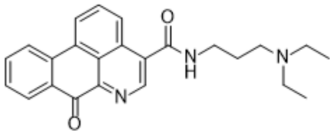
S130

Cat. No.:	HY-112818
CAS No.:	1160852-22-1
Molecular Formula:	$C_{24}H_{25}N_3O_2$
Molecular Weight:	387.47
Target:	Cathepsin; Autophagy; Apoptosis; Atg4
Pathway:	Metabolic Enzyme/Protease; Autophagy; Apoptosis
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (322.61 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.5808 mL	12.9042 mL	25.8084 mL
	5 mM	0.5162 mL	2.5808 mL	5.1617 mL
	10 mM	0.2581 mL	1.2904 mL	2.5808 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: ≥ 2.25 mg/mL (5.81 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.25 mg/mL (5.81 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.37 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

S130 is a high affinity, selective inhibitor of ATG4B (a major cysteine protease) with an IC_{50} of 3.24 μM. S130 suppresses autophagy flux[1].

IC_{50} & Target

IC50: 3.24 μM (ATG4B)[1]

In Vitro

S130 suppresses autophagy and activates apoptosis by inhibiting ATG4B, leads to enhanced cytotoxicity[1].
S130 (10 μM; 6 hours) suppresses autophagy at the early LC3 priming step or late autolysosome degradation stage[1].

S130 accumulates autolysosomes with more lipidated LC3[1].
S130 (0-25 μM; 48 hours) induces cell death through inhibiting the activity of ATG4B at a dose higher than 6.3 μM. And such cytotoxicity might not cause cell death through necroptosis[1].
Nutrient deprivation enhances S130-induced cytotoxicity[1].
S130 (0-10μM; 24 hours) suppresses approximately 79% of the cleavage of full-length LC3-GST at the 10 μM, while no substrates were processed in ATG4B KO cells. S130 displays obvious inhibitory effects on ATG4B[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Cytotoxicity Assay[1]

Cell Line:	HeLa cells, HCT116 cells, HL60 cells
Concentration:	0 μM, 3.1 μM, 6.3 μM, 12.5 μM, 25 μM
Incubation Time:	48 hours
Result:	Had significant cytotoxic effects on HeLa cells (IC_{50} =16.1 μM), HCT116 cells(IC_{50} =9.0 μM) and HL60 cells (IC_{50} =4.7 μM) at a dose higher than 6.3 μM. And such cytotoxicity might not cause cell death through necroptosis.

Cell Autophagy Assay[1]

Cell Line:	HeLa cells and MEF cells
Concentration:	10 μM
Incubation Time:	6 hours
Result:	Suppressed autophagy at the early LC3 priming step or late autolysosome degradation stage.

Western Blot Analysis[1]

Cell Line:	HeLa cells
Concentration:	0 μM, 5 μM, 10 μM
Incubation Time:	24 hours
Result:	Suppressed approximately 79% of the cleavage of full-length LC3-GST at 10 μM, while no substrates were processed in ATG4B KO cells.

In Vivo

S130 (20 mg/kg; i.p.; daily; 3 weeks) suppresses tumor growth, and shows an efficient in vivo antitumor effect with a sound safety on vital organs[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	BALB/c nude female mice (4 weeks), with HCT116 cells xenograft[1]
Dosage:	20 mg/kg
Administration:	Intraperitoneal injection; daily; 3 weeks
Result:	Was able to suppress tumor growth and with a sound safety on vital organs.

REFERENCES

[1]. Fu Y, et al. Discovery of a small molecule targeting autophagy via ATG4B inhibition and cell death of colorectal cancer cells in vitro and in vivo. Autophagy. 2018 Sep 20:1-17.

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