Nelotanserin

Cat. No.: HY-10559

CAS No.: 839713-36-9

Molecular Formula: $C_{18}H_{15}BrF_2N_4O_2$

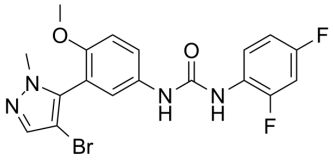
Molecular Weight: 437.24

Target: 5-HT Receptor

Pathway: GPCR/G Protein; Neuronal Signaling

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 32 mg/mL (73.19 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.2871 mL	11.4354 mL	22.8707 mL
5 mM	0.4574 mL	2.2871 mL	4.5741 mL
10 mM	0.2287 mL	1.1435 mL	2.2871 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

Nelotanserin is a potent 5-HT_{2A} inverse agonist, a moderately potent 5-HT_{2C} partial inverse agonist and a weak 5-HT_{2B} inverse agonist, with IC_{50}s of 1.7, 79, 791 nM in IP accumulation assays, respectively.

IC_{50} & Target

5-HT_{2A} Receptor	5-HT_{2C} Receptor	5-HT_{2B} Receptor
1.7 nM (IC_{50})	79 nM (IC_{50})	791 nM (IC_{50})

In Vitro

Results from IP accumulation assays suggest that Nelotanserin is a potent 5-HT_{2A} full inverse agonist (IC_{50}=1.7 nM), a moderately potent 5-HT_{2C} partial inverse agonist (IC_{50}=79 nM) (maximal response was 62% of the response obtained for the reference inverse agonist clozapine), and a weak 5-HT_{2B} inverse agonist (IC_{50}=791 nM). Nelotanserin displays high affinity for recombinant human 5-HT_{2A} receptors (K_i=0.35 nM), moderate affinity for human 5-HT_{2C} receptors (K_i=100 nM), and low affinity for human 5-HT_{2B} receptors (2000 nM) stably expressed in HEK293 cells. The results suggest that Nelotanserin has a 262-fold higher affinity for human 5-HT_{2A} than 5-HT_{2C} receptors and a 6610-fold higher affinity for human 5-HT_{2A} than 5-HT_{2B} receptors[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo	Each compound is tested in a minimum of five rats by oral gavage with administration occurring in the middle of the inactive period, 6 h after light onset. The delta power during non-REM sleep (NREMS) is significantly different between all the analogues tested and the vehicle control. Nelotanserin (Compound 39) produces significant increases in delta power that persist for the first 4 h following dosing. Significant differences are found, however, in NREMS bout length. Nelotanserin significantly increases NREMS bout length during the first hour following dosing, and 3 does so during the second hour. In conjunction with this increased NREM bout duration, the number of NREM bouts decrease during the first hour for Nelotanserin ($p<0.01$) as well as for compound 15 ($p<0.05$)[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- ACS Chem Neurosci. 2019 Nov 20;10(11):4476-4491.

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REFERENCES

[1]. Al-Shamma HA et al. Nelotanserin, a novel selective human 5-hydroxytryptamine2A inverse agonist for the treatment of insomnia. J Pharmacol Exp Ther. 2010 Jan;332(1):281-90.

[2]. Teegarden BR et al. Discovery of 1-[3-(4-bromo-2-methyl-2h-pyrazol-3-yl)-4-methoxyphenyl]-3-(2,4-difluorophenyl)urea (nelotanserin) and related 5-hydroxytryptamine2A inverse agonists for the treatment of insomnia. J Med Chem. 2010 Mar 11;53(5):1923-36.

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