# TOCRIS a biotechne brand

### Print Date: Sep 23rd 2019

# **Certificate of Analysis**

## www.tocris.com

Batch No.: 1

Catalog No.: 7027

## Product Name: LY 2033298

CAS Number: 886047-13-8

IUPAC Name: 3-Amino-5-chloro-*N*-cyclopropyl-6-methoxy-4-methylthieno[2,3-*b*]pyridine-2-carboxamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C<sub>13</sub>H<sub>14</sub>CIN<sub>3</sub>O<sub>2</sub>S 311.79 White solid DMSO to 100 mM ethanol to 20 mM Store at +4°C

Storage: **Batch Molecular Structure:** 

NH<sub>2</sub> CI

### 2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis:

Shows 99.8% purity Consistent with structure Consistent with structure

Carbon Hydrogen Nitrogen

Theoretical	50.08	4.53	13.48
Found	49.99	4.52	13.45

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

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### **Description:**

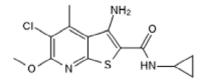
Selective positive allosteric modulator of  $M_4$  receptor ( $K_B = 200$  nM,  $\alpha = 35$ ); increases the potency of acetylcholine by 40-fold. Exhibits no effect at hM<sub>1/3/5</sub> receptors and a small effect at hM<sub>2</sub> ( $K_B = 1 \ \mu M \ \alpha = 3.7$ ). Potentiates other full and partial orthosteric agonists, including Carbachol, Oxotremorine-M, and McN-A343. Does not affect binding of antagonist NMS. Active in vivo. Antipsychotic.  $\alpha$  indicates the degree of allosteric enhancement when both orthosteric and allosteric sites are occupied (derived from the allosteric ternary complex model). Please see product datasheet on www.tocris.com for full description.

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

Batch Molecular Formula: C<sub>13</sub>H<sub>14</sub>ClN<sub>3</sub>O<sub>2</sub>S Batch Molecular Weight: 311.79 Physical Appearance: White solid

Minimum Purity: >98%

**Batch Molecular Structure:** 



### Storage: Store at +4°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).

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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:

**Huynh** *et al* (2015) Synthesis and pharmacological evaluation of M<sub>4</sub> muscarinic receptor positive allosteric modulators derived from VU10004. ACS Chem. Neurosci. *6* 838. PMID: 25857219.

Leach et al (2010) Molecular mechanisms of action and *in vivo* validation of an  $M_4$  muscarinic acetylcholine receptor allosteric modulator with potential antipsychotic properties. Neuropsychopharmacology **35** 855. PMID: 19940843.

**Chan** *et al* (2008) Allosteric modulation of the muscarinic M<sub>4</sub> receptor as an approach to treating schizophrenia Proc.Natl.Acad.Sci.U.S.A. **105** 10978. PMID: 18678919.

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