1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** \(\text{C}_{19}\text{H}_{16}\text{F}_{2}\text{N}_{6}\text{O}.\text{HCl.} \frac{1}{4}\text{H}_{2}\text{O}\)
- **Batch Molecular Weight:** 423.33
- **Physical Appearance:** Pale yellow solid
- **Solubility:**
  - water to 25 mM
  - DMSO to 100 mM
- **Storage:** Store at +4°C

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:**
  - Theoretical: Carbon 53.91, Hydrogen 4.17, Nitrogen 19.85
  - Found: Carbon 53.89, Hydrogen 4.03, Nitrogen 19.83
Product Information

Product Name: AR-C 102222
Catalog No.: 3969
Batch No.: 1

CAS Number: 1781934-50-6
IUPAC Name: 5-[(4'-Amino-5',8'-difluoro[1H]-quinazolin-1-yl)carbonyl]-2-pyridinecarbonitrile hydrochloride

Description:
Inducible nitric oxide synthase (iNOS) inhibitor; selective for iNOS over eNOS (IC_{50} values are 0.037 and >100 μM for iNOS and eNOS respectively). Exhibits antinociceptive and anti-inflammatory activity in rodent pain models.

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Batch Molecular Weight: 423.33
Physical Appearance: Pale yellow solid
Minimum Purity: >98%

Storage: Store at +4°C

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).

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:
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References: