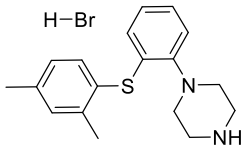
Product data sheet

MedKoo Cat#: 314242 Name: Vortioxetine HBr CAS#: 960203-27-4 (HBr) Chemical Formula: $C_{18}H_{23}BrN_2S$ Exact Mass: 378.07653 Molecular Weight: 379.36	
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:
Vortioxetine, also known as Lu AA21004, is an atypical antidepressant, and was approved in 2013 by the U.S. FDA for the treatment of major depressive disorder (MDD) in adults. Vortioxetine is a so-called "serotonin modulator and stimulator." It has been shown to possess the following pharmacological actions: Serotonin transporter (SERT) blocker (i.e. serotonin reuptake inhibitor (SRI)) — Ki (binding affinity) = 1.6 nM, IC50 = 5.4 nM; Norepinephrine transporter (NET) blocker — Ki = 113 nM; 5-HT1A receptor high-efficacy partial agonist/near-full agonist — Ki = 15 nM, IA = 80%; 5-HT1B receptor partial agonist — Ki = 33 nM; 5-HT1D receptor antagonist — Ki = 54 nM; 5-HT3A receptor antagonist — Ki = 3.7 nM; 5-HT7 receptor antagonist — Ki = 19 nM.

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	52.0	137.07
DMSO:PBS (pH 7.2) (1:3)	0.25	0.66
DMF	30.0	79.08
Ethanol	22.0	57.99

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.64 mL	13.18 mL	26.36 mL
5 mM	0.53 mL	2.64 mL	5.27 mL
10 mM	0.26 mL	1.32 mL	2.64 mL
50 mM	0.05 mL	0.26 mL	0.53 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

1. Waller JA, Chen F, Sánchez C. Vortioxetine promotes maturation of dendritic spines in vitro: A comparative study in hippocampal cultures. Neuropharmacology. 2016 Apr;103:143-54. doi: 10.1016/j.neuropharm.2015.12.012. Epub 2015 Dec 15. PMID: 26702943.
2. Bang-Andersen B, Ruhland T, Jørgensen M, Smith G, Frederiksen K, Jensen KG, Zhong H, Nielsen SM, Hogg S, Mørk A, Stensbøl TB. Discovery of 1-[2-(2,4-dimethylphenylsulfanyl)phenyl]piperazine (Lu AA21004): a novel multimodal compound for the treatment of major depressive disorder. J Med Chem. 2011 May 12;54(9):3206-21. doi: 10.1021/jm101459g. Epub 2011 Apr 12. PMID: 21486038.

In vivo study

Product data sheet

1. Turan Yücel N, Kandemir Ü, Demir Özkay Ü, Can ÖD. 5-HT1A Serotonergic, α-Adrenergic and Opioidergic Receptors Mediate the Analgesic Efficacy of Vortioxetine in Mice. Molecules. 2021 May 28;26(11):3242. doi: 10.3390/molecules26113242. PMID: 34071269.
2. Martis LS, Højgaard K, Holmes MC, Elfving B, Wiborg O. Vortioxetine ameliorates anhedonic-like behaviour and promotes strategic cognitive performance in a rodent touchscreen task. Sci Rep. 2021 Apr 27;11(1):9113. doi: 10.1038/s41598-021-88462-7. PMID: 33907240; PMCID: PMC8079376.

7. Bioactivity

Biological target:

Vortioxetine hydrobromide is a multimodal serotonergic agent, inhibits 5-HT1A, 5-HT1B, 5-HT3A, 5-HT7 receptor and SERT with Ki values of 15 nM, 33 nM, 3.7 nM, 19 nM and 1.6 nM, respectively.

In vitro activity

Relative to vehicle-treated neurons, vortioxetine promoted an increase in total spine area (1.30 ± 0.05 μm2; ****, $p < 0.0001$), spine width (1.16 ± 0.04 μm; ****, $p < 0.0001$), spine breadth (1.10 ± 0.03 μm; ***, $p = 0.0003$), which is comparable to spine head width in MetaMorph software, and spine length (1.16 ± 0.03 μm; ****, $p < 0.0001$) (Fig. 2A,B, Table 1). There was an increased proportion of large, mushroom-like spines with an area greater than 2.0 μm2 with vortioxetine treatment in comparison to vehicle (Fig. 6A). In contrast to the increase in spine density following subchronic and chronic vortioxetine treatment reported in vivo, there were no changes in the density of spines per 10 μm dendritic segment (7.50 ± 0.41 (VOR) vs. 7.07 ± 0.30 (VEH)) (Fig. 2A,C, Table 1). Interestingly, the proportion of spines that were closely apposed to or co-localized with the presynaptic vesicle marker synapsin I was greater with vortioxetine than in vehicle-treated neurons (45.44 ± 3.09% (VOR) vs. 34.47 ± 2.65% (VEH); *, $p = 0.0145$) (Fig. 2A,C, Table 1).

Reference: Neuropharmacology. 2016 Apr;103:143-54. https://pubmed.ncbi.nlm.nih.gov/21486038/

In vivo activity

The analgesic activity of vortioxetine was evaluated by the tail-clip, tail-immersion and hot-plate tests. In the tail-clip tests, animals administered vortioxetine at 10 and 20 mg/kg had significantly longer reaction time than saline-administered control mice. Moreover, MPE% and AUC values were also significantly higher with respect to the control groups. 5 mg/kg dose of this drug was only effective at 60th minute (Figure 2). In the tail-clip method, the clamp-biting reaction of animals is known to be associated with spinal transmission of nociception. Therefore, these findings suggest that the analgesic activity of vortioxetine is related to its effect on spinal nociceptive pathways that carry painful mechanical stimuli.

Reference: Molecules. 2021 May 28;26(11):3242. https://www.mdpi.com/1420-3049/26/11/3242/htm

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.