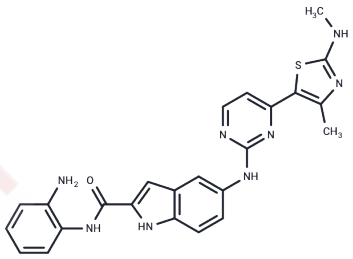
Data Sheet (Cat.No.T207433)

TargetMol

CDK9/HDAC1/HDAC3-IN-1

Chemical Properties



CAS No. : 2197029-81-3

Formula: C24H22N8OS

Molecular Weight: 470.55

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	CDK9/HDAC1/HDAC3-IN-1 is a dual inhibitor targeting CDK9 and HDAC enzymes. It potently suppresses the activity of CDK9, HDAC1, and HDAC3, with IC50 values of 0.17 μM, 1.73 μM, and 1.11 μM, respectively. The compound inhibits cancer cell growth by inducing apoptosis and causing cell cycle arrest at the G2/M phase. In a mouse model using TNBC MDA-MB-231 xenografts, it effectively hinders tumor progression. This compound exhibits broad-spectrum anticancer effects, notably against breast cancer, cervical cancer, and liver cancer.
Targets(IC50)	Apoptosis,HDAC,CDK
In vitro	CDK9/HDAC1/HDAC3-IN-1 (Compound 13EA) exhibits potent antiproliferative activity across various cancer cell lines, with IC50 values of 1.51 μM in HeLa, 2.47 μM in MDA-MB-231, and 4.52 μM in HepG2 cells. In MDA-MB-231 cells at concentrations ranging from 0.625 to 5 μM over 24 hours, it suppresses p-Ser2 mRNA expression in a time- and dose-dependent manner. Additionally, CDK9/HDAC1/HDAC3-IN-1 significantly reduces p-Ser2 (a substrate of CDK9) protein expression while increasing Ac-H3 (a substrate of HDAC) protein levels in both MDA-MB-231 and HeLa cells. The compound, at concentrations of 0.625 to 5 μM over 24 hours, induces concentration-dependent mitochondrial apoptosis, elevates cleaved PARP expression, and causes cell cycle arrest at the G2/M phase in MDA-MB-231 and HeLa cells.
In vivo	CDK9/HDAC1/HDAC3-IN-1, administered via intraperitoneal injection at a dosage of 30 mg/kg once daily for 10 days, significantly inhibits tumor growth in the MDA-MB-231 xenograft mouse model.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.1252 mL	10.6259 mL	21.2517 mL
5 mM	0.425 mL	2.1252 mL	4.2503 mL
10 mM	0.2125 mL	1.0626 mL	2.1252 mL
50 mM	0.0425 mL	0.2125 mL	0.425 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.