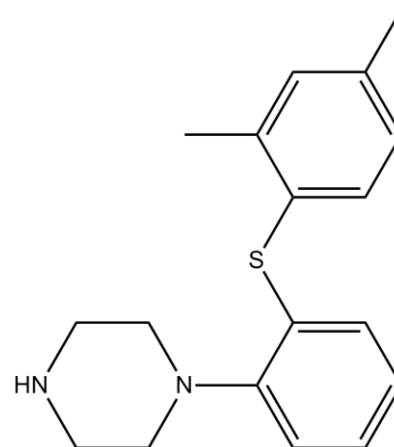


Product Data Sheet

Chemical Properties

Product Name:	Vortioxetine
Cas No.:	508233-74-7
M.Wt:	298.45
Formula:	C ₁₈ H ₂₂ N ₂ S
Synonyms:	Lu AA 21004;Lu AA21004



Chemical Name:	1-[2-(2,4-dimethylphenyl)sulfanylphenyl]piperazine
Canonical SMILES:	<chem>CC1=CC(=C(C=C1)SC2=CC=CC=C2N3CCNCC3)C</chem>
Solubility:	≥14.9mg/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 is a novel multimodal antidepressant currently under development for the treatment of MDD. The serotonergic system plays an important role in cognitive functions via various 5-HT receptors.

In vitro: Vortioxetine (Lu AA21004) was the lead compound, displaying high affinity for recombinant human 5-HT_{1A} (K_i = 15 nM), 5-HT_{1B} (K_i = 33 nM), 5-HT_{3A} (K_i = 3.7 nM), 5-HT₇ (K_i =

19 nM), and noradrenergic β_1 ($K_i = 46$ nM) receptors, and SERT ($K_i = 1.6$ nM). Vortioxetine displayed antagonistic properties at 5-HT_{3A} and 5-HT₇ receptors, partial agonist properties at 5-HT_{1B} receptors, agonistic properties at 5-HT_{1A} receptors, and potent inhibition of SERT [1]. In vivo: In conscious rats, vortioxetine significantly increased extracellular 5-HT levels in the brain after acute and 3 days of treatment. Following the 3-day treatment (5 or 10 mg/kg/day) SERT occupancies were only 43% and 57%, respectively [1].

Clinical trial: Drugs were administered in the evening of 15 consecutive days. Vortioxetine did not cause cognitive or psychomotor impairment. However, mirtazapine impaired cognitive and psychomotor performance on day 2. Most of these effects disappeared after multiple doses of mirtazapine [2].

Reference:

[1] 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;54(9):3206-21.*

[2] Theunissen EL, Street D, Højer AM, Vermeeren A, van Oers A, Ramaekers JG. *A randomized trial on the acute and steady-state effects of a new antidepressant, vortioxetine (Lu AA21004), on actual driving and cognition. Clin Pharmacol Ther. 2013;93(6):493-501.*

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. Short-term 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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