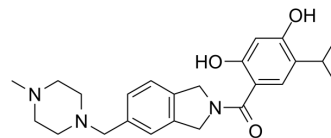


## Onalespib

<b>Cat. No.:</b>	HY-14463		
<b>CAS No.:</b>	912999-49-6		
<b>Molecular Formula:</b>	C <sub>24</sub> H <sub>31</sub> N <sub>3</sub> O <sub>3</sub>		
<b>Molecular Weight:</b>	409.52		
<b>Target:</b>	HSP		
<b>Pathway:</b>	Cell Cycle/DNA Damage; Metabolic Enzyme/Protease		
<b>Storage:</b>	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	2 years
		-20°C	1 year



### SOLVENT & SOLUBILITY

#### In Vitro

DMSO : 50 mg/mL (122.09 mM; ultrasonic and warming and heat to 60°C)

Concentration	Mass		
	1 mg	5 mg	10 mg
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

Please refer to the solubility information to select the appropriate solvent.

#### In Vivo

- Add each solvent one by one: 50% PEG300 >> 50% saline  
Solubility: 16.67 mg/mL (40.71 mM); Suspended solution; Need ultrasonic
- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline  
Solubility: ≥ 2.5 mg/mL (6.10 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)  
Solubility: ≥ 2.5 mg/mL (6.10 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil  
Solubility: ≥ 2.5 mg/mL (6.10 mM); Clear solution

### BIOLOGICAL ACTIVITY

#### Description

Onalespib (AT13387) is a long-acting second-generation Hsp90 inhibitor with a K<sub>d</sub> of 0.71 nM.

#### IC<sub>50</sub> & Target

HSP90  
0.71 nM (K<sub>d</sub>)

<b>In Vitro</b>	<p>Onalespib (Compound 35) is a potent inhibitor of Hsp90, with <math>K_d</math> of 0.71 nM. Onalespib shows potent antiproliferative activity in HCT116 cells, with an <math>IC_{50}</math> of 31 nM. Onalespib also strongly inhibits the proliferation of a panel of human tumor cell lines, showing <math>IC_{50}</math> of &lt; 100 nM<sup>[1]</sup>. Onalespib exhibits cytotoxic activity against many of the PPTP cell lines, with median <math>IC_{50}</math> of 41 nM<sup>[2]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>
<b>In Vivo</b>	<p>Onalespib (60 mg/kg, ip 3 days on and 3 days off for four cycles) shows antitumor activity in nude BALB/c mice bearing early stage HCT116 human colon carcinoma xenografts<sup>[1]</sup>. Onalespib (40 or 60 mg/kg, i.p.) induces significant differences in EFS distribution compared to controls in 17% evaluable solid tumor xenografts, but in none of the ALL xenografts<sup>[2]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>

## PROTOCOL

<b>Cell Assay</b> <sup>[2]</sup>	<p>In vitro testing is performed using DIMSCAN. Cells are incubated in the presence of Onalespib for 96 hours at concentrations from 1 nM to 10 <math>\mu</math>M<sup>[2]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>
<b>Animal Administration</b> <sup>[1]</sup>	<p>HCT116 cells are injected SC into the right hind flank of male nude BALB/c mice. Tumours are apparent 7 to 10 days later. Mice are arranged into matched groups of 12 according to tumour volume giving a group mean of approximately 100 mm<sup>[3]</sup> at initiation of dosing. Tumour volumes are measured every 2 days. Statistical significance between groups is assessed using nonparametric one-way ANOVA. Mice are given the lactate salt of Onalespib using a repeated cycle of dosing of once per day for three days, no dose for three days, once per day for three days etc., for four dosing cycles at 60 mg/kg/dose (as free base equivalents) dissolved in 17.5% hydroxypropyl-<math>\beta</math>-cyclodextrin via the IP route. Control mice receive dose vehicle only via the same route. Tolerability is assessed by recording body weight, clinical observations and survival<sup>[1]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>

## CUSTOMER VALIDATION

- Theranostics. 2019 Aug 12;9(20):5769-5783.
- Nano Res. 07 May 2022.
- Immunology. 2021 Jan;162(1):84-91.
- Sci Rep. 2017 Mar 15;7(1):201.
- J Appl Toxicol. 2017 Nov;37(11):1325-1332.

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## REFERENCES

[1]. Woodhead AJ, et al. Discovery of (2,4-dihydroxy-5-isopropylphenyl)-[5-(4-methylpiperazin-1-ylmethyl)-1,3-dihydroisindol-2-yl]methanone (AT13387), a novel inhibitor of the molecular chaperone Hsp90 by fragment based drug design. J Med Chem. 2010 Aug 26;53

[2]. Kang MH, et al. Initial testing (Stage 1) of AT13387, an HSP90 inhibitor, by the pediatric preclinical testing program. Pediatr Blood Cancer. 2012 Jul 15;59(1):185-8.

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**Caution: Product has not been fully validated for medical applications. For research use only.**

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