

Certificate of Analysis

Print Date: Jan 9th 2020

www.tocris.com

Product Name: LY 2119620 Catalog No.: 6964 Batch No.: 1

CAS Number: 886047-22-9

IUPAC Name: 3-Amino-5-chloro-*N*-cyclopropyl-4-methyl-6-[2-(4-methyl-1-piperazinyl)-2-oxoethoxy]-thieno[2,3-*b*]pyridine-2-

carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₂₄ClN₅O₃S

Batch Molecular Weight: 437.94

Physical Appearance: White solid

Solubility: DMSO to 100 mM

1eq. HCl to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 52.11 5.52 15.99 Found 51.7 5.53 15.77

Tel: +44 (0)1235 529449 www.tocris.com/distri Tel:+1 612 379 2956



Product Information

Print Date: Jan 9th 2020

www.tocris.com

Product Name: LY 2119620 Catalog No.: 6964 Batch No.: 1

CAS Number: 886047-22-9

IUPAC Name: 3-Amino-5-chloro-N-cyclopropyl-4-methyl-6-[2-(4-methyl-1-piperazinyl)-2-oxoethoxy]-thieno[2,3-b]pyridine-2-

carboxamide

Description:

Positive allosteric modulator of M_2 and M_4 muscarinic receptors. Potentiates activity of agonist at receptor in G protein-coupled functional assay. Cooperativity factor, α = 19.5 and 79.4 for M_2 and M_4 in presence of ACh, respectively. Binds in extracellular site

Physical and Chemical Properties:

Batch Molecular Formula: C₁₉H₂₄ClN₅O₃S

Batch Molecular Weight: 437.94 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM 1eq. HCl 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:

Croy *et al* (2014) Characterization of the novel positive allosteric modulator, LY2119620, at the muscarinic M(2) and M(4) receptors. Mol.Pharmacol. *86* 106. PMID: 24807965.

Kruse et al (2013) Activation and allosteric modulation of a muscarinic acetylcholine receptor. Nature. 504 101. PMID: 24256733.