1. PHYSICAL AND CHEMICAL PROPERTIES

   Batch Molecular Formula: \( \text{C}_{15}\text{H}_{12}\text{N}_{2}\text{O}_{2} \cdot 0.1\text{H}_{2}\text{O} \)

   Batch Molecular Weight: 254.07

   Physical Appearance: Yellow solid

   Solubility: DMSO to 100 mM

   Storage: Desiccate at +4°C

   Batch Molecular Structure:

2. ANALYTICAL DATA

   TLC: \( R_f = 0.2 \) (Ethyl acetate:iso-Hexane [2:3])

   HPLC: Shows 99.5% purity

   \(^1\text{H} \text{NMR:}\) 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>Carbon</td>
<td>70.91</td>
<td>70.92</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.84</td>
<td>4.76</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>11.03</td>
<td>11.01</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: BYK 204165

CAS Number: 1104546-89-5

IUPAC Name: 4-[(1-Methyl-1H-pyrrol-2-yl)methylene]-1,3(2H,4H)-isoquinolinedione

Description:
Potent and selective poly(ADP-ribose) polymerase (PARP)-1 inhibitor (pIC₅₀ values are 5.38 and 7.35 for PARP-2 and PARP-1 respectively).

Physical and Chemical Properties:
Batch Molecular Formula: C₁₉H₁₂N₂O₄·0.1H₂O
Batch Molecular Weight: 254.07
Physical Appearance: Yellow solid

Minimum Purity: >99%

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: