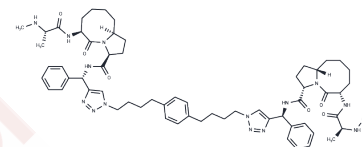


SM-164

Chemical Properties

CAS No. :	957135-43-2
Formula:	C62H84N14O6
Molecular Weight:	1121.42
Storage:	Store at low temperature, Keep away from moisture Powder: -20°C for 3 years In solvent: -80°C for 1 year <i>Actual storage temperature shall be subject to the COA.</i>



Biological Description

Description	SM-164 binds to XIAP protein containing both the BIR2 and BIR3 domains (IC50: 1.39 nM). It acts as an extremely potent antagonist of XIAP.
Targets(IC50)	Apoptosis, IAP
In vitro	SM-164 binds to XIAP being 300 and 7000-times more potent than its monovalent counterparts and the natural Smac AVPI peptide, respectively. The binding affinities of SM-164 to XIAP, cIAP-1, and cIAP-2 proteins are determined using fluorescence-polarization based assays. SM-164 concurrently interacts with both BIR domains in XIAP and functions as an ultra-potent antagonist of XIAP in both cell-free functional and cell-based assays. SM-164 targets cellular XIAP and effectively induces apoptosis at concentrations as low as 1 nM in leukemia cancer cells while having minimal toxicity to normal human primary cells at 10,000 nM. SM-164 has a Ki value of 0.56 nM to XIAP protein containing both BIR2 and BIR3 domains. SM-164 has a Ki value of 0.31 nM to a cIAP-1 protein containing both BIR2 and BIR3 domains. SM-164 binds to cIAP-2 BIR3 protein with Ki values of 1.1 nM [1][2].
In vivo	SM-164 is highly effective in the inhibition of tumor growth and capable of achieving tumor regression in the MDA-MB-231 xenograft model. SM-164 (1 mg/kg) treatment fully inhibits tumor growth during the treatment. SM-164 (5 mg/kg) treatment reduces the tumor volume from 147±54 mm ³ at the beginning of the treatment (day 25) to 54±32 mm ³ at the end of the treatment (day 36), a reduction of 65%. The strong antitumor activity by SM-164 is long-lasting and not transient. SM-164 (5 mg/kg) is statistically more effective than Taxotere at the end of the treatment (P<0.01) or when the tumor size in the control group reached 750 mm ³ (P<0.02) [2].

Solubility Information

Solubility	H2O: < 1 mg/mL (insoluble) DMSO: 50 mg/mL (44.59 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween-80+45% Saline: 1 mg/mL (0.89 mM), Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one.</i>

A DRUG SCREENING EXPERT

In vivo Formulation	<i>Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>
---------------------	--

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	0.8917 mL	4.4586 mL	8.9173 mL
5 mM	0.1783 mL	0.8917 mL	1.7835 mL
10 mM	0.0892 mL	0.4459 mL	0.8917 mL
50 mM	0.0178 mL	0.0892 mL	0.1783 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

- Sun H, et al. Design, synthesis, and characterization of a potent, nonpeptide, cell-permeable, bivalent Smac mimetic that concurrently targets both the BIR2 and BIR3 domains in XIAP. *J Am Chem Soc.* 2007 Dec 12;129(49): 15279-94.
- Huang F, Liang J, Lin Y, et al. Repurposing of Ibrutinib and Quizartinib as potent inhibitors of necroptosis. *Communications Biology.* 2023, 6(1): 972.
- Lu J, et al. SM-164: a novel, bivalent Smac mimetic that induces apoptosis and tumor regression by concurrent removal of the blockade of cIAP-1/2 and XIAP. *Cancer Res.* 2008 Nov 15;68(22):9384-93.
- Li J, Liu X, Liu Y, et al. Saracatinib inhibits necroptosis and ameliorates psoriatic inflammation by targeting MLKL. *Cell Death & Disease.* 2024, 15(2): 122.
- Chen D, Chen Y, Feng J, et al. Guanine nucleotide exchange factor RABGEF1 facilitates TNF-induced necroptosis by targeting cIAP1. *Biochemical and Biophysical Research Communications.* 2024: 149669.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

This product is for Research Use Only · Not for Human or Veterinary or Therapeutic Use

Tel: 781-999-4286 E_mail: info@targetmol.com Address: 34 Washington Street, Wellesley Hills, MA 02481