

## Certificate of Analysis

**Product Name:** VU 0409106

**Catalog No.:** 5322

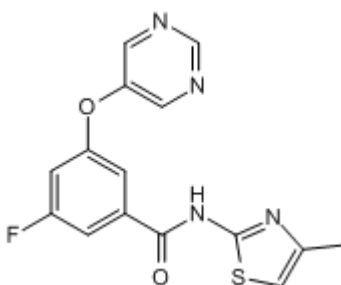
**Batch No.:** 1

CAS Number: 1276617-62-9

IUPAC Name: 3-Fluoro-N-(4-methyl-2-thiazolyl)-5-(5-pyrimidinyloxy)benzamide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>15</sub>H<sub>11</sub>FN<sub>4</sub>O<sub>2</sub>S  
**Batch Molecular Weight:** 330.34  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.65 (Dichloromethane:Methanol [95:5])  
**HPLC:** Shows >99.8% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	54.54	3.36	16.96
Found	54.58	3.32	16.94

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

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**Description:**

Potent and selective mGlu<sub>5</sub> negative allosteric modulator (IC<sub>50</sub> = 49 nM at human mGlu<sub>5</sub>). Selective for mGlu<sub>5</sub> over a panel of GPCRs and ion channels. Exhibits no significant nonspecific binding in rat brain homogenates in vitro. Inhibits marble burying behavior in mice. Brain penetrant.

**Physical and Chemical Properties:**

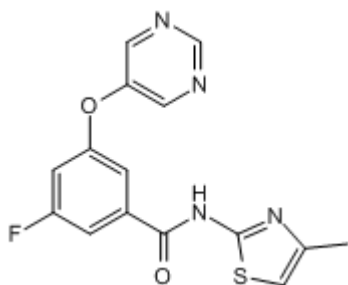
Batch Molecular Formula: C<sub>15</sub>H<sub>11</sub>FN<sub>4</sub>O<sub>2</sub>S

Batch Molecular Weight: 330.34

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Felts et al** (2013) Discovery of VU0409106: A negative allosteric modulator of mGlu<sub>5</sub> with activity in a mouse model of anxiety. *Bioorg.Med.Chem.Lett.* **23** 5779. PMID: 24074843.

**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO 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.

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**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

Tel:+1 612 379 2956