Print Date: Dec 13th 2017

Certificate of Analysis

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Product Name: **GSK J1** **Catalog No.: 4593** **Batch No.: 1**

CAS Number: 1373422-53-7

IUPAC Name: *N*-[2-(2-Pyridinyl)-6-(1,2,4,5-tetrahydro-3*H*-3-benzazepin-3-yl)-4-pyrimidinyl]-β-alanine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{23}N_5O_2.3H_2O$

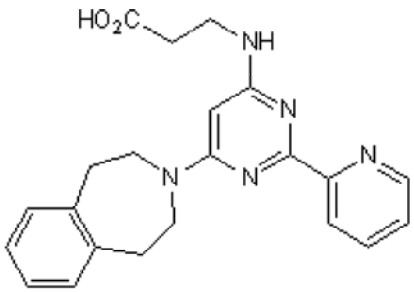
Batch Molecular Weight: 443.5

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.19 (Dichloromethane:Methanol [9:1])

HPLC: Shows >99.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.58	6.59	15.79
Found	59.7	6.3	15.94

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Product Information

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Description:

Potent inhibitor of the H3K27 histone demethylases JMJD3 (KDM6B) and UTX (KDM6A) (IC_{50} values are 28 and 53 nM respectively). Also inhibits KDM5B, KDM5C and KDM5A (IC_{50} values are 170, 550 and 6,800 nM respectively). Exhibits no activity against a panel of other histone demethylases (IC_{50} >20 μM), and displays no significant inhibitory activity against 100 protein kinases at a concentration of 30 μM. Ethyl ester derivative and Negative Control also available.

Physical and Chemical Properties:

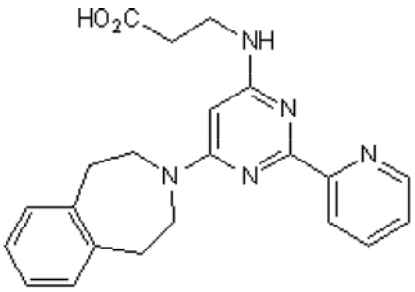
Batch Molecular Formula: $C_{22}H_{23}N_5O_2.3H_2O$

Batch Molecular Weight: 443.5

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at RT

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 GSK J1 probe summary on the SGC website.

References:

Heinemann *et al* (2014) Inhibition of demethylases by GSK-J1/J4. Nature ***514*** E1. PMID: 25279926.

Kruidenier *et al* (2012) A selective jumonji H3K27 demethylase inhibitor modulates the proinflammatory macrophage response. Nature ***488*** 404. PMID: 22842901.