



Certificate of Analysis

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Product Name: GS 6201 Catalog No.: 4727 Batch No.: 2

CAS Number: 752222-83-6

IUPAC Name: 3-Ethyl-3,9-dihydro-1-propyl-8-[1-[[3-(trifluoromethyl)phenyl]methyl]-1*H*-pyrazol-4-yl]-1*H*-purine-2,6-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{21}F_3N_6O_2$

Batch Molecular Weight: 446.43

Physical Appearance: White solid

Solubility: DMSO to 5 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

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

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 56.5 4.74 18.82 Found 56.43 4.74 18.86



Product Information

Print Date: Jan 14th 2016

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Description:

Selective antagonist of adenosine A_{2B} receptors (K_i values are 22, 1070, 1940 and 3280 nM for human A_{2B} , A_3 , A_1 and A_{2A} receptors respectively). Attenuates allergen-, NECA- and AMP-induced airway reactivity in an allergic mouse model of asthma. Also shown to attenuate the inflammatory response during acute myocardial infarction in mice; reduces caspase-1 activity in the heart.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₁H₂₁F₃N₆O₂ Batch Molecular Weight: 446.43 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at -20°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:

Mustafa et al (2007) Effect of a specific and selective A_{2B} adenosine receptor antagonist on adenosine agonist AMP and allergen-induced airway responsiveness and cellular influx in a mouse model of asthma. J.Pharmacol.Exp.Ther. **320** 1246. PMID: 17159162.

Elzein et al (2008) Discovery of a novel A_{2B} adenosine receptor antagonist as a clinical candidate for chronic inflammatory airway diseases. J.Med.Chem. **51** 2267. PMID: 18321039.

Toldo *et al* (2012) GS-6201, a selective blocker of the A_{2B} adenosine receptor, attenuates cardiac remodeling after acute myocardial infarction in the mouse. J.Pharmacol.Exp.Ther. **343** 587. PMID: 22923737.