

Certificate of Analysis

Print Date: Jul 28th 2018

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Product Name: Theophylline Catalog No.: 2795 Batch No.: 1

CAS Number: 58-55-9 EC Number: 200-385-7

IUPAC Name: 3,7-Dihydro-1,3-dimethyl-1*H*-purine-2,6-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_7H_8N_4O_2$ Batch Molecular Weight:180.16Physical Appearance:White solidSolubility:water to 25

water to 25 mM DMSO to 100 mM 1.1eq. NaOH to 100 mM 1eq. HCl to 25 mM ethanol to 10 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

Melting Point: At 272°C

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 46.67 4.48 31.09 Found 46.67 4.44 30.59



Product Information

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IUPAC Name: 3,7-Dihydro-1,3-dimethyl-1*H*-purine-2,6-dione

Description:

Bronchodilator, anti-inflammatory and immunomodulator. Antagonizes adenosine receptors and is a weak non-selective inhibitor of phosphodiesterases (PDEs).

Physical and Chemical Properties:

Batch Molecular Formula: C₇H₈N₄O₂ Batch Molecular Weight: 180.16 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

water to 25 mM DMSO to 100 mM 1.1eq. NaOH to 100 mM 1eq. HCl to 25 mM ethanol to 10 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:

Barnes (2003) Theophylline. New perspectives for an old drug. Am.J.Respir.Care Med. 167 813.

Page (1999) Recent advances in our understanding of the use of theophylline in the treatment of asthma. J.Clin.Pharmacol. 39 237. PMID: 10073321.

Coward et al (1998) Asthma, adenosine, mast cells and theophylline. Clin. Exp. Allery 28 (Suppl. 3) 42.