1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{21}\text{H}_{24}\text{ClN}_{5}\text{O}_{2} \)

Batch Molecular Weight: 413.9

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

2. ANALYTICAL DATA

TLC: \( R_t = 0.67 \) (Dichloromethane:Methanol [9:1])

HPLC: Shows 98% purity

\(^1\)H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th>Component</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>60.94</td>
<td>60.63</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.84</td>
<td>5.84</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>16.92</td>
<td>16.74</td>
</tr>
</tbody>
</table>
**Product Name:** EC 144  
**CAS Number:** 911397-80-3  
**IUPAC Name:** 5-[2-Amino-4-chloro-7-[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]-7H-pyrrolo[2,3-d]pyrimidin-5-yl]-2-methyl-4-pentyn-2-ol

**Description:**
High affinity, potent and selective Hsp90 inhibitor (K_0 = 0.2 nM and IC_50 = 1.1 nM). Exhibits selectivity for Hsp90 over Grp94 and TRAP1 (K_0 values are 61 and 255 nM respectively) and has no effect (IC_50 > 10 μM) against a panel of 285 kinases. Depgrades Her-2 in MCF-7 breast cancer cells (EC_50 = 14 nM). Blocks tumor growth and induces partial tumor regression in an N87 gastric tumor mouse model. Also inhibits LPS-induced TNFα release in an LPS shock mouse model and suppresses disease development in a rat model of collagen-induced arthritis. Exhibits <20-fold efficacy over BIIB 021 (Cat. No. 4608) in mice. Orally available and brain penetrant.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C_{21}H_{23}ClN_{6}O_{2}
- **Batch Molecular Weight:** 413.9
- **Physical Appearance:** Pale yellow solid
- **Minimum Purity:** >98%

**Storage:** Store at -20°C

**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:**