1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $\text{C}_{19}\text{H}_{16}\text{F}_2\text{N}_6\text{O}.\text{HCl}\cdot\frac{1}{4}\text{H}_2\text{O}$

**Batch Molecular Weight:** 423.33

**Physical Appearance:** Pale yellow solid

**Solubility:**
- Water to 25 mM
- DMSO to 100 mM

**Storage:** Store at $+4^\circ\text{C}$

**Batch Molecular Structure:**

![Molecular Structure](image)

2. ANALYTICAL DATA

**TLC:** $R_f = 0.4$ (Chloroform:Methanol [9:1])

**HPLC:** Shows 98.9% 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>53.91</td>
<td>53.89</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.17</td>
<td>4.03</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>19.85</td>
<td>19.83</td>
</tr>
</tbody>
</table>
Product Information

**Product Name:** AR-C 102222

**Catalog No.:** 3969  **Batch No.:** 1

**CAS Number:** 253771-21-0  
**IUPAC Name:** 5-[(4'-Amino-5',8'-difluorospiro[piperidine-4,2'(1'H)-quinaxolin]-1-yl)carbonyl]-2-pyridinecarbonitrile hydrochloride

**Description:**
Inducible nitric oxide synthase (iNOS) inhibitor; selective for iNOS over eNOS (IC₅₀ values are 0.037 and >100 μM for iNOS and eNOS respectively). Exhibits antinociceptive and anti-inflammatory activity in rodent pain models.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C₄₀H₃₅F₄N₁₀O₂·HCl·H₂O
- **Batch Molecular Weight:** 423.33
- **Physical Appearance:** Pale yellow solid
- **Minimum Purity:** >98%

**Solubility & Usage Info:**
- **water** to 25 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).

**References:**

**Storage:** Store at +4°C

**Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use**