

Certificate of Analysis

Print Date: May 10th 2022

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Product Name: GSK 319347A Catalog No.: 5672 Batch No.: 1

CAS Number: 862812-98-4

IUPAC Name: 5-(5,6-Dimethoxy-1*H*-benzimidazol-1-yl)-3-[[2-(methylsulfonyl)phenyl]methoxy]-2-thiophenecarbonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{19}N_3O_5S_2.\frac{1}{4}H_2O$

Batch Molecular Weight: 474.03

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.25$ (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.74 4.15 8.86 Found 55.59 4.27 8.87



Product Information

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Description:

GSK 319347A is a potent and selective IKK ϵ inhibitor (pIC $_{50}$ = 7.4). Exhibits >100-fold selectivity for IKK ϵ over IKK α IKK β , and a range of other kinases.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₂H₁₉N₃O₅S₂.¹/₄H₂O

Batch Molecular Weight: 474.03

Physical Appearance: Pale yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:

N S CN

MeO Neo

Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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:

Bamborough *et al* (2006) 5-(1*H*-Benzimidazol-1-yl)-3-alkoxy-2-thiophenecarbonitriles as potent, selective, inhibitors of IKK-ε kinase. Bioorg.Med.Chem.Lett. *16* 6236. PMID: 16997559.