# **Certificate of Analysis**

### www.tocris.com

#### Product Name: FITM

Catalog No.: 6859 B

Batch No.: 1

CAS Number: IUPAC Name:

Storage:

932737-65-0

4-Fluoro-N-[4-[6-(isopropylamino)pyrimidin-4-yl]-1,3-thiazol-2-yl]-N-methylbenzamide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C<sub>18</sub>H<sub>18</sub>FN<sub>5</sub>OS 371.43 White solid DMSO to 100 mM ethanol to 20 mM Store at -20°C

2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis: Shows 99.3% purity Consistent with structure Consistent with structure

	Carbon Hydrogen Nitrogen				
Theoretical	58.21	4.88	18.86		
Found	58.21	4.88	18.68		

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

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Batch Molecular Structure:

Print Date: Aug 5th 2019

# TOCRIS a biotechne brand

# **Product Information**

## www.tocris.com

Print Date: Aug 5th 2019

#### Product Name: FITM

CAS Number: 932737-65-0

4-Fluoro-N-[4-[6-(isopropylamino)pyrimidin-4-yl]-1,3-thiazol-2-yl]-N-methylbenzamide

#### **Description:**

**IUPAC Name:** 

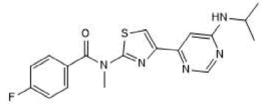
Potent and selective negative allosteric modulator of mGlu<sub>1</sub> receptors (IC<sub>50</sub> = 5.1 nM). Displays >1300-fold selectivity for mGlu<sub>1</sub> over other metabotropic glutamate receptors (IC<sub>50</sub> values are 7  $\mu$ M and >10  $\mu$ M for mGlu<sub>5</sub> and mGlu<sub>2</sub> or mGlu<sub>8</sub>, respectively). Antagonizes methamphetamine-induced locomotion in mice.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>18</sub>H<sub>18</sub>FN<sub>5</sub>OS Batch Molecular Weight: 371.43 Physical Appearance: White solid

#### Minimum Purity: >98%

#### **Batch Molecular Structure:**



#### Storage: Store at -20°C

Solubility & Usage Info: DMSO to 100 mM ethanol to 20 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  $45-60^{\circ}C$  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:**

**Wu** *et al* (2014) Structure of a class C GPCR metabotropic glutamate receptor 1 bound to an allosteric modulator. Science. **344** 58. PMID: 24603153.

**Satoh** *et al* (2009) Discovery and *in vitro* and *in vivo* profiles of 4-fluoro-*N*-[4-[6-(isopropylamino)pyrimidin-4-yl]-1,3-thiazol-2-yl] -*N*-methylbenzamide as novel class of an orally active metabotropic glutamate receptor 1 (mGluR<sub>1</sub>) antagonist. Bioorg.Med.Chem.Lett. **19** 5464. PMID: 19674894.

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