Data Sheet (Cat.No.T78708)

TargetMol

JAK/HDAC-IN-2

Chemical Properties

CAS No. :

Formula: C28H38N6O5S

Molecular Weight: 570.7

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	JAK/HDAC-IN-2, a potent 2-amino-4-phenylaminopyrimidine dual-target inhibitor, effectively suppresses JAK1/2 and HDAC3/6 at nanomolar concentrations. This compound exhibits proapoptotic properties, inhibits histone deacetylation, and impedes STAT3 phosphorylation, demonstrating notable antiproliferative activity against various hematological malignancies and solid tumors [1].
Targets(IC50)	Apoptosis,HDAC,JAK
In vitro	JAK/HDAC-IN-2 exhibited potent antiproliferative effects against K562, HL-60, and HEL cell lines with IC50 values of 1.87, 2.26, and 0.33 μM, respectively; it also inhibited the proliferation of solid tumor cell lines MCF-7, HeLa, A549, and PC-3 with IC50 values of 1.83, 2.88, 0.73, and 2.52 μM [1]. Additionally, JAK/HDAC-IN-2 demonstrated excellent pro-apoptotic activity in HEL cells and moderate pro-apoptotic activity in A549 cells at a concentration of 1.5 μM over 24 hours [1]. The compound effectively suppressed histone deacetylation and STAT3 phosphorylation in hematological malignancy HEL cells and solid tumor A549 cells at the same concentration and duration by inhibiting HDAC and JAK pathways [1].
In vivo	JAK/HDAC-IN-2 (Compound 21; 50 mg/kg; intraperitoneal injection; once daily; for 18 consecutive days) demonstrated effective antitumor activity in vivo against hematologic malignancy HEL and solid tumor A549 [1]. The pharmacokinetic parameters of LSD1-IN-14 in male Sprague-Dawley rats were as follows [1]: IV (3 mg/kg) and PO (15 mg/kg) yielded Tmax values of 2.912 hours and Cmax levels at 93.328 ng/mL, respectively. AUC0-t was 656.241 ng/mL*h for IV and 745.249 ng/mL*h for PO administration. The t1/2 was 0.128 hours for IV and 2.084 hours for PO, with clearance (CL) of 4.571 L/kg*h IV and 4.56 L/kg*h PO, and a steady-state volume of distribution (Vss) of 0.845 L/kg. The oral bioavailability (F) was determined to be 22.71%.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.7522 mL	8.7612 mL	17.5223 mL
5 mM	0.3504 mL	1.7522 mL	3.5045 mL
10 mM	0.1752 mL	0.8761 mL	1.7522 mL
50 mM	0.035 mL	0.1752 mL	0.3504 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.

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