

# **Certificate of Analysis**

Print Date: Jan 11th 2016

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Product Name: HC 030031 Catalog No.: 2896 Batch No.: 4

CAS Number: 349085-38-7

IUPAC Name: 2-(1,3-Dimethyl-2,6-dioxo-1,2,3,6-tetrahydro-7*H*-purin-7-yl)-*N*-(4-isopropylphenyl)acetamide

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{21}N_5O_3$ Batch Molecular Weight:355.39Physical Appearance:White solid

**Solubility:** DMSO to 100 mM ethanol to 5 mM

Storage: Store at RT

**Batch Molecular Structure:** 

# 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.5$  (Chloroform:Methanol [9:1])

HPLC: Shows 100% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 60.83 5.96 19.71 Found 60.82 5.98 19.61



# **Product Information**

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## **Description:**

Selective TRPA1 channel blocker that antagonizes AITC- and formalin-evoked calcium influx (IC $_{50}$  values are 6.2 and 5.3  $\mu$ M respectively). Does not block currents mediated by TRPV1, TRPV3, TRPV4, hERG or Na $_{\rm V}$ 1.2 channels. Inhibits AITC- and formalin-induced flinching in vivo.

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

Batch Molecular Formula: C<sub>18</sub>H<sub>21</sub>N<sub>5</sub>O<sub>3</sub> Batch Molecular Weight: 355.39 Physical Appearance: White solid

Minimum Purity: >99%

#### **Batch Molecular Structure:**

Storage: Store at RT

# Solubility & Usage Info:

DMSO to 100 mM ethanol to 5 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:

McNamara et al (2007) TRPA1 mediates formalin-induced pain. Proc.Natl.Acad.Sci.USA 104 13525.

**Taylor-Clark** *et al* (2008) Prostaglandin-induced activation of nociceptive neurons via direct interactions with TRPA1. Mol.Pharmacol. **73** 274. PMID: 18000030.