

## Certificate of Analysis

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**Product Name:** AZD 9272

**Catalog No.:** 5613

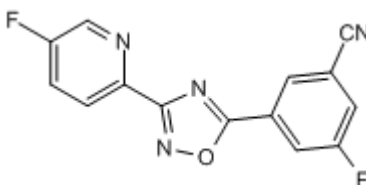
**Batch No.:** 1

CAS Number: 327056-26-8

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

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>14</sub>H<sub>6</sub>F<sub>2</sub>N<sub>4</sub>O  
**Batch Molecular Weight:** 284.22  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 50 mM  
**Storage:** Store at RT  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.82 (Dichloromethane:Methanol [1:4])  
**HPLC:** Shows 99.3% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	59.16	2.13	19.71
Found	59.39	2.09	19.6

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**Description:**

Potent and selective mGlu<sub>5</sub> antagonist (IC<sub>50</sub> values are 2.6 and 7.6 nM for rat and human receptors, respectively). Exhibits >3900-fold selectivity for mGlu<sub>5</sub> over other mGlu receptors. Also selective over a panel of other targets. Displays discriminative effects in rats. Orally bioavailable and brain penetrant.

**Physical and Chemical Properties:**

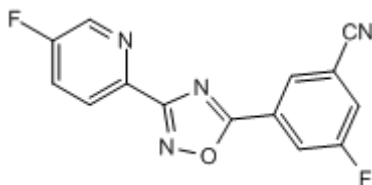
Batch Molecular Formula: C<sub>14</sub>H<sub>6</sub>F<sub>2</sub>N<sub>4</sub>O

Batch Molecular Weight: 284.22

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Raboisson et al** (2012) Discovery and characterization of AZD9272 and AZD6538-Two novel mGluR5 negative allosteric modulators selected for clinical development. *Bioorg.Med.Chem.Lett.* **22** 6974. PMID: 23046966.

**Swedberg and Raboisson** (2014) AZD9272 and AZD2066: selective and highly central nervous system penetrant mGluR5 antagonists characterized by their discriminative effects. *J.Pharmacol.Exp.Ther.* **350** 212. PMID: 24876235.

**Storage:** Store at RT

**Solubility & Usage Info:**

DMSO to 50 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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