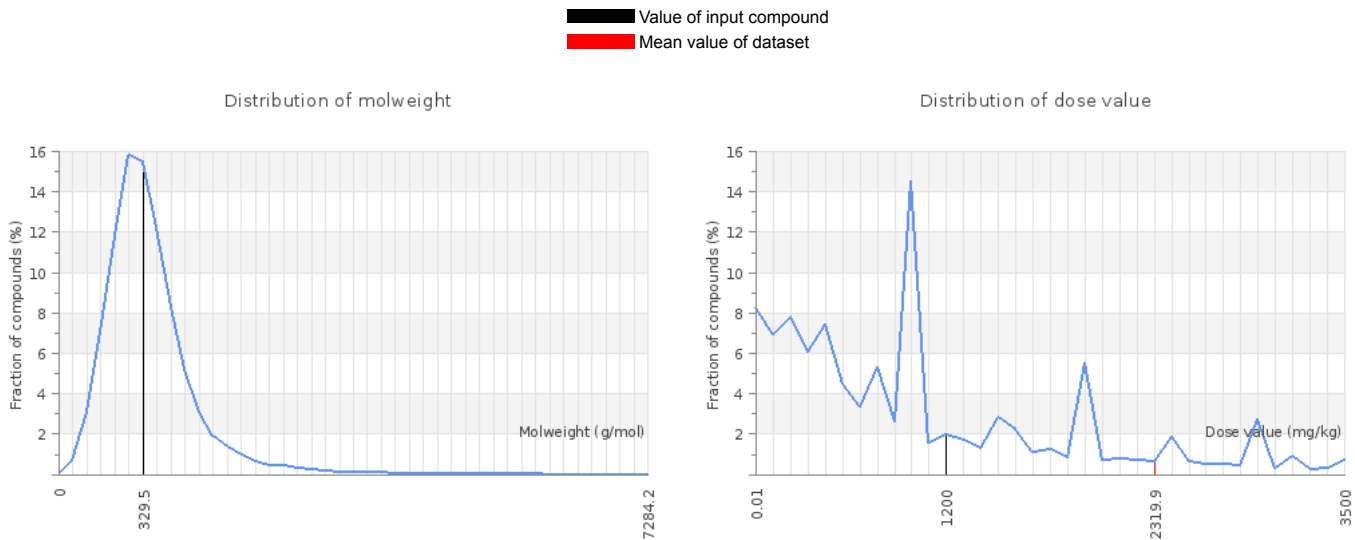
Average similarity: 66.06%

Prediction accuracy: 68.07%

20%40%60%80%

Name	CCC[NH+] (CC)CC(O)CC(C)Nc1ccc
Molweight	329.5
Number of hydrogen bond acceptors	2
Number of hydrogen bond donors	1
Number of atoms	25
Number of bonds	26
Number of rings	2
Number of rotatable bonds	9
Total charge	1
Molecular Polar Surface Area	36.7

Comparison of input compound with dataset compounds



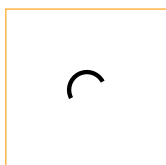
+

Similar compounds

Toxicity Model Report

Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Not Calculated	Not Calculated
Toxicity end points	Carcinogenicity	carcino	Not Calculated	Not Calculated
Toxicity end points	Immunotoxicity	immuno	Not Calculated	Not Calculated
Toxicity end points	Mutagenicity	mutagen	Not Calculated	Not Calculated
Toxicity end points	Cytotoxicity	cyto	Not Calculated	Not Calculated
Tox21-Nuclear receptor signalling pathways	Aryl hydrocarbon Receptor (AhR)	nr_ahr	Not Calculated	Not Calculated
Tox21-Nuclear receptor signalling pathways	Androgen Receptor (AR)	nr_ar	Not Calculated	Not Calculated
Tox21-Nuclear receptor signalling pathways	Androgen Receptor Ligand Binding Domain (AR-LBD)	nr_ar_lbd	Not Calculated	Not Calculated
Tox21-Nuclear receptor signalling pathways	Aromatase	nr_aromatase	Not Calculated	Not Calculated
Tox21-Nuclear receptor signalling pathways	Estrogen Receptor Alpha (ER)	nr_er	Not Calculated	Not Calculated
Tox21-Nuclear receptor signalling pathways	Estrogen Receptor Ligand Binding Domain (ER-LBD)	nr_er_lbd	Not Calculated	Not Calculated

Tox21-Nuclear receptor signalling pathways	Peroxisome Proliferator Activated Receptor Gamma (PPAR-Gamma)	nr_ppar_gamma	Not Calculated	Not Calculated
Tox21-Stress response pathways	Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE)	sr_are	Not Calculated	Not Calculated
Tox21-Stress response pathways	Heat shock factor response element (HSE)	sr_hse	Not Calculated	Not Calculated
Tox21-Stress response pathways	Mitochondrial Membrane Potential (MMP)	sr_mmp	Not Calculated	Not Calculated
Tox21-Stress response pathways	Phosphoprotein (Tumor Suppressor) p53	sr_p53	Not Calculated	Not Calculated
Tox21-Stress response pathways	ATPase family AAA domain-containing protein 5 (ATAD5)	sr_atad5	Not Calculated	Not Calculated



The toxicity radar chart is intended to quickly illustrate the confidence of positive toxicity results compared to the average of its class. Click the thumbnail to access the plot once it has finished loading.

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

Last updated: March 2020

Disclaimer: Compound structures submitted will not be released under any circumstances. This work is licensed under a [Creative Commons Attribution-Noncommercial License](#).