Product Name: U0126 Catalo
g
No.: 1144 Batch No.: 5
CAS Number: 109511-58-2
IUPAC Name: 1,4-Diamo-no-2,3-dicyano-1,4-bis[2-aminophenylthio]butadiene

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{18}H_{16}N_{6}S_{2} \cdot 0.75C_{2}H_{5}OH \)
Batch Molecular Weight: 415.04
Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
Storage: Desiccate at +4°C

2. ANALYTICAL DATA

HPLC: Shows 99.0% purity
\(^1\)H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
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</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>56.43</td>
<td>56.23</td>
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<tr>
<td>Hydrogen</td>
<td>4.98</td>
<td>4.82</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>20.25</td>
<td>19.95</td>
</tr>
</tbody>
</table>

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

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**Product Information**

**Product Name:** U0126  
**CAS Number:** 109511-58-2  
**IUPAC Name:** 1,4-Diamino-2,3-dicyano-1,4-bis[2-aminophenylthio]butadiene

**Description:**  
Potent and selective non-competitive inhibitor of MAP kinase kinase. Inhibits MEK-1 and MEK-2 (IC50 values of 0.07 and 0.06 μM respectively) with little or no effect on the activities of PKC, Abl, Raf, MEKK, ERK, JNK, M KK-3, M KK-4/SEK, M KK-6, Cdk2 or Cdk4. Brain penetrant. Helps maintain human pluripotent stem cells in undifferentiated state. Also available as part of the MAPK Cascade Inhibitor Tocriset™ and MAPK Inhibitor Tocriset™. Negative control U0124 (Cat. No. 1868) also available.

**Physical and Chemical Properties:**  
**Batch Molecular Formula:** C16H16N6S2.0.75C2H5OH  
**Batch Molecular Weight:** 415.04  
**Physical Appearance:** Off White solid

**Batch Molecular Structure:**

![Molecular Structure](image)

**Storage:** Desiccate at +4°C

**Solubility & Usage Info:**  
DMSO to 100 mM  
CAUTION - This product has been shown to isomerise relatively rapidly once in solution, affecting its activity. Therefore, we recommend that, as far as possible, solutions should be made up and used within 24 hours. This product contains 1 molar equivalent of ethanol *Duncia et al (1998) MEK inhibitors: the chemistry and biological activity of U0126, its analogs, and cyclization products. Bioorg.Med.Chem.Lett. 8 2839.*

**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:**  