

Certificate of Analysis

Print Date: Jan 15th 2016

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Product Name: YM 230888 Catalog No.: 2986 Batch No.: 1

CAS Number: 446257-23-4

IUPAC Name: 4-(Cycloheptylamino)-*N*-[[(2*R*)-tetrahydro-2-furanyl]methyl]-thieno[2,3-*d*]pyrimidine-6-methanamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{28}N_4OS$

Batch Molecular Weight: 360.52
Physical Appearance: Beige solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.8% purity
Chiral HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 63.3 7.83 15.54 Found 63.29 7.82 15.51



Product Information

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IUPAC Name: 4-(Cycloheptylamino)-N-[[(2R)-tetrahydro-2-furanyl]methyl]-thieno[2,3-d]pyrimidine-6-methanamine

Description:

Selective mGlu₁ antagonist ($K_i = 13$ nM). Inhibits mGlu₁-mediated inositol phosphate production in rat cerebellar granule cells ($IC_{50} = 13$ nM). Displays antinociceptive and analgesic effects in vitro; exhibits no significant sedative effect on locomotor activity.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₉H₂₈N₄OS Batch Molecular Weight: 360.52 Physical Appearance: Beige solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM ethanol 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.

References:

Kohara *et al* (2007) Antinociceptive profile of a selective metabotropic glutamate receptor 1 antagonist YM-230888 in chronic pain rodent models. Eur.J.Pharmacol. *571* 8. PMID: 17597604.

Satow *et al* (2008) Pharmacological effects of the metabotropic glutamate receptor 1 antagonist compared with those of the metabotropic glutamate receptor 5 antagonist and metabotropic glutamate receptor 2/3 agonist in rodents: detailed investigations with a selective allosteric metabotropic receptor 1 antagonist, FTIDC [4-[1-(2-Fluoropyridine-3-yl)-5-methyl-1*H*-1,2,3-triazol-4-yl]-*N*-isopropyl-*N*-methyl-3,6-dihydropyridine-1(2*H*)-carboxamide. J.Pharmacol.Exp.Ther. **326** 577. PMID: 18487514.