Certificate of Analysis

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Print Date: Dec 13th 2017

Product Name: GSK J4

Catalog No.: 4594

Batch No.: 2

CAS Number: 1373423-53-0

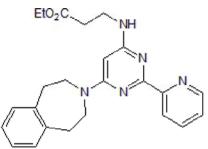
IUPAC Name: N-[2-(2-Pyridinyl)-6-(1,2,4,5-tetrahydro-3*H*-3-benzazepin-3-yl)-4-pyrimidinyl]- β -alanine ethyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

 $C_{24}H_{27}N_5O_2$ 417.5 White solid DMSO to 100 mM ethanol to 100 mM Store at RT

Storage: **Batch Molecular Structure:**



2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: **Microanalysis:**

Shows >99.6% purity Consistent with structure Consistent with structure

	Carbon	Hydrogen	Nitrogen
Theoretical	69.04	6.52	16.77
Found	69.15	6.74	16.62

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

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CAS Number: 1373423-53-0

N-[2-(2-Pyridinyl)-6-(1,2,4,5-tetrahydro-3H-3-benzazepin-3-yl)-4-pyrimidinyl]-β-alanine ethyl ester

Description:

IUPAC Name:

Histone lysine demethylase (KDM) inhibitor; blocks demethylation of histone H3K27. Attenuates lipopolysaccharide (LPS)-induced proinflammatory cytokine production in primary human macrophages (IC₅₀ = 9 μ M for the inhibition of TNF α release). Cell permeable. Ethyl ester derivative of GSK J1. Negative Control also available.

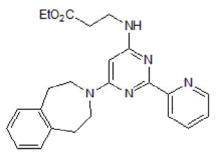
Physical and Chemical Properties:

Batch Molecular Formula: $C_{24}H_{27}N_5O_2$ Batch Molecular Weight: 417.5 Physical Appearance: White solid

Minimum Purity: >99%

References:

Batch Molecular Structure:



Storage: Store 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 of GSK J4, a cell permeable derivative of GSK J1, please visit the GSK J1 probe summary on the SGC website.

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.

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