# Nelotanserin

**Cat. No.:** HY-10559

**CAS No.:** 839713-36-9

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

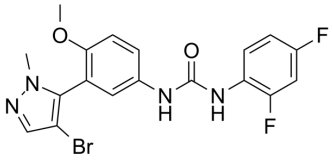
**Molecular Weight:** 437.24

**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].<br>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.



Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA