Product Name: VU 0360172 hydrochloride
Catalog No.: 4323
Batch No.: 3
CAS Number: 1309976-62-2
IUPAC Name: N-Cyclobutyl-6-[2-(3-fluorophenyl)ethynyl]-3-pyridinecarboxamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{18}\text{H}_{15}\text{FN}_2\text{O.HCl} \)
Batch Molecular Weight: 330.78
Physical Appearance: Off White solid
Solubility: DMSO to 50 mM
ethanol to 25 mM
Storage: Store at +4°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.45 \) (Ethyl acetate:Petroleum ether [2:3])
HPLC: Shows 98.9% purity
\(^1\)H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis: Carbon Hydrogen Nitrogen
Theoretical 65.36 4.88 8.47
Found 65.09 5.01 8.49
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**IUPAC Name:** N-Cyclobutyl-6-[2-(3-fluorophenyl)ethynyl]-3-pyridinecarboxamide hydrochloride

**Description:**
Positive allosteric modulator of mGlu$_5$ receptors ($EC_{50} = 16$ nM; $K_i = 195$ nM). Selective for mGlu$_5$; displays no significant activity at mGlu$_1$, mGlu$_2$ or mGlu$_4$ receptors. Exhibits antipsychotic-like activity in a rodent model. Also reduces spontaneous spike and wave discharges without affecting motor behaviour in a rat model of absence epilepsy.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C$_{18}$H$_{15}$FN$_2$O.HCl
- **Batch Molecular Weight:** 330.78
- **Physical Appearance:** Off White solid
- **Minimum Purity:** >98%
- **Batch Molecular Structure:**

![Molecular Structure](image)

**Storage:** Store at +4°C

**Solubility & Usage Info:**
- DMSO to 50 mM
- Ethanol to 25 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:**