1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{25}\text{H}_{23}\text{F}_3\text{N}_4\text{O}_2\cdot\frac{1}{4}\text{H}_2\text{O} \)

Batch Molecular Weight: 472.97

Physical Appearance: Off White solid

Solubility: DMSO to 75 mM

Storage: Store at +4°C

2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

\(^1\text{H NMR:}\) Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical: 63.49</td>
<td>5.01</td>
<td>11.85</td>
</tr>
<tr>
<td>Found: 63.38</td>
<td>4.85</td>
<td>11.81</td>
</tr>
</tbody>
</table>
Product Name: TAK 165
Catalog No.: 3599  Batch No.: 2
CAS Number: 366017-09-6
IUPAC Name: 1-[4-[[2-[(1E)-2-[4-(trifluoromethyl)phenyl]ethenyl]-4-oxazolyl]methoxy]phenyl]butyl]-1H-1,2,3-triazole

Description:
Potent, irreversible human epithelial growth factor receptor 2 (ErbB2) inhibitor (IC\textsubscript{50} = 6 nM) that displays > 4000-fold selectivity over EGFR, FGFR, PDGFR, JAK1 and Src. Exhibits potent antiproliferative effects in ErbB2-overexpressing cancer cell lines (IC\textsubscript{50} = 5 nM in BT474 breast cancer cells) and significantly inhibits bladder, breast and prostate cancer xenograft growth in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C\textsubscript{29}H\textsubscript{29}F\textsubscript{3}N\textsubscript{4}O\textsubscript{2}.\frac{1}{4}H\textsubscript{2}O
Batch Molecular Weight: 472.97
Physical Appearance: Off White solid
Minimum Purity: >99%

Storage:
Store at +4°C

Solubility & Usage Info:
DMSO to 75 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: