

Product Name: VU 0360172 hydrochloride

Catalog No.: 4323

Batch No.: 2

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: C₁₈H₁₅FN₂O.HCl

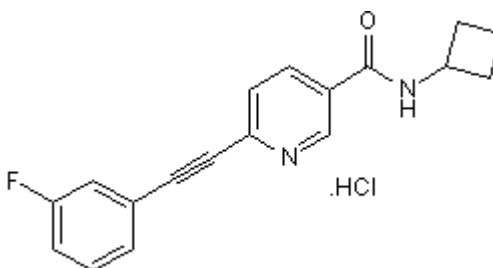
Batch Molecular Weight: 330.78

Physical Appearance: Yellow solid

Solubility: DMSO to 50 mM
ethanol to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.45 (Ethyl acetate:Petroleum ether [2:3])

HPLC: Shows 98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.36	4.88	8.47
Found	65.16	4.93	8.51

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Description:

Positive allosteric modulator of mGlu₅ receptors (EC₅₀ = 16 nM; K_i = 195 nM). Selective for mGlu₅; displays no significant activity at mGlu₁, mGlu₂ or mGlu₄ 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:

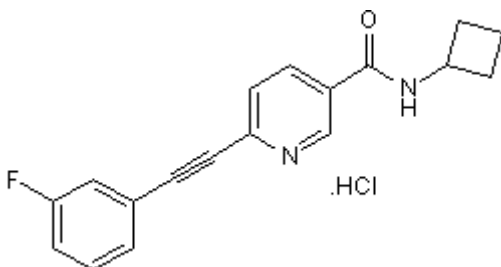
Batch Molecular Formula: C₁₈H₁₅FN₂O.HCl

Batch Molecular Weight: 330.78

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



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:

Rodriguez et al (2010) Discovery of novel allosteric modulators of metabotropic glutamate receptor subtype 5 reveals chemical and functional diversity and in vivo activity in rat behavioral models of anxiolytic and antipsychotic activity. *Mol.Pharmacol.* **78** (6) 1105. PMID: 20923853.

D'Amore et al (2013) Potentiation of mGlu₅ receptors with the novel enhancer, VU0360172, reduces spontaneous absence seizures in WAG/Rij rats. *Neuropharmacology* **66** 330. PMID: 22705340.

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