



Certificate of Analysis

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Product Name: GSK J4 Catalog No.: 4594 Batch No.: 1

CAS Number: 1373423-53-0

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{27}N_5O_2$

Batch Molecular Weight: 417.5

Physical Appearance: White solid

Solubility: DMSO to 100 mM ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.36$ (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 69.04 6.52 16.77 Found 69.04 6.4 16.7



Product Information

Print Date: Oct 4th 2012

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Description:

Histone demethylase JMJD3/UTX inhibitor; blocks demethylation of histone H3K27. Attenuates lipopolysaccharide (LPS)-induced proinflammatory cytokine production in primary human macrophages (IC $_{50}$ = 9 μ M for the inhibition of TNF α release). Cell permeable. Ethyl ester derivative of GSK J1 (Cat. No. 4593).

Physical and Chemical Properties:

Batch Molecular Formula: C₂₄H₂₇N₅O₂ Batch Molecular Weight: 417.5 Physical Appearance: White solid

Minimum Purity: >99%

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.

References:

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

