Product Data Sheet

Product Name: AT13387
Cat. No.: GC13414

Chemical Properties

Cas. No.	912999-49-6		
Chemical Name	(2,4-dihydroxy-5-propan-2-ylphenyl)-[5-[(4-methylpiperazin-1-yl)methyl]-1,3-dihydroisoindol-2-yl]methanone		
SMILES	CC(C)C1=C(C=C(C(=C1)C(=O)N2CC3=C(C2)C=C(C=C3)CN4CCN(CC4)C)O)O		
Formula	$C_{24}H_{31}N_3O_3$	M.Wt	409.5
Solubility	≥ 13.25 mg/mL in DMSO, ≥ 47.7 mg/mL in EtOH with ultrasonic	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	AT13387		

Protocol

Cell experiment [1]:

Cell lines	LN229, U251HF and A172 Glioblastoma cell lines
Preparation Method	LN229, U251HF and A172 cells were seeded into 96 well plates and exposed to vehicle control (DMSO) or increasing concentrations of AT13387 (0.1 - 2.5μM) for 72h. Cell viability was measured using the WST-1 assay as per manufacturer’s instructions.

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Reaction Conditions	0.1 - 2.5μM, 72h
Applications	AT13387 inhibited cell proliferation in a dose-dependent manner, with an IC_{50} ≤ 0.25μM.
Animal experiment [2]:	
Animal models	Radiosensitive HCT116 human adenocarcinoma xenograft mouse model
Preparation Method	Female nu/nu Balb/c mice were housed under standard laboratory conditions and fed ad libitum. Tumor xenografts were formed by subcutaneous inoculation of approximately $1×10^6$ HCT116 cells suspended in 100μL serum free cell culture medium in the right posterior leg. After approximately 10 days tumors had established (> $80mm^3$) and the treatment schedule started. HCT116 xenografted mice were divided into the following treatment groups: (i) control (N = 10), (ii) radiotherapy (N = 10) 3 × 2 Gy, (iii) AT13387 (N = 10) 3 × 10mg/kg AT13387, (iiii) AT13387 and 3 × 10mg/kg combined with 3 × 2 Gy (N = 10), (iv) AT13387 3 × 5mg/kg (N = 10), (v) AT13387 3 × 5mg/kg combined with 3 × 2 Gy (N = 10). Mice were injected intraperitoneally with 100μL AT13387 or (controls and radiation groups) with 100μL 17.5% β-Cyclodextrin on day 1, 2, and 3. Radiotherapy was given 6h after the drug treatment, performed under anesthesia on day 1, 2, and 3. Tumor size was measured every day with a digital caliper and survival analysis was performed after reaching the study endpoint of $1000mm^3$ tumor size.
Dosage form	5, 10mg/kg/day; 3 days; i.p.

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Applications	AT13387 significantly reduced tumor growth and prolonged both median and overall survival in the HCT116 mouse model.

References:

[1] Canella A, Welker A M, Yoo J Y, et al. Efficacy of onalespib, a long-acting second-generation HSP90 inhibitor, as a single agent and in combination with temozolomide against malignant gliomas[J]. Clinical Cancer Research, 2017, 23(20): 6215-6226.

[2] Spiegelberg D, Abramenkovs A, Mortensen A C L, et al. The HSP90 inhibitor Onalespib exerts

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synergistic anti-cancer effects when combined with radiotherapy: an in vitro and in vivo approach[J]. Scientific Reports, 2020, 10(1): 5923.

Background

AT13387 is a small-molecule, non-ansamycin HSP90 (heat shock protein 90) inhibitor that acts by targeting the AKT and ERK signaling pathways[1]. AT13387 inhibits tumor cell growth and migration and exerts synergistic anti-cancer effects when combined with radiotherapy[2]. AT13387 is commonly used in the study of non-small cell lung cancer (NSCLC)[3].

AT13387 (0.1 - 2.5μM, 72h) inhibited cell proliferation in glioblastoma cell lines in a dose-dependent manner (IC_{50} ≤ 0.25μM). AT13387 (0.4μM, 24h) significantly inhibited the proliferation and angiogenic potential of glioma cells[4].

AT13387 (5, 10mg/kg/day; 3 days; i.p.) significantly reduced tumor growth and prolonged both median and overall survival in the radiosensitive HCT116 human adenocarcinoma xenograft mouse model[2].

References:
[1] Riess J W, Reckamp K L, Frankel P, et al. Erlotinib and onalespib lactate focused on EGFR exon 20 insertion non-small cell lung cancer (NSCLC): a California Cancer Consortium Phase I/II Trial (NCI 9878)[J]. Clinical lung cancer, 2021, 22(6): 541-548.
[2] Spiegelberg D, Abramenkovs A, Mortensen A C L, et al. The HSP90 inhibitor Onalespib exerts synergistic anti-cancer effects when combined with radiotherapy: an in vitro and in vivo approach[J]. Scientific Reports, 2020, 10(1): 5923.
[3] Mooradian M J, Cleary J M, Giobbie-Hurder A, et al. Dose-escalation trial of

combination dabrafenib, trametinib, and AT13387 in patients with BRAF-mutant solid tumors[J]. Cancer, 2023, 129(12): 1904-1918.
[4] Canella A, Welker A M, Yoo J Y, et al. Efficacy of onalespib, a long-acting second-generation HSP90 inhibitor, as a single agent and in combination with temozolomide against malignant gliomas[J]. Clinical Cancer Research, 2017, 23(20): 6215-6226.

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