1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{13}\text{H}_{11}\text{N}_{3}\text{O}_2\cdot\frac{1}{4}\text{H}_2\text{O} \)

Batch Molecular Weight: 245.75

Physical Appearance: Orange solid

Solubility: DMSO to 100 mM, ethanol to 20 mM

Storage: Store at +4°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.28 \) (Dichloromethane:Methanol:Ammonia soln. [98:1:1])

HPLC: Shows 99.9% purity

\(^1\text{H} \) NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>63.54</td>
<td>4.72</td>
<td>17.1</td>
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<tr>
<td>Found</td>
<td>63.84</td>
<td>4.58</td>
<td>17.07</td>
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</table>
Product Name: SU 9516  
Catalog No.: 2907  
Batch No.: 2

CAS Number: 377090-84-1  
IUPAC Name: (Z)-1,3-Dihydro-3-(1H-imidazol-4-ylmethylene)-5-methoxy-2H-indol-2-one

Description:
Cyclin-dependent kinase (cdk) inhibitor (reported IC\textsubscript{50} values are 0.02 - 0.03, 0.04 - 0.2, 0.2 - 1.7 and 0.9 \mu \text{M} for cdk2, cdk1, cdk4 and cdk9, respectively). Inhibits pRb phosphorylation causing enhanced pRB/E2F complex formation and induces G1 and G2-M cell cycle arrest. Transcriptionally downregulates Mcl-1 and has antiproliferative, cytostatic and pro-apoptotic effects in vitro.

Physical and Chemical Properties:
Batch Molecular Formula: C\textsubscript{13}H\textsubscript{11}N\textsubscript{2}O\textsubscript{.4}H\textsubscript{2}O
Batch Molecular Weight: 245.75
Physical Appearance: Orange solid
Minimum Purity: >99%

Storage: Store at +4°C

Solubility & Usage Info:
DMSO to 100 mM
ethanol to 20 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 aliquotted 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: