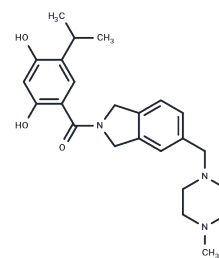


Onalespib

Chemical Properties

CAS No. :	912999-49-6
Formula:	C ₂₄ H ₃₁ N ₃ O ₃
Molecular Weight:	409.52
Storage:	Powder: -20°C for 3 years In solvent: -80°C for 1 year Actual storage temperature shall be subject to the COA.



Biological Description

Description	Onalespib (AT13387) is a synthetic, orally bioavailable, small-molecule inhibitor of heat shock protein 90 (Hsp90) with potential antineoplastic activity. Onalespib selectively binds to Hsp90, thereby inhibiting its chaperone function and promoting the degradation of oncogenic signaling proteins involved in tumor cell proliferation and survival. Hsp90, a chaperone protein upregulated in a variety of tumor cells, regulates the folding, stability and degradation of many oncogenic signaling proteins.
Targets(IC50)	HSP
In vitro	AT13387 is a potent inhibitor of the proliferation and survival of many different cell lines from a wide range of different tumor types (e.g., MES-SA cell line). In a panel of 30 tumor cell lines, AT13387 effectively inhibited cell proliferation with GI50 values in the range of 13-260 nM. AT13387 inhibited the proliferation of the non-tumorigenic human prostate epithelial cell line PNT2 with a GI50 value of 480 nM.
In vivo	AT13387 is a potent inhibitor of the proliferation and survival of many different cell lines from a wide range of different tumor types (e.g., MES-SA cell line). In a panel of 30 tumor cell lines, AT13387 effectively inhibited cell proliferation with GI50 values in the range of 13-260 nM. AT13387 inhibited the proliferation of the non-tumorigenic human prostate epithelial cell line PNT2 with a GI50 value of 480 nM.
Kinase Assay	HSP90 competition isothermal calorimetry: K _d values for AT13387 binding to HSP90 are determined with a competition Isothermal Calorimetry (ITC) format. ITC experiments are performed on a Micro Cal VP-ITC at 25 °C in a buffer comprising 25 mM Tris, 100 mM NaCl, 1 mM MgCl ₂ and 1 mM Tris(2-carboxy-ethyl)phosphine at pH 7.4 in order to maintain the higher affinity
Cell Research	The human cell lines including A375, 22RV1, T474, DU145, LNCaP, MCF-7, DA-MB-468 are seeded into 96-well plates before the addition of AT13387 in 0.1% (v/v) DMSO. GI50 are determined using a 10-point dose response curve for three cell doubling times. After AT13387 incubation 10% (v/v), Alamar blue is added, and cells are incubated for a further 4 hours. Fluorescence is read.(Only for Reference)

Solubility Information

Solubility	DMSO: 2.04 mg/mL (4.98 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 1 mg/mL (2.44 mM), Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. 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>
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.4419 mL	12.2094 mL	24.4188 mL
5 mM	0.4884 mL	2.4419 mL	4.8838 mL
10 mM	0.2442 mL	1.2209 mL	2.4419 mL
50 mM	0.0488 mL	0.2442 mL	0.4884 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

Lyons J, et al. Poser A217.

Wang Y, Ma H, Huang J, et al. Discovery of bardoxolone derivatives as novel orally active necroptosis inhibitors. European Journal of Medicinal Chemistry, 2021 Feb 15;212:113030

Graham B, et al. Cancer Sci. 2012, 103(3), 522-527.

Wang Y, Ma H, Huang J, et al. Discovery of bardoxolone derivatives as novel orally active necroptosis inhibitors[J]. European Journal of Medicinal Chemistry. 2020: 113030.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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