Certificate of Analysis

Product Name: **VU 0424465** **Catalog No.: 6895** **Batch No.: 1**

CAS Number: 1428630-85-6

IUPAC Name: 5-[2-(2-(3-Fluorophenyl)ethynyl]-*N*-[(1*R*)-2-hydroxy-1,2-dimethylpropyl]-2-pyridinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{19}FN_2O_2$

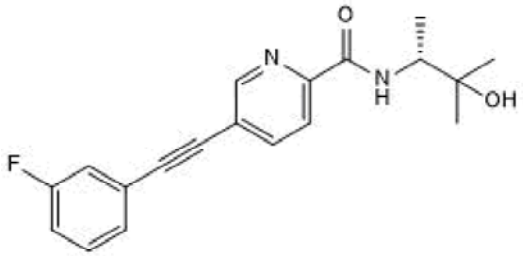
Batch Molecular Weight: 326.37

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99% purity

Chiral HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	69.92	5.87	8.58
Found	69.72	5.89	8.56

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Product Information

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IUPAC Name: 5-[2-(2-(3-Fluorophenyl)ethynyl]-*N*-[(1*R*)-2-hydroxy-1,2-dimethylpropyl]-2-pyridinecarboxamide

Description:

Potent $mGlu_5$ positive allosteric modulator (EC_{50} = 1.5 nM) and agonist (EC_{50} = 171 nM; maximum effect is 65% that of glutamate). Binds allosteric site with high affinity (K_i = 11.8 nM). Increases maximum response to glutamate by 30%. Exhibits bias towards signaling via IP_1 and ERK1/2 over iCa^{2+} in HEK293 and neuronal cells, and activates G_s in HEK 293 cells. Induces epileptiform activity in CA3 hippocampal neurons in vitro and convulsions in vivo.

Physical and Chemical Properties:

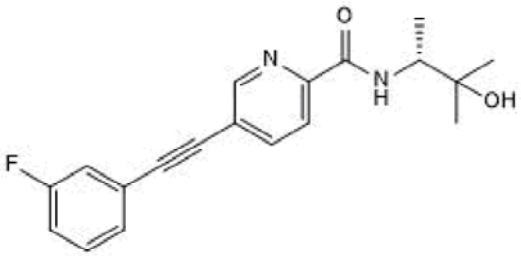
Batch Molecular Formula: $C_{19}H_{19}FN_2O_2$

Batch Molecular Weight: 326.37

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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.

References:

Nasrallah *et al* (2018) Direct coupling of detergent purified human $mGlu_5$ receptor to the heterotrimeric G proteins Gq and Gs. Sci.Rep. ***8*** 4407. PMID: 29535347.

Sengmany *et al* (2017) Biased allosteric agonism and modulation of metabotropic glutamate receptor 5: Implications for optimizing preclinical neuroscience drug discovery. Neuropharmacology ***115*** 60. PMID: 27392634.

Rook *et al* (2013) Unique signaling profiles of positive allosteric modulators of metabotropic glutamate receptor subtype 5 determine differences in *in vivo* activity. Biol.Psychiatry. ***73*** 501. PMID: 23140665.

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