TOCRIS b i o s c i e n c e

Certificate of Analysis

Print Date: Mar 4th 2014

Batch No.: 5

www.tocris.com

Catalog No.: 2752

Product Name: MRS 1754

CAS Number: IUPAC Name:

Storage:

264622-58-4

N-(4-Cyanophenyl)-2-[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1*H*-purin-8-yl)phenoxy]-acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

Batch Molecular Structure:

C₂₆H₂₆N₆O₄.^{1/2}H₂O 495.53 White solid DMSO to 5 mM with gentle warming DMSO to 10 mM with sonication Desiccate at RT

CN HN

2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: Microanalysis: R_f = 0.45 (Dichloromethane:Methanol [97.5:2.5]) Shows >99% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen

Theoretical	63.02	5.49	16.96
Found	62.96	5.4	16.92

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

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TOCRIS b i o s c i e n c e

Print Date: Mar 4th 2014

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Product Name: MRS 1754

Catalog No.: 2752 Batch No.: 5

CAS Number: 264622-58-4

IUPAC Name: N-(4-Cyanophenyl)-2-[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1*H*-purin-8-yl)phenoxy]-acetamide

Description:

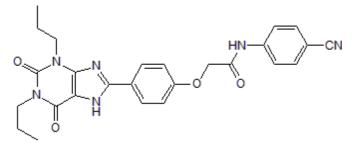
Selective adenosine A_{2B} receptor antagonist (K_i values are 1.97, 16.8, 403, 503, 570 and 612 nM for hA_{2B}, rA₁, hA₁, hA_{2A}, hA₃ and rA_{2A} receptors respectively).

Physical and Chemical Properties:

 $\begin{array}{l} \mbox{Batch Molecular Formula: } C_{26}H_{26}N_6O_4.\, \rlap{W}_2H_2O\\ \mbox{Batch Molecular Weight: 495.53}\\ \mbox{Physical Appearance: White solid} \end{array}$

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 5 mM with gentle warming DMSO to 10 mM with sonication

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).

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:

Kim *et al* (2000) Anilide derivatives of an 8-phenylxanthine carboxylic congener are highly potent and selective antagonists at human A_{2B} adenosine receptors. J.Med.Chem. **43** 1165. PMID: 10737749.

Ji *et al* (2001) [³H]MRS 1754, a selective antagonist radioligand for A_{2B} adenosine receptors. Biochem.Pharmacol. *61* 657. PMID: 11266650.

Nemeth et al (2007) Adenosine receptor activation ameliorates type I diabetes. FASEB J. 21 2380.

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