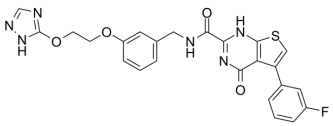
MMP13-IN-2

Cat. No.:	HY-122624
CAS No.:	935759-55-0
Molecular Formula:	$C_{24}H_{19}FN_6O_4S$
Molecular Weight:	506.51
Target:	MMP
Pathway:	Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (197.43 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9743 mL	9.8715 mL	19.7429 mL
	5 mM	0.3949 mL	1.9743 mL	3.9486 mL
	10 mM	0.1974 mL	0.9871 mL	1.9743 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

MMP13-IN-2 is a potent, selective and orally active MMP-13 inhibitor. MMP13-IN-2 exhibits excellent potency for MMP-13 (IC_{50}=0.036 nM) and selectivities (greater than 1,500-fold) over MMP-1, 3, 7, 8, 9, 14, and TACE. MMP13-IN-2 has the ability to block the release of collagen from cartilage in vitro. MMP13-IN-2 has the potential for collagenase related disease research[1] .

IC_{50} & Target

MMP-13	MMP-2	MMP-3
0.036 nM (IC_{50})	180 nM (IC_{50})	1100 nM (IC_{50})

In Vitro

In a bovine nasal cartilage (BNC) assay, the chondrocyte-mediated degradation of cartilage was studied using bovine nasal cartilage slices cultured for up to 14 days. MMP13-IN-2 (0.01-1 μM) is effective at preventing the IL-1/OSM induced in vitro degradation of BNC (-17.6%, 48.4% and 70.8% inhibition of cartilage degradation, respectively).[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

MMP13-IN-2 (oral gavage; 1 mg/kg) shows the best combination of CYP3A4 inhibition risk and oral exposure at a dose of 1 mg/kg in rats and mice (F% = 33 and 38, respectively)[1].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Hiroshi Nara, et al. Discovery of Novel, Highly Potent, and Selective Matrix Metalloproteinase (MMP)-13 Inhibitors with a 1,2,4-Triazol-3-yl Moiety as a Zinc Binding Group Using a Structure-Based Design Approach. J Med Chem. 2017 Jan 26;60(2):608-626.

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