Product Data Sheet

Chemical Properties

**Product Name:** Vortioxetine (Lu AA21004) HBr

**Cas No.:** 960203-27-4

**M.Wt:** 379.36

**Formula:** C18H22N2S.HBr

**Chemical Name:** 1-[2-(2,4-dimethylphenyl)sulfanylphenyl]piperazine;hydrobromide

**Canonical SMILES:** CC1=CC(=C(C=C1)SC2=CC=CC=C2N3CCNCC3)C.Br

**Solubility:** \( \geq 18.968 \text{mg/mL} \) in DMSO

**Storage:** Store at -20°C

**General tips:** For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

**Shopping Condition:** Evaluation sample solution: ship with blue ice
All other available size: ship with RT, or blue ice upon request

Biological Activity

**Targets:** Neuroscience

**Pathways:** 5-HT Receptor

**Description:**

Vortioxetine (Lu AA21004) HBr (vortioxetine) is an antidepressant, [1] [2] and a serotonin (5-HT) receptor modulator [1] [3] with Ki values of 3.7 nM, 19 nM, 200 nM, 33 nM, 15 nM, and 1.6 nM, to human (h) 5-HT3A receptor, h5-HT7 receptor, rat (r) 5-HT7 receptor, h5-HT1B receptor, h5-HT1A receptor and h5-HT transporter (hSERT), respectively, with an IC50 value of 2080 nM to r5-HT7 receptor, and with an EC50 value of 460 nM to h5-HT1B receptor [3].

5-HT is important in brain, acting as a neurotransmitter in neuromodulation [4].
In HELA cells expressing h5-HT1B receptors stably, Lu AA21004 displayed a partial agonistic response with an EC50 value of 460±110 nM and an IA of 22%. In a polyclonal HEK-293 cell line expressing the r5-HT7 receptor, Lu AA21004 bound to the r5-HT7 receptor with a Ki value of 200±27 nM and was a functional antagonist at the r5-HT7 receptor with an IC50 value of 2080±18 nM [3].

In rats, subcutaneous (sc) administration of Lu AA21004 resulted in ED50 values of 0.4 mg/kg and 3.2 mg/kg to the rSERT and the r5-HT1B receptor, respectively. Lu AA21004 acted as an antagonist of 5-HT3 receptor with an ED50 value of 0.11 mg/kg sc [3]. Treatment with vortioxetine at doses of 2.5 and 5 mg/kg prior to the acquisition of novel objects made rats show 29 and 33 s, respectively, as average exploration values [5].

Reference:

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.

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