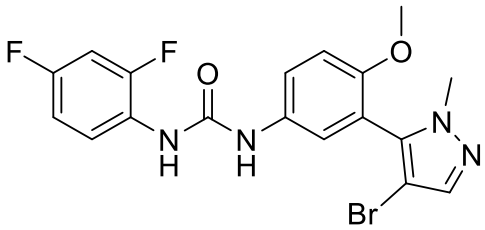
Product data sheet

MedKoo Cat#: 319837 Name: Nelotanserin CAS#: 839713-36-9 Chemical Formula: $C_{18}H_{15}BrF_2N_4O_2$ Exact Mass: 436.0346 Molecular Weight: 437.24	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
Nelotanserin, also known as APD125, is a potent and selective human 5-hydroxytryptamine2A inverse agonist for the treatment of insomnia. Nelotanserin has low nanomolar potency on the 5-HT(2A) receptor with at least 30- and 5000-fold selectivity compared with 5-HT(2C) and 5-HT(2B) receptors, respectively. Nelotanserin produced statistically significant improvements in objective parameters of sleep maintenance and sleep consolidation and was well tolerated in adults with primary chronic insomnia.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	32.0	73.2

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.29 mL	11.44 mL	22.87 mL
5 mM	0.46 mL	2.29 mL	4.57 mL
10 mM	0.23 mL	1.14 mL	2.29 mL
50 mM	0.05 mL	0.23 mL	0.46 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

TBD

In vivo study

1. Teegarden BR, Li H, Jayakumar H, Strah-Pleynet S, Dosa PI, Selaya SD, Kato N, Elwell KH, Davidson J, Cheng K, Saldana H, Frazer JM, Whelan K, Foster J, Espitia S, Webb RR, Beeley NR, Thomsen W, Morairty SR, Kilduff TS, Al-Shamma HA. 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. doi: 10.1021/jm9007328. PMID: 20143782.

7. Bioactivity
Biological target:

Nelotanserin is a potent 5-HT2A inverse agonist, a moderately potent 5-HT2C partial inverse agonist and a weak 5-HT2B inverse agonist, with IC50s of 1.7, 79, 791 nM in IP accumulation assays, respectively.

In vitro activity

Product data sheet

TBD

In vivo activity

Individual doses were selected for each of the four compounds to measure their effects in rat sleep pharmacology studies that were 2-fold higher than the compound's ED50 in the DOI model. The delta power during non-REM sleep (NREMS) was significantly different between all the analogues tested and the vehicle control (Figure 3). Compound 39 (Nelotanserin) produced significant increases in delta power that persisted for the first 4 h following dosing. No significant effects were found on either waking bout length or number of waking bouts. Significant differences were found, however, in NREMS bout length. Compound 39 significantly increased NREMS bout length during the first hour following dosing, and 3 did so during the second hour. In conjunction with this increased NREM bout duration, the number of NREM bouts decreased during the first hour for compound 39 ($p < 0.01$) as well as for compound 15 ($p < 0.05$).

Reference: J Med Chem. 2010 Mar 11;53(5):1923-36. https://pubmed.ncbi.nlm.nih.gov/20143782/