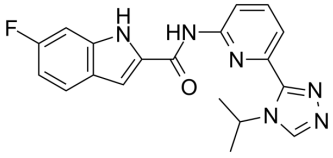
ASK1-IN-2

Cat. No.:	HY-131969
CAS No.:	2541792-70-3
Molecular Formula:	$C_{19}H_{17}FN_6O$
Molecular Weight:	364.38
Target:	Apoptosis; MAP3K
Pathway:	Apoptosis; MAPK/ERK Pathway
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 : 250 mg/mL (686.10 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.7444 mL	13.7219 mL	27.4439 mL
5 mM	0.5489 mL	2.7444 mL	5.4888 mL
10 mM	0.2744 mL	1.3722 mL	2.7444 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: ≥ 2.08 mg/mL (5.71 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.71 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ASK1-IN-2 is a potent and orally active inhibitor of apoptosis signal-regulating kinase 1 (ASK1), with an IC_{50} of 32.8 nM. ASK1-IN-2 can be used for the research of ulcerative colitis[1].

IC_{50} & Target

ASK1
32.8 nM (IC_{50})

In Vitro

ASK1-IN-2 (compound 19) (10 mM; 1 h) inhibits the luciferase reporter activity in AP1-HEK293 cells, with inhibition rate of 95.59%[1].

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

In Vivo

ASK1-IN-2 (25 mg/kg; p.o. daily for 7 d) improves dextran sulphate sodium (DSS)-induced ulcerative colitis (UC) in mice[1].
ASK1-IN-2 (25 mg/kg; p.o. daily for 7 d) blocks ASK1-p38/JNK signaling pathways and reduces inflammatory cytokine levels in DSS-induced mouse colon tissues[1].
ASK1-IN-2 (1 mg/kg; i.v.) shows low clearance (CL=1.38 L/h/kg) and moderate half-life ($T_{1/2}$=1.45 h) in rats[1].
ASK1-IN-2 (10 mg/kg; p.o.) shows high oral exposure (AUC_{last}=4517 h•ng/mL), 62.2% oral bioavailability and acceptable terminal half-life ($T_{1/2}$=2.31 h) in rats[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male ICR mice (18-22 g, 6-8 weeks) were given 3% DSS (w/v) orally in drinking water[1]
Dosage:	25 mg/kg
Administration:	P.o. daily for 7 days
Result:	Induced a significant recovery of body weight loss, with an increase of +11.2%. Decreased the disease activity index (DAI) score about a 2 unit. Significantly prevented colon shortening. Attenuated a severe colonic tissue damage and infiltration of inflammatory cells.

Animal Model:	Male SD rats [1]
Dosage:	1 mg/kg for i.v.; 10 mg/kg for p.o. (Pharmacokinetic Analysis)
Administration:	I.v. and p.o. administration
Result:	I.v.: CL=1.38 L/h/kg; $T_{1/2}$=1.45 h. P.o.: AUC_{last}=4517 h•ng/mL; F=62.2%; $T_{1/2}$=2.31 h.

REFERENCES

[1]. Hou S, et, al. Structure-based discovery of 1H-indole-2-carboxamide derivatives as potent ASK1 inhibitors for potential treatment of ulcerative colitis. Eur J Med Chem. 2020 Dec 24;211:113114.

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