TOCRIS
a bio-techne brand

Print Date: Jul 27th 2020

Certificate of Analysis

www.tocris.com

Product Name: **SGC 0946** **Catalog No.: 4541** **Batch No.: 2**

CAS Number: 1561178-17-3

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: $C_{28}H_{40}BrN_7O_4.¾H_2O$

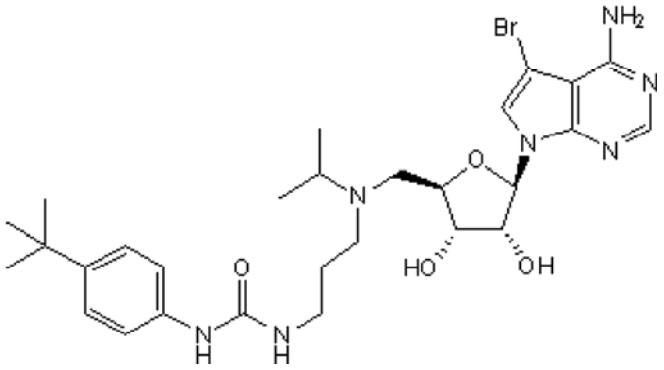
Batch Molecular Weight: 632.08

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.21	6.62	15.51
Found	52.84	6.55	15.26

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

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

Product Information

Product Name: **SGC 0946** **Catalog No.: 4541** **Batch No.: 2**

CAS Number: 1561178-17-3

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:

Highly 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. 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. To request the negative control for SGC0946, please fill out the SGC0649 request form on the SGC website.

Physical and Chemical Properties:

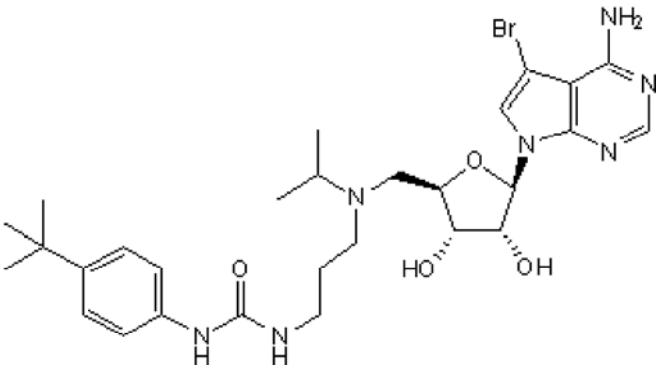
Batch Molecular Formula: $C_{28}H_{40}BrN_7O_4.¾H_2O$

Batch Molecular Weight: 632.08

Physical Appearance: Off 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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the SGC 0946 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.

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