1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{17}\text{H}_{13}\text{NO}_3\cdot\frac{1}{2}\text{H}_2\text{O} \)

Batch Molecular Weight: 288.3

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

![Molecular Structure Image]

2. ANALYTICAL DATA

TLC: \( R_f = 0.18 \) (Dichloromethane:Methanol [19:1])

HPLC: Shows 99.5% 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>70.82</td>
<td>4.89</td>
<td>4.86</td>
</tr>
<tr>
<td>Found</td>
<td>71.21</td>
<td>4.66</td>
<td>4.97</td>
</tr>
</tbody>
</table>
Product Name: UPF 1069
CAS Number: 1048371-03-4
IUPAC Name: 5-(2-Oxo-2-phenylethoxy)-3,4-dihydroisoquinolin-1(2H)-one

Description:
Selective poly(ADP-ribose) polymerase (PARP) 2 inhibitor (IC₅₀ values are 0.3 and 8.0 μM for PARP-2 and PARP-1 respectively).

Physical and Chemical Properties:
Batch Molecular Formula: C₁₇H₁₂NO₅·½H₂O
Batch Molecular Weight: 288.3
Physical Appearance: White solid
Minimum Purity: >99%

Storage: Store at RT

Solubility & Usage Info:
DMSO to 100 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: