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: C₁₈H₁₈FN₅OS 371.43 White solid DMSO to 100 mM ethanol to 20 mM Store at -20°C

2. ANALYTICAL DATA

HPLC: ¹H 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

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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:

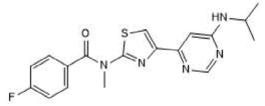
Potent and selective negative allosteric modulator of mGlu₁ receptors (IC₅₀ = 5.1 nM). Displays >1300-fold selectivity for mGlu₁ over other metabotropic glutamate receptors (IC₅₀ values are 7 μ M and >10 μ M for mGlu₅ and mGlu₂ or mGlu₈, respectively). Antagonizes methamphetamine-induced locomotion in mice.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₁₈FN₅OS 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 (mGluR₁) antagonist. Bioorg.Med.Chem.Lett. **19** 5464. PMID: 19674894.

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