1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{16}\text{H}_{19}\text{F}_{3}\text{N}_{4}\text{O}_{2}\cdot\text{HCl} \)

Batch Molecular Weight: 392.8

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Desiccate at RT

Batch Molecular Structure:

![Molecular Structure](image)

2. ANALYTICAL DATA

TLC: \( R_f = 0.25 \) (Chloroform:Methanol [9:1])

HPLC: Shows 99.2% purity

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

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>48.92</td>
<td>48.98</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.13</td>
<td>5.15</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>14.26</td>
<td>14.18</td>
</tr>
</tbody>
</table>
Product Information

**Product Name:** BIX NHE1 inhibitor

**Catalog No.:** 5512  
**Batch No.:** 1

**CAS Number:** 1422252-46-7  
**IUPAC Name:** 4-(1-Acetyl-4-piperidinyl)-N-(aminoiminomethyl)-3-(trifluoromethyl)benzamide hydrochloride

**Description:**

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C₁₇H₁₉F₃N₄O₄·HCl
- **Batch Molecular Weight:** 392.8
- **Physical Appearance:** White solid
- **Minimum Purity:** ≥98%
- **Batch Molecular Structure:**

![Molecular Structure](image)

**Storage:** Desiccate at RT

**Solubility & Usage Info:**
- **DMSO to 50 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:**