1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{35}H_{28}F_3N_5O_2 \cdot 1/4H_2O \)

Batch Molecular Weight: 612.12

Physical Appearance: Beige solid

Solubility: DMSO to 1 mM with gentle warming

Storage: Store at +4°C

2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

\(^1H\) 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>68.67</td>
<td>4.69</td>
<td>11.44</td>
</tr>
<tr>
<td>Found</td>
<td>68.61</td>
<td>4.47</td>
<td>11.33</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: Torin 1
Catalog No.: 4247  Batch No.: 5

CAS Number: 1222998-36-8
IUPAC Name: 1-[4-[4-(1-Oxopropyl)-1-piperazinyl]-3-(trifluoromethyl)phenyl]-9-(3-quinolinyl)-benzo[h]-1,6-naphthyridin-2(1H)-one

Description:
Potent and selective mTOR inhibitor (IC$_{50}$ = 2 - 10 nM for mTORC1 and mTORC2). Displays 200-fold selectivity for mTOR over DNA-PK, ATM and hVps34. Induces autophagy in HeLa cells.

Physical and Chemical Properties:
Batch Molecular Formula: C$_{35}$H$_{26}$F$_3$N$_5$O$_2$, ¼H$_2$O
Batch Molecular Weight: 612.12
Physical Appearance: Beige solid
Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:
DMSO to 1 mM with gentle warming

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.

Licensing Information:
Sold under license from Whitehead Institute for Biomedical Research.

References:
Peterson et al (2011) mTOR complex 1 regulates lipin 1 localization to control the SREBP pathway. Cell. 146 408. PMID: 21816276.