Data Sheet (Cat.No.T16124)

TargetMol

MMP13-IN-3

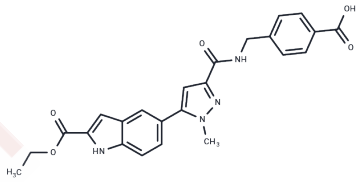
Chemical Properties

CAS No. : 1222173-37-6

Formula: C24H22N4O5

Molecular Weight: 446.46

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	MMP13-IN-3 is >1000 selective over other MMPs. MMP13-IN-3 is an effective, selective, and orally active MMP-13 inhibitor (IC50=1 nM) for the potential treatment of osteoarthritis.
Targets(IC50)	MMP
In vitro	MMP13-IN-3 inhibits MMP-2, MMP-9, MMP-10 and MMP-14 with IC50s of 18, 8.9, 16 and 8.3 μM, respectively. MMP13-IN-3 is effective in a full-length MMP-13 collagen degradation assay (11 nM) and is able to inhibit the degradation of bovine nasal cartilage (IC50: 31 nM) [1].
In vivo	MMP13-IN-3 has short terminal elimination half-life (t1/2=0.47 h for rat (1 mg/kg, i.v.) and rat (10 mg/kg, orally), respectively). MMP13-IN-3 reaches micromolar plasma levels (AUC=1109±64 nM h/mL) when dosed orally at 10 mg/kg or i.v. 1 mg/kg. It displays modest clearance (CL=34 mL/min/kg), and shows acceptable bioavailability (39%). The Vss is quite low at 0.26 mL/mi/kg rat pharmacokinetic profile [1].

Solubility Information

Solubility	DMSO: 100 mg/mL (223.98 mM),Sonication and heating to 60°C are recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.2398 mL	11.1992 mL	22.3984 mL
5 mM	0.448 mL	2.2398 mL	4.4797 mL
10 mM	0.224 mL	1.1199 mL	2.2398 mL
50 mM	0.0448 mL	0.224 mL	0.448 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

Taylor SJ, et al. Fragment-based discovery of indole inhibitors of matrix metalloproteinase-13. J Med Chem. 2011 Dec 8;54(23):8174-87.
Ruminski PG, et al. Discovery of N-(4-Fluoro-3-methoxybenzyl)-6-(2-(((2S,5R)-5-(hydroxymethyl)-1,4-dioxan-2-yl) methyl)-2H-tetrazol-5-yl)-2-methylpyrimidine-4-carboxamide. A Highly Selective and Orally Bioavailable Matrix Metalloproteinase-13 Inhibitor for the Potential Treatment of Osteoarthritis. J Med Chem. 2016 Jan 14;59(1):313-27.