1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{23}H_{18}N_4O_3 \cdot \frac{3}{4}H_2O \)
Batch Molecular Weight: 411.92
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM, ethanol to 50 mM
Storage: Store at +4°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.15 \) (Dichloromethane:Methanol:NH4OH [94:5:1])
HPLC: Shows 99.0% purity
\(^1\)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>67.06</td>
<td>4.77</td>
<td>13.6</td>
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<tr>
<td>Found</td>
<td>67.38</td>
<td>4.56</td>
<td>13.74</td>
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</table>
Product Name: D 4476

CAS Number: 301836-43-1
IUPAC Name: 4-[4-(2,3-Dihydro-1,4-benzodioxin-6-yl)-5-(2-pyridinyl)-1H-imidazol-2-yl]benzamide

Description:
Selective inhibitor of casein kinase 1 (CK1) and TGF-β type-I receptor (ALK5) that displays > 20-fold selectivity over SAPK2/p38 and a much greater selectivity over all other protein kinases tested. Suppresses site-specific phosphorylation and nuclear exclusion of FOXO1a.

Physical and Chemical Properties:
Batch Molecular Formula: C_{23}H_{19}N,O_{3.4}H_{2}O
Batch Molecular Weight: 411.92
Physical Appearance: Yellow solid
Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:
DMSO to 100 mM
ethanol to 50 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: