1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $\text{C}_9\text{H}_8\text{N}_2\text{O}_2\text{S}_2$

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:

![Molecular Structure](image)

2. ANALYTICAL DATA

HPLC: Shows >98.7% purity

$^1$H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>48.2%</td>
<td>48.2%</td>
</tr>
<tr>
<td>H</td>
<td>3.59%</td>
<td>3.6%</td>
</tr>
<tr>
<td>N</td>
<td>12.49%</td>
<td>12.44%</td>
</tr>
</tbody>
</table>

Certificate of Analysis

Print Date: Apr 3rd 2013

www.tocris.com

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: SC 514
Catalog No.: 3318
Batch No.: 1

Product Information

CAS Number: 354812-17-2
IUPAC Name: 4-Amino-[2',3'-bithiophene]-5-carboxamide

Description:
Orally active, ATP-competitive IKK β inhibitor (IC₅₀ = 3 - 12 μM) that displays > 10-fold selectivity over 28 other kinases including JNK, p38, MK2 and ERK. Attenuates NF-κB-induced gene expression of IL-6, IL-8 and COX-2 in synovial fibroblasts (IC₅₀ values are 20, 20 and 8 μM respectively). Reduces iNOS induction and exhibits anti-inflammatory activity in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C₁₂H₁₀N₄O₃S₂
Batch Molecular Weight: 224.3
Physical Appearance: Pale yellow solid
Minimum Purity: >98%

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.

References:

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