

Certificate of Analysis

Print Date: Mar 7th 2019

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Product Name: Fenobam Catalog No.: 2386 Batch No.: 1

CAS Number: 57653-26-6

IUPAC Name: N-(3-Chlorophenyl)-N'-(4,5-dihydro-1-methyl-4-oxo-1*H*-imidazol-2-yl)urea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₁H₁₁N₄O₂Cl

Batch Molecular Weight: 266.69

Physical Appearance: Pale orange solid
Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

¹H NMR: Consistent with structure

¹³C NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 49.54 4.16 21 Found 49.36 4.12 20.84

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



Product Information

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IUPAC Name: N-(3-Chlorophenyl)-N'-(4,5-dihydro-1-methyl-4-oxo-1H-imidazol-2-yl)urea

Description:

Potent and selective non-competitive mGlu $_5$ negative allosteric modulator (NAM) that also displays inverse agonist properties; blocks mGlu $_5$ constitutive activity in vitro (IC $_{50}$ = 87 nM). Acts at an allosteric modulatory site shared with MPEP and binds the mGlu $_5$ receptor with K $_d$ values of 54 and 31 nM for rat and human receptors respectively. Displays anxiolytic activity following oral administration in vivo; also exhibits analgesic properties.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{11}H_{11}N_4O_2CI$

Batch Molecular Weight: 266.69

Physical Appearance: Pale orange solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

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.

References:

Kufahl *et al* (2013) Positive or negative allosteric modulation of metabotropic glutamate receptor 5 (mGluR5) does not alter expression of behavioral sensitization to methamphetamine F1000Res. *1* 10.12688/f1000resear. PMID: 24358885.

Montana *et al* (2009) The metabotropic glutamate receptor subtype 5 antagonist fenobam is analgesic and has improved in vivo selectivity compared with the prototypical antagonist 2-methyl-6-(phenylethynyl)-pyridine. J.Pharmacol.Exp.Ther. *330* 834. PMID: 19515968.

Porter et al (2005) Description of a clinically validated anxiolytic with mGlu5 antagonist properties. Neuropharmacology 49 (Suppl. 1)

Porter *et al* (2005) Fenobam: a clinically validated nonbenzodiazepine anxiolytic is a potent, selective, and noncompetitive mGlu5 receptor antagonist with inverse agonist activity. J.Pharmacol.Exp.Ther. *315* 711. PMID: 16040814.

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