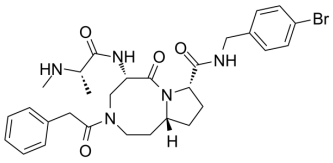
SM-1295

Cat. No.:	HY-124181
CAS No.:	1562375-46-5
Molecular Formula:	$C_{29}H_{36}BrN_5O_4$
Molecular Weight:	598.53
Target:	IAP
Pathway:	Apoptosis
Storage:	-20°C, sealed storage, away from moisture * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 310 mg/mL (517.94 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.6708 mL	8.3538 mL	16.7076 mL
	5 mM	0.3342 mL	1.6708 mL	3.3415 mL
	10 mM	0.1671 mL	0.8354 mL	1.6708 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: ≥ 7.75 mg/mL (12.95 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 7.75 mg/mL (12.95 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

SM-1295 is an inhibitor of apoptosis protein (IAP) antagonist, with K_d values of 3077 nM, 3.2 nM and 9.5 nM for XIAP-BIR3, c-IAP1-BIR3 and c-IAP2-BIR3, respectively[1][2].

IC_{50} & Target

Kd: 3077 nM (XIAP-BIR3), 3.2 nM (c-IAP1-BIR3), 9.5 nM (c-IAP2-BIR3)[2].

In Vitro

SM-1295 (compound 5) binds to both cIAP1 and cIAP2 proteins with K_i values of <10 nM and displays a selectivity of >900-fold for cIAP1 over XIAP[1].

SM-1295 (compound 5) exhibits an IC_{50} of 46 nM in MDA-MB-231[1].

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

REFERENCES

[1]. Haiying Sun, et al. Potent and Selective Small-Molecule Inhibitors of cIAP1/2 Proteins Reveal That the Binding of Smac Mimetics to XIAP BIR3 Is Not Required for Their Effective Induction of Cell Death in Tumor Cells. ACS Chem Biol. 2014 Apr 18;9(4):994-1002.

[2]. Hui Cong, et al. Inhibitor of Apoptosis Protein (IAP) Antagonists in Anticancer Agent Discovery: Current Status and Perspectives. J Med Chem. 2019 Jun 27;62(12):5750-5772.

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