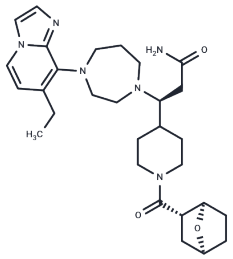
Data Sheet (Cat.No.T10907)

TargetMol

CXCR7 modulator 2

Chemical Properties



CAS No. : 2227426-37-9

Formula: C29H42N6O3

Molecular Weight: 522.68

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	CXCR7 modulator 2 is a 7-type C-X-C chemokine receptor (CXCR7) modulator with a Ki of 13 nM.
Targets(IC50)	Others
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 induces cardiac fibrosis, evidenced by a fourfold increase in collagen deposition detected by Pixirius red staining relative to the control group. Treatment with CXCR7 modulator 2 significantly reduces cardiac fibrosis, demonstrating its protective effect on CXCR7 modulation in isoproterenol-induced cardiac injury.

Solubility Information

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

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.9132 mL	9.5661 mL	19.1322 mL
5 mM	0.3826 mL	1.9132 mL	3.8264 mL
10 mM	0.1913 mL	0.9566 mL	1.9132 mL
50 mM	0.0383 mL	0.1913 mL	0.3826 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.

Reference

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.