Product Data Sheet

Product Name: S1RA
Cat. No.: GC10407

Chemical Properties

Cas. No.	878141-96-9		
Chemical Name	4-(2-((5-methyl-1-(naphthalen-2-yl)-1H-pyrazol-3-yl)oxy)ethyl)morpholine		
SMILES	CC1=CC(OCCN2CCOCC2)=NN1C3=CC4=CC=CC=C4C=C3		
Formula	$C_{20}H_{23}N_3O_2$	M.Wt	337.42
Solubility	≥ 10.35mg/mL in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	S1RA		

Background

S1RA is a potent and selective antagonist of σ1 receptor (σ1R) with Ki value of 17nM [1].

S1RA is the first σ1 receptor antagonist with potent antinociceptive activities in various pain models. In the binding assay, S1RA shows good affinity to human σ1 receptor transfected in HEK293 membranes with Ki value of 17nM. The Ki value for guinea pig brain membrane σ1 receptor is higher than 1μM. S1RA also shows no significant affinity to another 170 molecular targets including receptors, ion channels and enzymes [1, 2].

In the mouse tests, S1RA exhibits potent analgesic effects on capsaicin-induced mechanical hypersensitivity and formalin-induced pain. Besides that, S1RA inhibits both mechanical allodynia and thermal hypersensitivity with ED50 values of 23.4mg/kg and 18.8mg/kg in the partial sciatic nerve ligation model in mice [1].

References:
[1] Díaz J L, Cuberes R, Berrocal J, et al. Synthesis and Biological Evaluation of the 1-

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Arylpyrazole Class of σ1 Receptor Antagonists: Identification of 4-{2-[5-Methyl-1-(naphthalen-2-yl)-1 H-pyrazol-3-yloxy] ethyl} morpholine (S1RA, E-52862). Journal of medicinal chemistry, 2012, 55(19): 8211-8224.
[2] Wunsch B. The σ1 Receptor Antagonist S1RA Is a Promising Candidate for the Treatment of Neurogenic PainJ. Journal of medicinal chemistry, 2012, 55(19): 8209-8210.

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