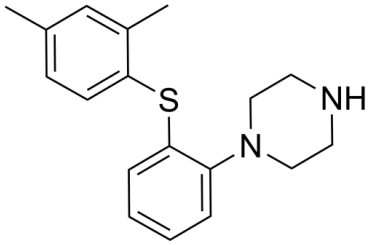
Data Sheet

Product Name:	Vortioxetine
Cat. No.:	CS-1471
CAS No.:	508233-74-7
Molecular Formula:	$C_{18}H_{22}N_2S$
Molecular Weight:	298.45
Target:	5-HT Receptor; Serotonin Transporter
Pathway:	GPCR/G Protein; Neuronal Signaling
Solubility:	DMSO : 50 mg/mL (ultrasonic)



BIOLOGICAL ACTIVITY:

Vortioxetine (Lu AA 21004) is a inhibitor of **5-HT_{1A}, 5-HT_{1B}, 5-HT_{3A}, 5-HT_7** receptor and **SERT**, with **K_i** values of 15 nM, 33 nM, 3.7 nM, 19 nM and 1.6 nM, respectively. IC50 & Target: Ki: 15 nM (5-HT_{1A}); 33 nM (5-HT_{1B}); 3.7 nM (5-HT_{3A}); 19 nM (5-HT_7); 1.6 nM (SERT)[1]. ***In Vitro:*** Vortioxetine (Compound 5m) is a multimodal serotonergic agent, inhibits 5-HT_{1A}, 5-HT_{1B}, 5-HT_{3A}, 5-HT_7 receptor and SERT with K_i values of 15 nM, 33 nM, 3.7 nM, 19 nM and 1.6 nM, respectively. Vortioxetine displays antagonistic properties at 5-HT_{3A} and 5-HT_7 receptors, partial agonist properties at 5-HT_{1B} receptors, agonistic properties at 5-HT_{1A} receptors, and potent inhibition of $SERT_{[1]}$. Vortioxetine is a partial h5-HT_{1B} receptor agonist with EC_{50} of 460 nM and intrinsic activity of 22% using a whole-cell cAMP-based assay. Vortioxetine binds to the r5-HT_7 receptor with a K_i value of 200 nM and is a functional antagonist at the r5-HT_7 receptor with an IC_{50} of 2 μM in an in vitro whole-cell cAMP assay[5]. ***In Vivo:*** Vortioxetine (Lu AA21004) occupies the r5-HT_{1B} receptor and rSERT (ED_{50}= 3.2 and 0.4 mg/kg, respectively) after subcutaneous administration and is a 5-HT_3 receptor antagonist[6]. Vortioxetine significantly increases cell proliferation and cell survival and stimulates maturation of immature granule cells in the sub granular zone of the dentate gyrus of the hippocampus after 21 days of treatment[3]. Vortioxetine does not cause cognitive or psychomotor impairment[4].

References:

[1]. Bang-Andersen B, et al. 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.

[2]. Guilloux JP, et al. Antidepressant and anxiolytic potential of the multimodal antidepressant vortioxetine (Lu AA21004) assessed by behavioural and neurogenesis outcomes in mice. Neuropharmacology. 2013 May 28;73C:147-159.

[3]. Theunissen EL, et al. 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 Jun;93(6):493-501.

[4]. Rothschild AJ, et al. Vortioxetine (Lu AA21004) 5mg in generalized anxiety disorder: results of an 8-week randomized, double-blind, placebo-controlled clinical trial in the United States. Eur Neuropsychopharmacol. 2012 Dec;22(12):858-66.

[5]. Mrk A, et al. Pharmacological effects of Lu AA21004: a novel multimodal compound for the treatment of major depressive disorder. J Pharmacol Exp Ther. 2012 Mar;340(3):666-75.

CAIndexNames:

Piperazine, 1-[2-[(2,4-dimethylphenyl)thio]phenyl]-

SMILES:

CC1=CC=C(SC2=CC=CC=C2N3CCNCC3)C(C)=C1

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 610-426-3128 Fax: 888-484-5008 E-mail: sales@ChemScene.com
Address: 1 Deer Park Dr, Suite F, Monmouth Junction, NJ 08852, USA