TOCRIS
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Print Date: Mar 23rd 2021

Certificate of Analysis

www.tocris.com

Product Name: **BAY 598** **Catalog No.: 5991** **Batch No.: 1**

CAS Number: 1906919-67-2

IUPAC Name: *N*-[(4*S*)-1-[(Cyanoamino)[[3-(difluoromethoxy)phenyl]imino]methyl]-3-(3,4-dichlorophenyl)-4,5-dihydro-1*H*-pyrazol-4-yl]-*N*-ethyl-2-hydroxyacetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{20}Cl_2F_2N_6O_3$

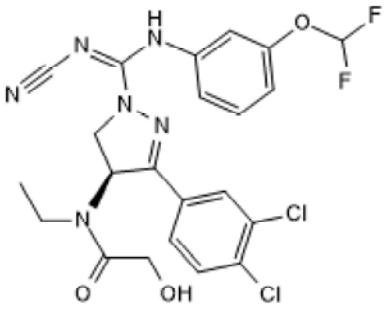
Batch Molecular Weight: 525.34

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol to 20 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

Chiral HPLC: Shows 98.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -89.9 (Concentration = 0.44, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.3	3.84	16
Found	50.46	3.82	15.89

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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), which displays >100-fold selectivity for SMYD2 over a panel of 32 other methyltransferases including SMYD3, SUV420H1, and SUV420H2. BAY 598 enhances apoptotic responses to doxorubicin (Cat. No. 2252) in cancer cell lines, and decreases p53K370me levels in HEK293 cells. It also reduces methylation in tumor cells in a mouse xenograft model. To request the negative control for BAY 598, please fill out the BAY 369 request form on the SGC website. Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:

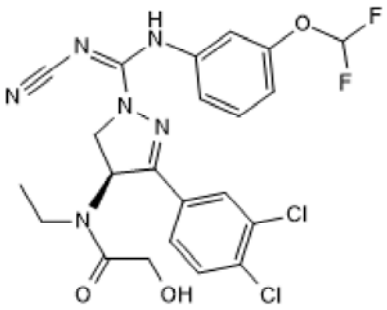
Batch Molecular Formula: $C_{22}H_{20}Cl_2F_2N_6O_3$

Batch Molecular Weight: 525.34

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 20 mM with gentle warming

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the BAY 598 probe summary on the SGC website.

References:

Scheer *et al* (2019) A chemical biology toolbox to study protein methyltransferases and epigenetic signaling. Nat.Commun. ***10*** 19. PMID: 30604761.

Eggert *et al* (2016) 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. ***59*** 4578. PMID: 27075367.