MMP2-IN-1

Cat. No.:	HY-146754		
CAS No.:	2764598-01	-6	
Molecular Formula:	$C_{15}H_{13}NO_{5}S$		
Molecular Weight:	319.33		
Target:	ММР; Арор	tosis	
Pathway:	Metabolic E	inzyme/F	Protease; Apoptosis
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	6 months
		-20°C	1 month

SOLVENT & SOLUBILITY

In Vitro	DMSO : 100 mg/mL (3	.00 mg/mL (313.16 mM; Need ultrasonic)			
		Solvent Mass Concentration	1 mg	5 mg	10 mg
	Preparing Stock Solutions	1 mM	3.1316 mL	15.6578 mL	31.3156 mL
		5 mM	0.6263 mL	3.1316 mL	6.2631 mL
		10 mM	0.3132 mL	1.5658 mL	3.1316 mL
	Please refer to the so	lubility information to select the app	propriate solvent.		
In Vivo	1. Add each solvent Solubility: 2.5 mg/	one by one: 10% DMSO >> 40% PEC (mL (7.83 mM); Clear solution; Need	G300 >> 5% Tween-8 ultrasonic	0 >> 45% saline	
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: 2.5 mg/mL (7.83 mM); Clear solution; Need ultrasonic				
	3. Add each solvent Solubility: 2.5 mg/	one by one: 10% DMSO >> 90% cor /mL (7.83 mM); Clear solution; Need	n oil ultrasonic		

BIOLOGICALACITY	
Description	MMP2-IN-1 is a moderate potenet MMP2 inhibitor with IC ₅₀ of 6.8 μM. MMP2-IN-1 exhibits remarkable antiproliferative activity in certain cancer cells by arresting the cell cycle and inducing apoptosis ^[1] .
IC ₅₀ & Target	MMP2 6.8 μM (IC ₅₀)
In Vitro	MMP2-IN-1 (compound 4a) (0-10 μ M; 74 hours) exhibits IC ₅₀ values of 0.07 μ M, 0.11 μ M, and 0.18 μ M against MDA-MB-231,

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Product Data Sheet

A549, and HeLa cancer cells, respectively, and over 10 μ M in Hep 5G cells^[1]. MMP2-IN-1 (10 μ M; 24 hours) induces cell cycle arrest in the S phase^[1]. MMP2-IN-1 (0.01 μ M, 0.1 μ M, 1 μ M and 10 μ M; 24 hours) induces a dose-dependent increment in early-and late-stage apoptosis of MDA-MB-231 cells, and increased the early-stage apoptosis percentage from 4.66% to 10.9% at 10 μ M^[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay

Cell Line:	MDA-MB-231, A549, HeLa and Hep 5G cells ^[1]
Concentration:	0-10 μΜ
Incubation Time:	74 hours
Result:	Exhibited IC $_{50}$ values of 0.07 μ M, 0.11 μ M, and 0.18 μ M against MDA-MB-231, A549, and HeLa cancer cells, respectively, and over 10 μ M in Hep 5G cells.

Cell Cycle Analysis

Cell Line:	MDA-MB-231 ^[1]
Concentration:	10 µM
Incubation Time:	24 hours
Result:	Induced cell cycle arrest in the S phase.

Apoptosis Analysis

Cell Line:	MDA-MB-231 ^[1]
Concentration:	0.01 uM, 0.1 uM, 1 uM and 10 uM
Incubation Time:	24 nours
Result:	Induced a dose-dependent increment in early-and late-stage apoptosis of MDA-MB-231 cells, and increased the early-stage apoptosis percentage from 4.66% to 10.9% at 10 μ M.

In Vivo

MMP2-IN-1 (100 mg/kg, 150 mg/kg, 200 mg/kg, 250 mg/kg; IP, single) causes 0%, 30%, 50% and 60% mortality rate at dosing 100 mg/kg, 150 mg/kg, 200 mg/kg and 250 mg/kg respectively^[1].

MMP2-IN-1 (10 mg/kg; IP, daily, for 14 days) significantly inhibits tumor growth in metastatic 4T1 murine breast cancer model^[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Kunming mice (n = 10, half male and half female) ^[1]
Dosage:	100 mg/kg, 150 mg/kg, 200 mg/kg, 250 mg/kg
Administration:	IP, single
Result:	No mortality occurred after administration of 100 mg/kg, and the mortality rate was 30%, 50% and 60% at dosing 150 mg/kg, 200 mg/kg, 250 mg/kg respectively.
Animal Model:	Orthotopic 4T1 tumor-bearing mice ^[1]
Dosage:	10 mg/kg

Administration:	IP, daily, for 14 days
Result:	Significantly inhibited tumor growth in metastatic 4T1 murine breast cancer model.

REFERENCES

[1]. Chen C, Luo Y, Yin H, et al. Design, synthesis, and antitumor activity evaluation of novel acyl sulfonamide spirodienones. Bioorg Med Chem. 2022;60:116626.

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

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