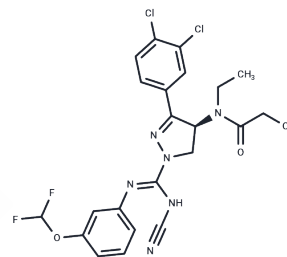


BAY-598

Chemical Properties

CAS No. : 1906919-67-2
 Formula: C₂₂H₂₀Cl₂F₂N₆O₃
 Molecular Weight: 525.34
 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	BAY 598 is a potent and selective competitive inhibitor of SMYD2 lysine methyltransferase, IC ₅₀ values are 27 and 58 nM for biochemical and cellular activity assays, respectively.
Targets(IC ₅₀)	Histone Methyltransferase
In vitro	METHODS: PDAC cells SW1990 and MIA PaCa2 were treated with BAY-598 (10 μM) and doxorubicin (1 μM) for 48 h. Cell viability was determined by MTT assay. RESULTS: PDAC cells were highly sensitive to acute treatment with the low-dose combination of doxorubicin and BAY-598. [1]
In vivo	METHODS: To detect antitumor activity in vivo, BAY-598 (50 mg/kg once daily) and gemcitabine (100 mg/kg every three days) were administered intraperitoneally to NSG mice bearing SW1990 xenografts for 27 days. RESULTS: The combination of gemcitabine and BAY-598 attenuated the growth of SW1990 xenografts compared to monotherapy. [1] METHODS: To assay anti-tumor activity in vivo, BAY-598 (10-100 mg/kg, PEG 400/water 8:2) was administered orally to BALB/c nude mice bearing KYSE-150 xenografts once daily for three days. RESULTS: BAY-598 was able to inhibit SMYD2 methylation activity in tumor cells in vivo. [2]

Solubility Information

Solubility	DMSO: 125 mg/mL (237.94 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 4 mg/mL (7.61 mM), Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.9035 mL	9.5176 mL	19.0353 mL
5 mM	0.3807 mL	1.9035 mL	3.8071 mL
10 mM	0.1904 mL	0.9518 mL	1.9035 mL
50 mM	0.0381 mL	0.1904 mL	0.3807 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.

Reference

Reynoird N, et al. Coordination of stress signals by the lysine methyltransferase SMYD2 promotes pancreatic cancer. *Genes Dev.* 2016 Apr 1; 30(7):772-85.

Eggert E, et al. Discovery and Characterization of a Highly Potent and Selective Aminopyrazoline-Based in Vivo Probe (BAY-598) for the Protein Lysine Methyltransferase SMYDJ *Med Chem.* 2016 May 26; 59(10):4578-600.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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