

Product Name: EPZ 004777

Catalog No.: 5567

Batch No.: 2

CAS Number: 1338466-77-5

IUPAC Name: 7-[5-Deoxy-5-[[3-[[[4-(1,1-dimethylethyl)phenyl]amino]carbonyl]amino]propyl](1-methylethyl)amino]-β-D-ribofuranosyl]-7H-pyrrolo[2,3-d]pyrimidin-4-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₄₁N₇O₄ · 1¼H₂O

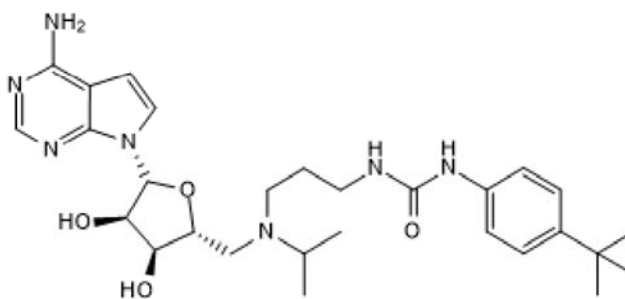
Batch Molecular Weight: 562.19

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.82	7.8	17.44
Found	59.76	7.87	17.4

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Description:

Highly potent DOT1L inhibitor (IC₅₀ = 0.4 nM). Exhibits >1000-fold selectivity for DOT1L over a panel of other methyltransferases. Selectively inhibits proliferation and induces apoptosis of MLL-rearranged cells in vitro. Prolongs survival in a MLL xenograft mouse model. Enhances efficiency of Yamanaka-factor factor reprogramming of fibroblasts by 3-4-fold.

Physical and Chemical Properties:

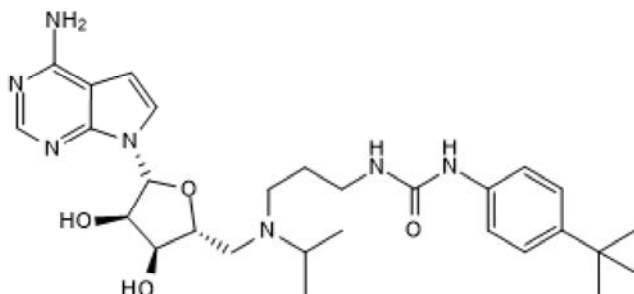
Batch Molecular Formula: C₂₈H₄₁N₇O₄·1¼H₂O

Batch Molecular Weight: 562.19

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Onder *et al* (2012) Chromatin-modifying enzymes as modulators of reprogramming. *Nature* **483** 598. PMID: 22388813.

Yu *et al* (2012) Catalytic site remodelling of the DOT1L methyltransferase by selective inhibitors. *Nat.Commun.* **3** 1288. PMID: 23250418.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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°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:

Sold under license from Epizyme, Inc.

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