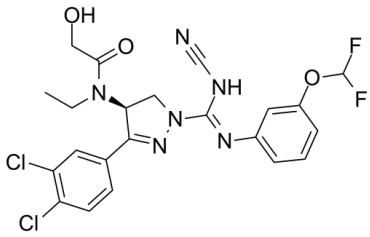
Data Sheet

Product Name:	BAY-598
Cat. No.:	CS-0015642
CAS No.:	1906919-67-2
Molecular Formula:	C22H20Cl2F2N6O3
Molecular Weight:	525.34
Target:	Histone Methyltransferase
Pathway:	Epigenetics
Solubility:	DMSO : 125 mg/mL (237.94 mM; Need ultrasonic); H2O : < 0.1 mg/mL (insoluble)



BIOLOGICAL ACTIVITY:

BAY-598 is selective small molecule inhibitor of **SMYD2** with an **IC_{50}** of 27 nM[1][2]. IC50 & Target: IC50: 27 nM (SMYD2)[2] **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].

PROTOCOL (Extracted from published papers and Only for reference)

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]. **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].

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.

CAIndexNames:

Acetamide, N-[(4S)-1-[(cyanoamino)[[3-(difluoromethoxy)phenyl]imino]methyl]-3-(3,4-dichlorophenyl)-4,5-dihydro-1H-pyrazol-4-yl]-N-ethyl-2-hydroxy-

SMILES:

ClC1=C(Cl)C=CC(C2=NN(/C(NC#N)=N/C3=CC=CC(OC(F)F)=C3)C[C@@H]2N(C(CO)=O)CC)=C1

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

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