

Certificate of Analysis

Print Date: Sep 29th 2017

www.tocris.com

Product Name: AM 0902 Catalog No.: 5914 Batch No.: 1

CAS Number: 1883711-97-4

IUPAC Name: 1-[[3-[2-(4-Chlorophenyl)ethyl]-1,2,4-oxadiazol-5-yl]methyl]-1,7-dihydro-7-methyl-6*H*-purin-6-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₅CIN₆O₂

Batch Molecular Weight: 370.79

Physical Appearance: Light brown solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.22$ (Dichloromethane:Methanol [95:5])

HPLC: Shows 98.7% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.07 4.08 22.66 Found 54.9 4.03 22.61



Product Information

Print Date: Sep 29th 2017

www.tocris.com

Product Name: AM 0902 Catalog No.: 5914 Batch No.: 1

CAS Number: 1883711-97-4

IUPAC Name: 1-[[3-[2-(4-Chlorophenyl)ethyl]-1,2,4-oxadiazol-5-yl]methyl]-1,7-dihydro-7-methyl-6*H*-purin-6-one

Description:

Potent and selective TRPA1 antagonist (IC_{50} = 0.02 μ M for human TRPA1). Exhibits no significant activity against human TRPV1 or TRPV4, and rat TRPV1, TRPV3 or TRPM8. Exhibits efficacy in a rat pain model. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{17}H_{15}CIN_6O_2$

Batch Molecular Weight: 370.79

Physical Appearance: Light brown solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

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:

Schenkel *et al* (2016) Optimization of a novel quinazolinone-based series of transient receptor potential A1 (TRPA1) antagonists demonstrating potent *in vivo* activity. J.Med.Chem. **59** 2794. PMID: 26942860.