

Certificate of Analysis

Print Date: Jul 25th 2019

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Product Name: SC 514 Catalog No.: 3318 Batch No.: 1

CAS Number: 354812-17-2

IUPAC Name: 4-Amino-[2',3'-bithiophene]-5-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_9H_8N_2OS_2$

Batch Molecular Weight: 224.3

Physical Appearance: Pale yellow solid
Solubility: DMSO to 100 mM

ethanol to 10 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.7% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 48.2 3.59 12.49 Found 48.2 3.6 12.44



Product Information

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IUPAC Name: 4-Amino-[2',3'-bithiophene]-5-carboxamide

Description:

Orally active, ATP-competitive IKK β inhibitor (IC $_{50}$ = 3 - 12 μ M) that displays > 10-fold selectivity over 28 other kinases including JNK, p38, MK2 and ERK. Attenuates NF- κ B-induced gene expression of IL-6, IL-8 and COX-2 in synovial fibroblasts (IC $_{50}$ values are 20, 20 and 8 μ M respectively). Reduces iNOS induction and exhibits anti-inflammatory activity in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₉H₈N₂OS₂ Batch Molecular Weight: 224.3

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:

$$H_2N$$
 H_2N
 S

Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM ethanol to 10 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:

Sold for research purposes under agreement from AstraZeneca

References:

Gomez *et al* (2005) Selective inhibition of kappa B kinase-β aborgates induction of nitric oxide synthase in lipopolysaccharide-stimulated rat aortic smooth muscle cells. Br.J.Pharmacol. *146* 217. PMID: 15997236.

Baxter *et al* (2004) Hit-to-lead studies: the discovery of potent, orally active thiophenecarboxamide IKK-2 inhibitors. Bioorg.Med.Chem.Letts. *14* 2817.

Kishore *et al* (2003) A selective IKK-2 inhibitor blocks NF-κB-dependent gene expression in interleukin-1β-stimulated synovial fibroblasts. J.Biol.Chem. **278** 32861. PMID: 12813046.