

Product Name: SGC 0946

Catalog No.: 4541

Batch No.: 1

IUPAC Name: 1-[3-[[[(2*R*,3*S*,4*R*,5*R*)-5-(4-Amino-5-bromo-7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl](isopropyl)amino]propyl]-3-[4-(2,2-dimethylethyl)phenyl]urea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₄₀BrN₇O₄·½H₂O

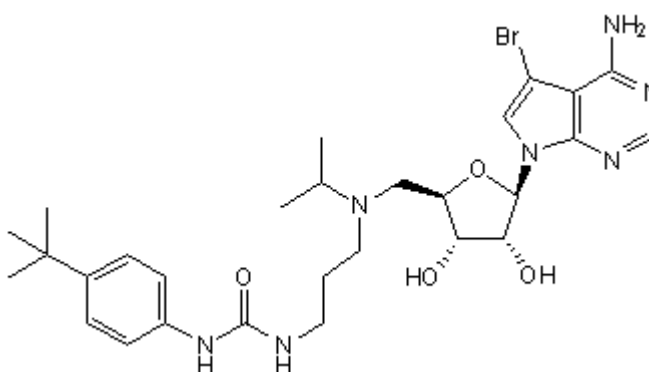
Batch Molecular Weight: 627.58

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.61 (Dichloromethane:Methanol:Ammonia soln. [90:9:1])

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	53.59	6.58	15.62
Found	53.76	6.64	15.34

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

Tocris Bioscience is an R&D Systems company
USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373
www.RnDSystems.com

R&D
SYSTEMS®

Product Name: SGC 0946

Catalog No.: 4541

Batch No.: 1

IUPAC Name: 1-[3-[[[(2*R*,3*S*,4*R*,5*R*)-5-(4-Amino-5-bromo-7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl](isopropyl)amino]propyl]-3-[4-(2,2-dimethylethyl)phenyl]urea

Description:

Potent DOT1L methyltransferase inhibitor ($K_D = 0.06$ nM, $IC_{50} = 0.3$ nM in a radioactive assay); blocks H3K79 methylation in A431 cells and MCF10A cells (IC_{50} values are 2.65 and 8.8 nM respectively). Inactive at 12 histone methyltransferases and DNMT1. Selectively kills cells transformed with the MLL-AF9 fusion oncogene in an in vitro model of leukemia; lowers levels of MLL target genes HOXA9 and Meis1.

Physical and Chemical Properties:

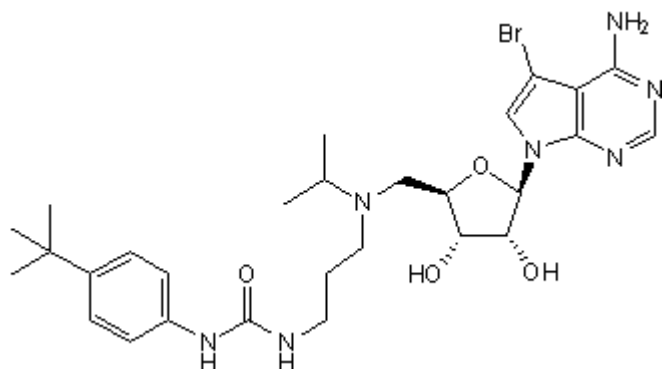
Batch Molecular Formula: $C_{28}H_{40}BrN_7O_4 \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 627.58

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



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.

References:

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

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

Tocris Bioscience is an R&D Systems company
USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373
www.RnDSystems.com

R&D
SYSTEMS®