

Certificate of Analysis

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Product Name: GSK J2

Catalog No.: 4688

Batch No.: 1

CAS Number: 1394854-52-4

IUPAC Name: *N*-[2-(3-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: C₂₂H₂₃N₅O₂·½H₂O

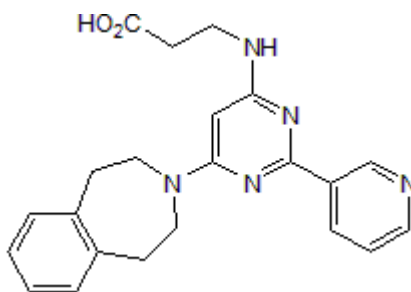
Batch Molecular Weight: 398.46

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
1eq. HCl to 50 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

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

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.32	6.07	17.58
Found	66.02	5.85	17.38

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Description:

Inactive control of GSK J1 (Cat No.4593) ($IC_{50} > 100 \mu M$ for inhibition of JMJD3/UTX). Cell permeable ester derivative, GSK J5 (Cat. No. 4689), also available.

Physical and Chemical Properties:

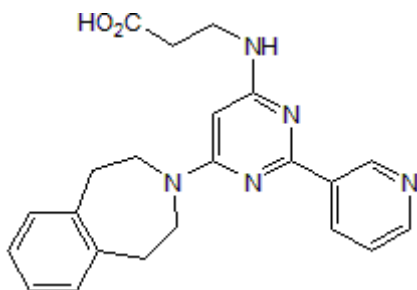
Batch Molecular Formula: $C_{22}H_{23}N_5O_2 \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 398.46

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 100 mM

1eq. HCl to 50 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.

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