Smurf1-IN-1

Cat. No.: HY-149316

CAS No.: 1824708-03-3

Molecular Formula: $C_{24}H_{29}ClN_6O_2$

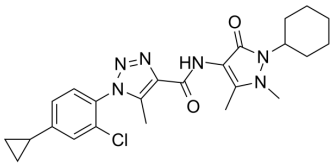
Molecular Weight: 468.98

Target: E1/E2/E3 Enzyme

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 (213.23 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.1323 mL	10.6614 mL	21.3229 mL
5 mM	0.4265 mL	2.1323 mL	4.2646 mL
10 mM	0.2132 mL	1.0661 mL	2.1323 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 (5.33 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (5.33 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (5.33 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

Smurf1-IN-1 is an orally active and selective inhibitor of specific E3 ubiquitin protein ligase 1 (SMURF1) with an IC_{50} of 92 nM. Smurf1-IN-1 has significant efficacy in rats model of pulmonary hypertension[1].

IC_{50} & Target

IC50: 92 nM Specific E3ubiquitin protein ligase 1 (SMURF1)[1]

In Vivo

Smurf1-IN-1 (Compound 38) (1, 3, 10 mg/kg for p.o.) has significant efficacy in rats model of pulmonary hypertension[1].
Smurf1-IN-1 (1 mg/kg for i.v., 3 mg/kg for p.o.) shows a $T_{1/2}$ of 7.9, and oral bioavailability of 82%[1].

Pharmacokinetic parameters for Smurf1-IN-1 (Compound 38) in rats [1]

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

dose and route	oral bioavailability (%)	p.o. AUC_{last} (nM • h /mL)	p.o. C_{max} (nM/L)	half-life (h)	claearance (mL/min/kg)	V_{ss} (1/kg)
3 mpg p.o./1 mpg i.v.	82	7383	2007	7.9	17.1	2.3

Animal Model:	Hypoxia-Sugen rat model of PAH[1]
Dosage:	1, 3, 10 mg/kg
Administration:	Oral gavage (p.o.)
Result:	Caused a 10% increase in muscularization at day 14 and progression to around 18% muscularization was observed in the vehicle group by the end of the study at a dose of 3 mg/kg.

REFERENCES

[1]. Shaw DE, et.al. Design and Synthesis of Inhibitors of the E3 Ligase SMAD Specific E3 Ubiquitin Protein Ligase 1 as a Treatment for Lung Remodeling in Pulmonary Arterial Hypertension. J Med Chem. 2023 Jun 22;66(12):8130-8139.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA