

Product Name: AS 99

Catalog No.: 7648

Batch No.: 1

CAS Number: 2323623-93-2

IUPAC Name: *N*-[[3-[3-(Aminothioxomethyl)phenyl]-1-[1-[(trifluoromethyl)sulfonyl]-4-piperidinyl]-1*H*-indol-6-yl]methyl]-1-methyl-3-azetidincarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₃₀F₃N₅O₃S₂·½H₂O

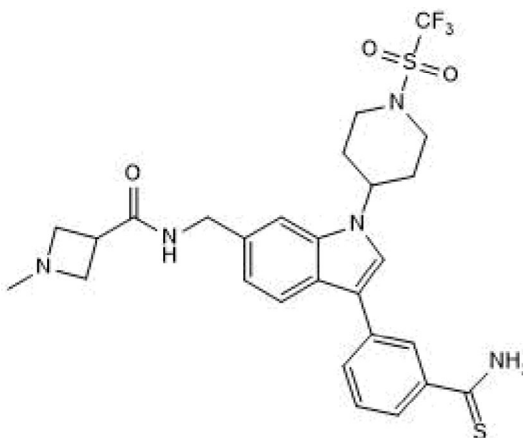
Batch Molecular Weight: 602.69

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.81	5.18	11.62
Found	53.25	4.88	11.38

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

AS 99 is a selective ASH1L histone methyltransferase inhibitor ($IC_{50} = 0.79 \mu M$); it binds to the autoinhibitory loop region in the SET domain ($K_d = 0.89 \mu M$). AS 99 exhibits >100-fold selectivity for ASH1L over a range of lysine methyltransferases; no significant inhibition is observed at 50 μM against a panel of 20 histone methyltransferases, including NSD1, NSD2, NSD3, and SETD2. In leukemia cells, AS 99 blocks H3K36 methylation, and causes a dose-dependent downregulation of MLL fusion target genes; it also induces apoptosis and differentiation and inhibits cell proliferation. AS 99 reduces leukemia burden in the xenotran... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

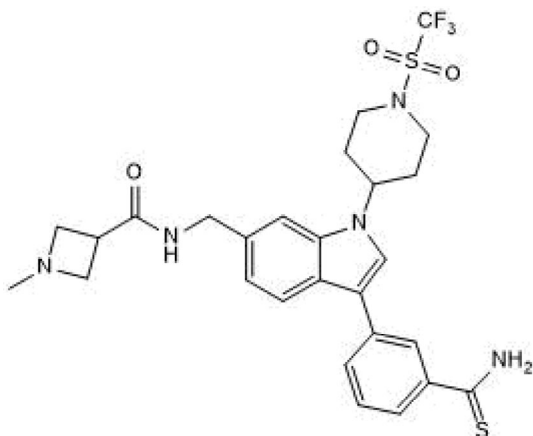
Batch Molecular Formula: $C_{27}H_{30}F_3N_5O_3S_2 \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 602.69

Physical Appearance: Yellow solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



References:

Rogawski *et al* (2021) Discovery of first-in-class inhibitors of ASH1L histone methyltransferase with anti-leukemic activity. *Nat. Commun* **12** 2792. PMID: 33990599.

Storage: Store at $-20^{\circ}C$

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

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

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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 $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:

Sold under license from the University of Michigan

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