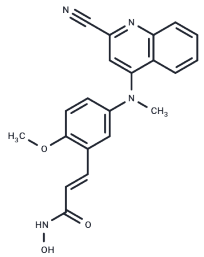
Data Sheet (Cat.No.T61524)

TargetMol
YOUR TARGET MOLECULES

Tubulin/HDAC-IN-1

Chemical Properties



CAS No. : 2413587-26-3

Formula: C21H18N4O3

Molecular Weight: 374.39

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	Tubulin/HDAC-IN-1 is a compound that functions as a dual inhibitor for tubulin and HDAC-IN-1. It achieves this by interacting with tubulin through CH/π interaction and with HDAC8 through hydrogen bond interaction. This compound 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. This compound is valuable for studying hematologic and solid tumors, including neuroblastoma and leukemia [1].
In vitro	Tubulin/HDAC-IN-1 (Compound 12a) demonstrates significant cytotoxicity across various human cancer cell lines, achieving an average IC 50 value of 0.6 nM. This compound induces G2/M phase cell cycle arrest and caspase-mediated apoptosis in HT29 cells, attributed to mitochondrial dysfunction, when applied at 2 nM for 24 hours. Moreover, Tubulin/HDAC-IN-1 selectively targets HDAC8 with an IC 50 value of 150 nM, while also inhibiting HDAC6 and HDAC11 at higher concentrations of 1 μM and 1.9 μM, respectively. At concentrations ranging from 0.5 to 100 nM over 24 hours or 30 minutes, it dose-dependently elevates γH2AX levels and acetylated SMC3 in HT-29 cells, indicating DNA damage and cell stress. Additionally, Tubulin/HDAC-IN-1 impedes tubulin polymerization in a dose-dependent manner, especially notable at concentrations between 5 and 15 μM, and at 250 nM, it effectively disassembles the cell microtubule network, though non-specifically. The compound also exhibits favorable in vitro metabolic stability, evidenced by its intrinsic clearance rates in both rat liver microsomes (RLM) and human liver microsomes (HLM). Its effects have been thoroughly evaluated through cell proliferation assays across various tumor cell lines and through western blot analysis in HT-29 cells, further demonstrating its potential as a therapeutic agent in cancer treatment.
In vivo	Tubulin/HDAC-IN-1 (Compound 12a), when administered via intratumoral injection at a dosage of 0.25 mg/kg three times weekly for two weeks, significantly reduced the growth of MCA205 tumors and improved overall survival in an allogeneic sarcoma mouse model using C57BL/6 mice. This study, referenced [1], evaluated dosages of 0.1, 0.25, and 0.50 mg/kg, revealing that treatment not only decreased tumor growth but also 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.

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