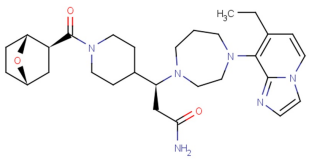
Data Sheet (Cat.No.T10907)

TargetMol
A DRUG SCREENING EXPERT

CXCR7 modulator 2

Chemical Properties



CAS No.:	2227426-37-9
Formula:	C29H42N6O3
Molecular Weight:	522.68
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	CXCR7 modulator 2 is a 7-type C-X-C chemokine receptor (CXCR7) modulator with a Ki of 13 nM.
Targets(IC_{50})	CXCR7: 13 nM (ki)
In vitro	CXCR7 modulator 2 showed strong CXCR7 binding affinity (Ki = 13 nM) and β-arrestin activity (EC50 = 11 nM). Compared with 11c, CXCR7 modulator 2 also showed improved selectivity in the GPCR panel and showed a higher therapeutic index in the hERG patch clamp assay. CXCR7 modulator 2 exhibited medium to high in vitro turnover in NADPH- supplemented mouse liver microsomes (MLM, 93 μL / min / mg) and hepatocytes (28 μL / min per million cells), which was shown to be more comparable in MDCK Poor passive absorption permeability type II permeability measurement method, and has good water solubility. CXCR7 regulator 2 is rapidly absorbed, with an average maximum plasma concentration (Cmax) of 682 ng / mL, which appears at 0.25 h (Tmax). The corresponding average area under the plasma concentration-time curve (AUC) is 740 ng / mL / h.
In vivo	The administration of isoproterenol for 9 days will lead to the development of cardiac fibrosis. This is because the amount of collagen deposition detected by Pixirius red staining has increased by about 4 times relative to that of the control group. proven. Treatment with CXCR7 modulator 2 can lead to a statistically significant reduction in cardiac fibrosis, thus demonstrating that CXCR7 modulator 2 has a protective effect on CXCR7 modulation in isoproterenol-induced cardiac injury.

Solubility Information

Solubility	DMSO: 250 mg/mL (478.30 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.913 mL	9.566 mL	19.132 mL
5 mM	0.383 mL	1.913 mL	3.826 mL
10 mM	0.191 mL	0.957 mL	1.913 mL
50 mM	0.038 mL	0.191 mL	0.383 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Menhaji-Klotz E, et al. Discovery of a Novel Small-Molecule Modulator of C-X-C Chemokine Receptor Type 7 as a Treatment for Cardiac Fibrosis. J Med Chem. 2018 Apr 26;61(8):3685-3696.

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