



# **Certificate of Analysis**

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Product Name: GSK J5 HCI Catalog No.: 6935 Batch No.: 1

CAS Number: 1797983-32-4

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

## 1. PHYSICAL AND CHEMICAL PROPERTIES

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

Batch Molecular Weight: 453.97

Physical Appearance: Off White solid
Solubility: DMSO to 50 mM

ethanol to 20 mM with gentle warming

Storage: Store at RT

**Batch Molecular Structure:** 

# 2. ANALYTICAL DATA

**HPLC:** Shows 99.4% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 63.5 6.22 15.43 Found 63.83 6.41 15.71



# **Product Information**

Print Date: Jun 28th 2019

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

#### **Description:**

Inactive isomer of GSK J4 (Cat. No. 4594); also cell permeable ester derivative of the inactive control, GSK J2 (Cat. No. 4688). Active Analog also available.

## **Physical and Chemical Properties:**

Batch Molecular Formula: C24H27N5O2.HCI

Batch Molecular Weight: 453.97 Physical Appearance: Off White solid

Minimum Purity: >98%

#### **Batch Molecular Structure:**

Storage: Store at RT

#### Solubility & Usage Info:

DMSO to 50 mM

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.

#### **Licensing Information:**

This compound is supplied in conjunction with the Structural Genomics Consortium. For further characterization details of GSK J5, a cell permeable inactive isomer of GSK J1, please visit the GSK J1 probe summary on the SGC website.

#### References:

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

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