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Print Date: Jul 24th 2024

Certificate of Analysis

www.tocris.com

Product Name: MRS 1754

Catalog No.: 2752 Batch No.: 5

CAS Number: **IUPAC Name:**

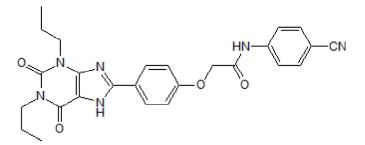
N-(4-Cyanophenyl)-2-[4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)phenoxy]-acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

264622-58-4

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: **Batch Molecular Structure:**

 $C_{26}H_{26}N_6O_4$.¹/₂H₂O 495.53 White solid DMSO to 5 mM with gentle warming Desiccate at RT



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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CAS Number: 264622-58-4

IUPAC Name:

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

Description:

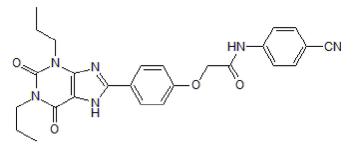
MRS 1754 is a selective adenosine A_{2B} receptor antagonist (K_i values are 1.97, 16.8, 403, 503, 570 and 612 nM for hA_{2B} , rA_1 , hA_1 , hA_{2A} , hA_3 and rA_{2A} receptors respectively).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{26}H_{26}N_6O_4$. $\frac{1}{2}H_2O$ Batch Molecular Weight: 495.53 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 5 mM with gentle warming

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

Licensing Information:

Sold with the permission of the University of Virginia Patent Foundation

References:

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

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

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.

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bio-techne.com	North America	China	Europe Middle East Africa	Rest of World
info@bio-techne.com techsupport@bio-techne.com	Tel: (800) 343 7475	info.cn@bio-techne.com Tel: +86 (21) 52380373	Tel: +44 (0)1235 529449	www.tocris.com/distributors Tel:+1 612 379 2956

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