Data Sheet (Cat.No.T74542)

TargetMol

YM458

Chemical Properties

CAS No. :	2770108-93-3
Formula:	C53H61ClN8O5S
Molecular Weight:	957.62
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	YM458, a potent dual inhibitor of EZH2 and BRD4, exhibits IC50 values of 490 nM and 34 nM, respectively. This compound effectively hinders cell proliferation and colony formation, while also inducing cell cycle arrest and apoptosis in solid tumor cells, making it a viable candidate for anticancer research [1].
Targets(IC50)	Apoptosis,Epigenetic Reader Domain,Histone Methyltransferase
In vitro	YM458 (compound D7) demonstrates antiproliferative effects on AsPC-1 pancreatic cancer cells, inhibiting growth with an IC50 value of 0.69 ± 0.16 μM after 6 days at concentrations ranging from 0 to 30 μM. At a dose of 1 μM over 72 hours, YM458 notably reduces H3K27me3 levels and c-Myc expression in AsPC-1 cells [1]. Furthermore, YM458 exhibits inhibitory activity against various solid tumor cell lines; specifically, it markedly diminishes the proliferation of A549 lung and HCT116 colorectal cancer cells at 1 μM within 4 to 6 days of treatment [1]. Additionally, YM458 at submicromolar ranges (0.05-0.4 μM) over 12 to 20 days dose-dependently impedes colony formation in AsPC-1, HCT116, and A549 cell lines [1].
In vivo	YM458 administered intraperitoneally (IP; 60 mg/kg; every other day, for 38 days) exhibited anticancer activity by inhibiting tumor growth in AsPC-1 and A549 cells, with rates of 38.6% and 62.3%, respectively [1]. In female BALB/c mice, pharmacokinetic parameters revealed after IP administration (80 mg/kg), YM458 had a half-life (t1/2) of 3.81 hours and reached its maximum concentration (Cmax) of 27126.3 ng/mL within 1 hour (Tmax), while oral administration (PO) of the same dosage resulted in a longer half-life (4.16 hours), lower peak concentration (4383.6 ng/mL), and a substantially reduced area under the curve (AUC 0-24) of 13509.1 ng/mL·h. The clearance rate (CL) was 4.88 mL/min/kg with an oral bioavailability (F) of 4.94% [1].

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.0443 mL	5.2213 mL	10.4426 mL
5 mM	0.2089 mL	1.0443 mL	2.0885 mL
10 mM	0.1044 mL	0.5221 mL	1.0443 mL
50 mM	0.0209 mL	0.1044 mL	0.2089 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.