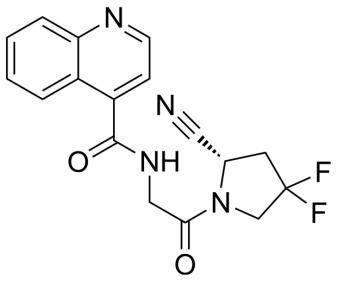
SP-13786

Cat. No.:	HY-100684		
CAS No.:	1448440-52-5		
Molecular Formula:	$C_{17}H_{14}F_2N_4O_2$		
Molecular Weight:	344.32		
Target:	Others		
Pathway:	Others		
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 (290.43 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.9043 mL	14.5214 mL	29.0428 mL
5 mM	0.5809 mL	2.9043 mL	5.8085 mL
10 mM	0.2904 mL	1.4521 mL	2.9043 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (7.26 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (7.26 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (7.26 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

SP-13786 is a highly potent and selective inhibitor of fibroblast activation protein (FAP) with an IC_{50} of 3.2 nM; also inhibits prolyl oligopeptidase (PREP) with an IC_{50} of 1.8 μM.

IC_{50} & Target

IC50: 3.2 nM (FAP), 1.8 μM (PREP)[1]

In Vitro

SP-13786 is also found to have better FAP/PREP selectivity and a very proficient ligand efficiency of 0.34.

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

In Vivo	SP-13786 is the most extensive and prolonged inhibitior of FAP in the PK studies. No tight binding behavior is observed, and the inhibitor proves to bind reversibly to FAP. Pharmacokinetic evaluation in mice of SP-13786 demonstrates high oral bioavailability, plasma half-life, and the potential to selectively and completely inhibit FAP in vivo[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Animal Administration [1]	Rats: The PK parameters are determined for inhibitors 4, 5, 60 (SP-13786), and 61 in rats. Six male rats are treated for each inhibitor tested, three of which received the compound via a single intravenous (iv) administration at 5 mg/kg. The other three animals are dosed per os (po) at 20 mg/kg. Blood samples are collected at 0.083, 0.25, 0.5, 1, 2, 4, 6, and 24 h after administration. Inhibitor concentrations are determined using UPLC–MS/MS, and pharmacokinetic parameters are calculated using standard algorithms[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Anal Chem. 2019 Dec 3;91(23):14873-14878.
- Mol Cancer Ther. 2022 Feb 11;molcanther.MCT-21-0518-A.2021.

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REFERENCES

[1]. Jansen K, et al. Extended structure-activity relationship and pharmacokinetic investigation of (4-quinolinoyl)glycyl-2-cyanopyrrolidine inhibitors of fibroblast activation protein (FAP). J Med Chem. 2014 Apr 10;57(7):3053-74.

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