**1. PHYSICAL AND CHEMICAL PROPERTIES**

- **Batch Molecular Formula:** $C_{29}H_{29}F_3N_4O_3 \cdot 2HCl \cdot 2H_2O$
- **Batch Molecular Weight:** 647.51
- **Physical Appearance:** White solid
- **Solubility:** Water to 100 mM, DMSO to 100 mM
- **Storage:** Store at +4°C

**Batch Molecular Structure:**

![Molecular Structure Image]

**2. ANALYTICAL DATA**

- **TLC:** $R_f = 0.23$ (Dichloromethane:Methanol [9:1] (V/V) 2M NH₃)
- **HPLC:** Shows >98.6% purity
- **Chiral HPLC:** Shows >99.5% purity
- **$^1$H NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Optical Rotation:** $[\alpha]_D = +17.7$ (Concentration = 1, Solvent = Methanol)
- **Microanalysis:**
  
<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>53.79</td>
<td>53.77</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.45</td>
<td>5.41</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>8.65</td>
<td>8.64</td>
</tr>
</tbody>
</table>

---

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: ML 786 dihydrochloride  
Catalog No.: 5036  
Batch No.: 1

CAS Number: 1237536-18-3  
IUPAC Name: 3-(1-Amino-1-methylethyl)-N-[(2R)-1,2,3,4-tetrahydro-7-oxo-1,8-naphthridin-4-yl)oxy]-2-naphthalenyl]-5-benzamide dihydrochloride

Description:
Potent Raf kinase inhibitor (IC₅₀ values are 2.1, 2.5 and 4.2 nM for B-RafV600E, C-Raf and wild-type B-Raf respectively). Also inhibits Abl-1, DDR2, EPHA2 and RET tyrosine kinase activity. Inhibits pERK formation and attenuates tumor growth in melanoma cell xenografts expressing the B-RafV600E mutation in vivo. Orally bioavailable.

Physical and Chemical Properties:
Batch Molecular Formula: C₂₃H₂₀F₃N₄O₉·2HCl·2H₂O  
Batch Molecular Weight: 647.51  
Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:
- water to 100 mM
- 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: