1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{21}\text{H}_{27}\text{N}_{3}\text{O}_{3}\text{S}.\text{2HCl} \)
Batch Molecular Weight: 474.44
Physical Appearance: White solid
Solubility:
- Water to 100 mM
- DMSO to 50 mM
Storage: Desiccate at RT

2. ANALYTICAL DATA

TLC: \( R_f = 0.25 \) (Dichloromethane:Methanol:Ammonia soln. [95:5:0.5])
HPLC: Shows >99.2% purity
\(^1\text{H NMR:}\) Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>53.16</td>
<td>53.05</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.16</td>
<td>6.33</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>8.85</td>
<td>8.76</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
**Product Name:** E-4031 dihydrochloride  
**Catalog No.:** 1808  
**Batch No.:** 3

### CAS Number: 113559-13-0  
### IUPAC Name:  
\[ N\text{-}\left[4\text{-}\left[1\text{-}\left[2\text{-}\left(6\text{-methyl}-2\text{-pyridinyl}\right)\text{ethyl}\right]-4\text{-piperidinyl}\right]\text{carbonyl}\right]\text{phenyl}\]\text{methanesulfonamid}e dihydrochloride

### Description:
Selective blocker of \(K\text{\textsubscript{1.1}}\) (hERG) channels; inhibits the rapid delayed-rectifier \(K^+\) current (\(I_{\text{Ks}}\)). Reversibly prolongs action potential duration in guinea pig papillary muscle and isolated ventricular myocytes, without affecting \(Na^+\) or \(Ca^{2+}\) inward currents. Class III antiarrhythmic agent.

### Physical and Chemical Properties:
- **Batch Molecular Formula:** \(C_{21}H_{22}N_6O_6S\cdot2HCl\)
- **Batch Molecular Weight:** 474.44
- **Physical Appearance:** White solid
- **Minimum Purity:** >98%
- **Batch Molecular Structure:**

![Molecular Structure Image]

### Storage:
Desiccate at RT

### Solubility & Usage Info:
- Water to 100 mM
- 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: