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产品名称：SP-13786
产品别名：SP-13786

生物活性：

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.
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].

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

*请根据产品在不同溶剂中的溶解度选择合适的溶剂配制储备液；一旦配成溶液，请分装保存，避免反复冻融造成的产品失效。

储备液的保存方式和期限：-80°C, 6 months; -20°C, 1 month。-80°C 储存时，请在 6 个月内使用，-20°C 储存时，请在 1 个月内使用。

In Vivo:

请根据您的实验动物和给药方式选择适当的溶解方案。以下溶解方案都请先按照 In Vitro 方式配制澄清的储备液，再依次添加助溶剂：

——为保证实验结果的可靠性，澄清的储备液可以根据储存条件，适当保存；体内实验的工作液，建议您现用现配，当天使用； 以下溶剂前显示的百分比是指该溶剂在您配制终溶液中的体积占比；如在配制过程中出现沉淀、析出现象，可以通过加热和/或超声的方式助溶

1.请依序添加每种溶剂： 10% DMSO→40% PEG300 →5% Tween-80 → 45% saline

Solubility: ≥ 2.5 mg/mL (7.26 mM); Clear solution

此方案可获得 ≥ 2.5 mg/mL (7.26 mM，饱和度未知) 的澄清溶液。

以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 400 μL PEG300 中，混合均匀；向上述体系中加入 50 μL Tween-80，混合均匀；然后继续加入 450 μL 生理盐水定容至 1 mL。

2.请依序添加每种溶剂： 10% DMSO→ 90% (20% SBE-β-CD in saline)

Solubility: ≥ 2.5 mg/mL (7.26 mM); Clear solution

此方案可获得 ≥ 2.5 mg/mL (7.26 mM，饱和度未知) 的澄清溶液。

以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 900 μL 20% 的 SBE-β-CD 生理盐水水溶液中，混合均匀。

	3.请依序添加每种溶剂： 10% DMSO →90% corn oil Solubility: ≥ 2.5 mg/mL (7.26 mM); Clear solution 此方案可获得 ≥ 2.5 mg/mL (7.26 mM，饱和度未知) 的澄清溶液，此方案不适用于实验周期在半个月以上的实验。 以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 900 μL 玉米油中，混合均匀。
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.

实验参考：

Animal Administration	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].
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.