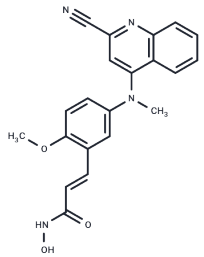
Data Sheet (Cat.No.T61524)

TargetMol

Tubulin/HDAC-IN-1

Chemical Properties



CAS No. : 2413587-26-3

Formula: C21H18N4O3

Molecular Weight: 374.39

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	Tubulin/HDAC-IN-1 is a dual inhibitor of tubulin and HDAC8, interacting with tubulin via CH/π interactions and with HDAC8 through hydrogen bonds. It effectively inhibits tubulin polymerization and selectively targets HDAC8 with an IC50 of 150 nM. Additionally, Tubulin/HDAC-IN-1 demonstrates cytotoxicity against various human cancer cells, induces cell cycle arrest in the G2/M phase, and triggers cell apoptosis, making it valuable for studying hematologic and solid tumors, including neuroblastoma and leukemia [1].
Targets(IC50)	Apoptosis,Others,Microtubule Associated,Mitochondrial Metabolism,HDAC
In vitro	Tubulin/HDAC-IN-1 (Compound 12a) exhibits pronounced cytotoxicity with an average IC50 of 0.6 nM across various human cancer cell lines. In HT29 cells, 2 nM application induces G2/M phase arrest and caspase-mediated apoptosis via mitochondrial dysfunction over 24 hours. The compound selectively inhibits HDAC8 with an IC50 of 150 nM, and also inhibits HDAC6 and HDAC11 at higher concentrations (1 μM and 1.9 μM, respectively). It increases γH2AX and acetylated SMC3 levels in a dose-dependent manner at 0.5-100 nM, indicating DNA damage and cell stress. Tubulin polymerization is impeded dose-dependently, particularly notable at 5-15 μM, and at 250 nM, it disrupts the microtubule network non-specifically. The compound shows good in vitro metabolic stability, observed in intrinsic clearance rates for rat and human liver microsomes. Comprehensive evaluation through cell proliferation assays and western blot analysis in HT-29 cells underscores its potential as a cancer therapeutic agent.
In vivo	Tubulin/HDAC-IN-1 (Compound 12a), administered intratumorally at 0.25 mg/kg three times weekly for two weeks, significantly reduced MCA205 tumor growth and improved overall survival in a C57BL/6 allogeneic sarcoma mouse model. The study [1] also evaluated 0.1 and 0.50 mg/kg dosages, showing decreased tumor growth and extended survival without evident adverse effects.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.671 mL	13.3551 mL	26.7101 mL
5 mM	0.5342 mL	2.671 mL	5.342 mL
10 mM	0.2671 mL	1.3355 mL	2.671 mL
50 mM	0.0534 mL	0.2671 mL	0.5342 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.

Tel:781-999-4286 E_mail:info@targetmol.com Address:34 Washington Street,Wellesley Hills,MA 02481