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Print Date: Jan 13th 2016

Certificate of Analysis

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Product Name: **MRS 1706** **Catalog No.: 1584** **Batch No.: 3**

CAS Number: 264622-53-9

IUPAC Name: *N*-(4-Acetylphenyl)-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: $C_{27}H_{29}N_5O_5 \cdot \frac{1}{2}H_2O$

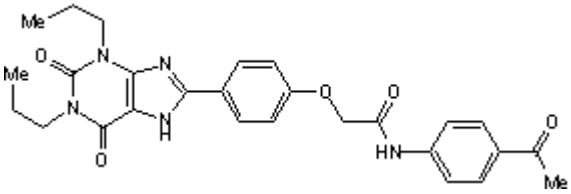
Batch Molecular Weight: 512.57

Physical Appearance: White solid

Solubility: DMSO to 5 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.44 (Dichloromethane:Methanol [95:5])

HPLC: Shows 96.4% purity

^{1}H NMR: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.21	5.9	13.66
Found	62.91	5.65	13.61

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Description:

Potent and selective adenosine A_{2B} receptor inverse agonist (K_i values are 1.39, 157, 112 and 230 nM for human A_{2B}, A_1, A_{2A} and A_3 receptors respectively).

Physical and Chemical Properties:

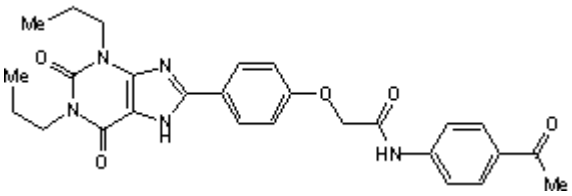
Batch Molecular Formula: $C_{27}H_{29}N_5O_5.½H_2O$

Batch Molecular Weight: 512.57

Physical Appearance: White solid

Minimum Purity: >96%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO 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:

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.

Kiec-Kononowicz *et al* (2001) New developments in A_1 and A_2 adenosine receptor antagonists. Pure Appl.Chem. ***73*** 1411.

Li *et al* (2007) ZM241385, DPCPX, MRS1706 are inverse agonists with different relative intrinsic efficacies on constitutively active mutants of the human adenosine A_{2B} receptor. J.Pharmacol.Exp.Ther. ***320*** 637. PMID: 17077318.

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