Data Sheet (Cat.No.T61939)

TargetMol

Topo I/COX-2-IN-1

Chemical Properties

CAS No. :

Formula: C21H18ClFN2O3

Molecular Weight: 400.83

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	Topo I/COX-2-IN-1 (1H-30) is a potent Topo I/COX-2 inhibitor with IC50 values of 0.24 μM for COX-2 and 4.42 μM for Topo I. It induces apoptosis and inhibits cancer cell migration, demonstrating anti-cancer activity.
Targets(IC50)	Apoptosis,Others,Prostaglandin Receptor,Topoisomerase
In vitro	Topo I/COX-2-IN-1 (1H-30) exhibits potent anti-tumor properties by halting tumor cell proliferation and inducing apoptosis through a dose-responsive increase in caspase-3 activity over 24 hours (0-100 μM). At 0.04 to 0.37 μM over 48 hours, it significantly reduces cell migration, especially at 0.37 μM, and lowers MMP-9 expression in HGC-27 and RKO cells. At 10 μM concentration and 48-hour exposure, it inhibits the NF-κB signaling pathway activation in cancer cells. In various colon cancer cell lines (HGC-27, RKO, HT-29, SGC-7901, and CT26.WT), it demonstrates significant cell proliferation inhibition, with notable IC50 values. Apoptosis analysis reveals a marked increase in caspase-3 positive cells at 10 μM, indicating its apoptotic potency. Additionally, it induces cell cycle arrest in the G2/M phase, underscoring its multifaceted action against cancer cell growth and metastasis.
In vivo	Topo I/COX-2-IN-1 (1H-30), administered via intraperitoneal injection at 100 mg/kg twice daily for 14 days, can inhibit tumor growth in BALB/c mice with CT26.WT colon cancer cells by increasing caspase-3 and reducing MMP-9 and COX-2 levels, promoting apoptosis. This regimen significantly decreased tumor size and weight without affecting body weight or organ health. In SD rats, a single dose with the same dosage showed pharmacokinetic parameters: half-life (t 1/2) of 1.56 hours, time to maximum concentration (T max) of 0.67 hours, maximum serum concentration (C max) of 20.19 μg/mL, area under the curve from zero to last measurable concentration (AUC 0-t) of 18.20 mg/L h, and area under the curve from zero to infinity based on observed data (AUC 0 inf_obs) of 18.60 mg/L h.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.4948 mL	12.4741 mL	24.9482 mL
5 mM	0.499 mL	2.4948 mL	4.9896 mL
10 mM	0.2495 mL	1.2474 mL	2.4948 mL
50 mM	0.0499 mL	0.2495 mL	0.499 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.