Data Sheet (Cat.No.T10102)

TargetMol
A DRUG SCREENING EXPERT

3,6-DMAD hydrochloride

Chemical Properties

CAS No.:	T10102
Formula:	C22H31N5xHCl
Molecular Weight:	365.52
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	3,6-DMAD hydrochloride is an inhibitor of the IRE1α-XBP1 pathway of the unfolded protein response.
Targets(IC_{50})	IRE1α: None
In vitro	3,6-DMAD inhibits both IRE1α oligomerization and in vitro endoribonuclease (RNase) activity.
In vivo	3,6-DMAD (10 mg/kg, i.p., once every 12 h, total thrice) significantly inhibits in vivo XBP1-luciferase activity assessed 3.5 days after the initial treatment. 3,6-DMAD-treatment significantly inhibits tumor xenograft growth.
Kinase Assay	IRE1α oligomerization assay is set up using the nuclease reaction buffer, 2 μM recombinant hIRE1α, 2 mM ADP, and 60 μM of 3,6-DMAD. All reactions are performed in 20 μL with 10% DMSO to account for the vehicle and incubated for 15 min at 30 °C to allow for oligomerization. The optical density of the sample is measured at 500 nm using a NanoDrop 2000.
Cell Research	2×10^4 cells per well are plated into 96-well plates and treatment started 0-12 hours after plating. RPMI 8226 and MM1.R human MM cells are treated with 0-6 μM 3,6-DMAD. After 24 hours of treatment, XTT reagent (ATCC) is added to the wells then cells are incubated for 2 hours and absorbance measured at both 475 nM and 660 nM using a plate reader.
Animal Research	5×10^6 RPMI 8226 cells are implanted subcutaneously into the flanks of 4-6 weeks' old NOD Scid mice. Drug treatment started when the sizes of the tumors reached 150 mm3. Four tumor-bearing mice per group are treated with 10 mg/kg 3,6-DMAD or vehicle (saline) intraperitoneally once every 2 days.

Solubility Information

Solubility	DMSO: 25 mg/mL (68.40 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.736 mL	13.679 mL	27.358 mL
5 mM	0.547 mL	2.736 mL	5.472 mL
10 mM	0.274 mL	1.368 mL	2.736 mL
50 mM	0.055 mL	0.274 mL	0.547 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Jiang D, et al. Acridine Derivatives as Inhibitors of the IRE1α-XBP1 Pathway Are Cytotoxic to Human Multiple Myeloma. Mol Cancer Ther. 2016 Sep;15(9):2055-65.

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