Product Name: HKI 357
Catalog No.: 3580
Batch No.: 2

CAS Number: 848133-17-5
IUPAC Name: (2E)-N-[4-[4-[3-Chloro-4-[3-fluorophenyl]methoxy]phenyl]amino]-3-cyano-7-ethoxy-6-quinolinyl]-4-(dimethylamino)-2-butenamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{31}H_{29}ClF_{5}N_{5}O_{3}
Batch Molecular Weight: 574.05
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM, ethanol to 25 mM
Storage: Store at -20°C

2. ANALYTICAL DATA

TLC: $R_f = 0.17$ (Chloroform:Methanol [9:1])
HPLC: Shows 99% purity
$^1$H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Elemental Composition</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>64.86</td>
<td>65.1</td>
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<tr>
<td>Hydrogen</td>
<td>5.09</td>
<td>4.98</td>
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<tr>
<td>Nitrogen</td>
<td>12.2</td>
<td>12.28</td>
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</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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**Description:**
Potent, irreversible inhibitor of ErbB2 (HER2) and EGFR (IC\textsubscript{50} values are 33 and 34 nM respectively). Suppresses ligand-induced EGFR autophosphorylation and cell proliferation in NCI-H1975 cells containing L858R and T790M mutations. Circumvents mechanisms of resistance to Iressa (Cat. No. 3000) in non-small-cell lung cancer cells.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C\textsubscript{37}H\textsubscript{50}ClFN\textsubscript{2}O\textsubscript{3}
- **Batch Molecular Weight:** 574.05
- **Physical Appearance:** Off-white solid
- **Minimum Purity:** >98%
- **Storage:** Store at -20°C

**Solubility & Usage Info:**
- DMSO to 100 mM
- Ethanol to 25 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:**