

Certificate of Analysis

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Product Name: VU 0285683

Catalog No.: 4381

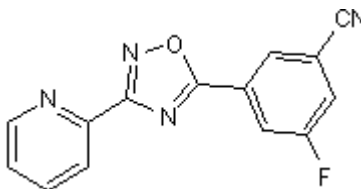
Batch No.: 1

CAS Number: 327056-22-4

IUPAC Name: 3-Fluoro-5-[3-(2-pyridinyl)-1,2,4-oxadiazol-5-yl]-benzonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₄H₇FN₄O
Batch Molecular Weight: 266.23
Physical Appearance: White solid
Solubility: DMSO to 50 mM
 ethanol to 25 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.35 (Ethyl acetate:Petroleum ether [3:7])
HPLC: Shows 99.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.16	2.65	21.04
Found	63.02	2.67	20.91

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

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CAS Number: 327056-22-4

IUPAC Name: 3-Fluoro-5-[3-(2-pyridinyl)-1,2,4-oxadiazol-5-yl]-benzonitrile

Description:

Negative allosteric modulator of mGlu₅ receptors. Displays high affinity for the MPEP (Cat. No. 1212) binding site; acts as a full antagonist and blocks the glutamate response to mGlu₅ (IC₅₀ = 24.4 nM). Selective for mGlu₅ over mGlu₁, mGlu₃ and mGlu₄. Exhibits anxiolytic activity in rodent models of anxiety. Analog available (Cat. No. 4323).

Physical and Chemical Properties:

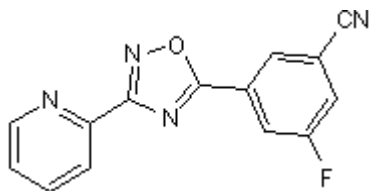
Batch Molecular Formula: C₁₄H₇FN₄O

Batch Molecular Weight: 266.23

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Rodriguez (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.

Storage: Store at RT

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.

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