

Certificate of Analysis

Print Date: Sep 12th 2019

www.tocris.com

Product Name: ZLD 1039 Catalog No.: 5847 Batch No.: 1

CAS Number: 1826865-46-6

IUPAC Name: 3-[Ethyl(tetrahydro-2*H*-pyran-4-yl)amino]-*N*-[(2,3,5,6,7,8-hexahydro-1-methyl-3-oxo-4-isoquinolinyl)methyl]-2-

methyl-5-[6-(4-methyl-1-piperazinyl)-3-pyridinyl]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{36}H_{48}N_6O_3.1/2H_2O$

Batch Molecular Weight: 621.81 **Physical Appearance:** White solid

Solubility: DMSO to 20 mM with gentle warming

ethanol to 20 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 69.54 7.94 13.52 Found 69.46 7.62 13.5



Product Information

Print Date: Sep 12th 2019

www.tocris.com

Product Name: ZLD 1039 Catalog No.: 5847 Batch No.: 1

CAS Number: 1826865-46-6

IUPAC Name: 3-[Ethyl(tetrahydro-2*H*-pyran-4-yl)amino]-*N*-[(2,3,5,6,7,8-hexahydro-1-methyl-3-oxo-4-isoquinolinyl)methyl]-2-

methyl-5-[6-(4-methyl-1-piperazinyl)-3-pyridinyl]benzamide

Description:

Potent and selective EZH2 inhibitor (IC_{50} = 5.6 nM). Displays selectivity against a panel of HMTs (inhibition less than 30% at 16 μ M). Blocks H3K27 methylation in breast cancer cell lines. Induces tumor regression and metastasis in breast cancer xenograft-bearing mice. Reactivates silenced tumor suppressors in vivo. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₃₆H₄₈N₆O₃.½H₂O

Batch Molecular Weight: 621.81 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 mM with gentle warming 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.

References:

Song et al (2016) Corrigendum: Selective inhibition of EZH2 by ZLD1039 blocks H3K27methylation and leads to potent anti-tumor activity in breast cancer. Sci.Rep. **29** 24893. PMID: 27128979.

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