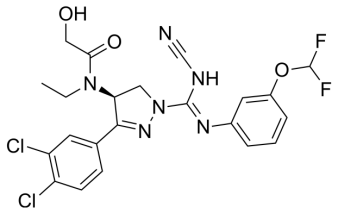
BAY-598

Cat. No.:	HY-19546
CAS No.:	1906919-67-2
Molecular Formula:	$C_{22}H_{20}Cl_2F_2N_6O_3$
Molecular Weight:	525.34
Target:	Histone Methyltransferase
Pathway:	Epigenetics
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (237.94 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
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

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (3.96 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (3.96 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BAY-598 is selective small molecule inhibitor of SMYD2 with an IC_{50} of 27 nM[1][2].

IC_{50} & Target

SMYD2

In Vitro

BAY-598 treatment blocks in vitro methylation of MAPKAPK3 by SMYD2 but has no activity against the SMYD2-related KMT SMYD3. BAY-598 treatment reduces the growth of Kras;p53 mutant PDAC cells after 9 d in culture but has little impact on the growth of Kras;p53;Smyd2 mutant cells[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Kinase Assay [1]	For SMYD2 inhibition, 10 μL of BAY-598 or DMSO is first incubated with recombinant SMYD2 in methylation buffer reaction for 1 h at 30°C, and then 2 μCi of ^{3}H-AdoMet is added to the mix and incubated overnight at 30°C. The reaction mixture is resolved by SDS-PAGE followed by autoradiography, Coomassie stain, or MS analysis[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Cell Assay [1]	Cells are seeded in 96-well plates at 2000 cells per well (optimum density for growth) in a total volume of 100 μL of medium containing 2% fetal bovine serum. Serially diluted BAY-598 in 100 μL of medium is added to the cells 12 h later. After 72 h of incubation, cell viability is assessed by an MTT assay according to the manufacturer's instructions[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Pharmacol Res. 2022 Feb 8;177:106122.
- Cell Death Dis. 2022 Jan 12;13(1):52.
- Acta Pharmacol Sin. 2021 Apr 13.
- Cells. 2022 Apr 8;11(8):1262.
- bioRxiv. 2023 Apr 3.

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REFERENCES

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

[2]. 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 SMYD2. J Med Chem. 2016 May 26;59(10):4578-600.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA