Data Sheet (Cat.No.T4229)

TargetMol

S1RA hydrochloride

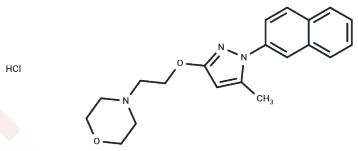
Chemical Properties

CAS No. : 1265917-14-3

Formula: C20H24ClN3O2

Molecular Weight: 373.87

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.



Biological Description

Description	S1RA hydrochloride (E-52862 hydrochloride) is an effective and specific sigma-1 receptor(σ1R, Ki: 17 nM) antagonist, and has good selectivity against σ2R (Ki > 1000 nM).
Targets(IC50)	5-HT Receptor,Sigma receptor
In vitro	S1RA showed high affinity for the guinea pig (Ki: 23.5 nM) and human (Ki: 17 nM) σ1 receptors but no marked affinity for the σ2 receptors (Ki > 1000 nM for guinea pig and rat σ2 receptors). Moderate affinity (Ki: 328 nM) and antagonistic activity with very low potency (IC50: 4700 nM) were found at the human 5-HT2B receptor. S1RA showed a low affinity (Ki > 1 μM, IC50>1 μM) for other additional 170 targets (transporters, receptors, ion channels and enzymes).
In vivo	Control (non-operated) and nerve-injured mice received a single or repeated (b.i.d, for 12 days) S1RA (25 mg/kg, i.p.), the same dose used for the assessment of behavioral hypersensitivity in the chronic treatment study. In the behavioral studies, acute treatment was given on day 12 post-surgery and repeated treatment with S1RA started the day of surgery. Intrathecal pre-treatment with idazoxan prevented the systemic S1RA antinociceptive effect, suggesting that the S1RA antinociception depends on the activation of spinal α2 -adrenoceptors which, in turn, could induce an inhibition of formalin-evoked glutamate release. When administered locally, intrathecal S1RA inhibited only the flinching behavior, whereas intracerebroventricularly or intraplantarly injected also attenuated the lifting/licking behavior.

Solubility Information

Solubility	DMSO: 50 mg/mL (133.74 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (5.35 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.6747 mL	13.3736 mL	26.7473 mL
5 mM	0.5349 mL	2.6747 mL	5.3495 mL
10 mM	0.2675 mL	1.3374 mL	2.6747 mL
50 mM	0.0535 mL	0.2675 mL	0.5349 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Díaz JL, et al. Synthesis and biological evaluation of the 1-arylpyrazole class of σ(1) receptor antagonists: identification of 4-{2-[5-methyl-1-(naphthalen-2-yl)-1H-pyrazol-3-yloxy]ethyl}morpholine (S1RA, E-52862). J Med Chem. 2012 Oct 11;55(19):8211-24.

Meng F, Xiao Y, Ji Y, et al. An open-like conformation of the sigma-1 receptor reveals its ligand entry pathway. Nature Communications. 2022, 13(1): 1-11.

Romero L, et al. Pharmacological properties of S1RA, a new sigma-1 receptor antagonist that inhibits neuropathic pain and activity-induced spinal sensitization. Br J Pharmacol. 2012 Aug;166(8):2289-306.

Vidal-Torres A, et al. Effects of the selective sigma-1 receptor antagonist S1RA on formalin-induced pain behavior and neurotransmitter release in the spinal cord in rats. J Neurochem. 2014 Jan 3.