Certificate of Analysis

Product Name: **GS 6201** **Catalog No.: 4727** **Batch No.: 4**

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: $C_{21}H_{21}F_3N_6O_2 \cdot \frac{1}{2}H_2O$

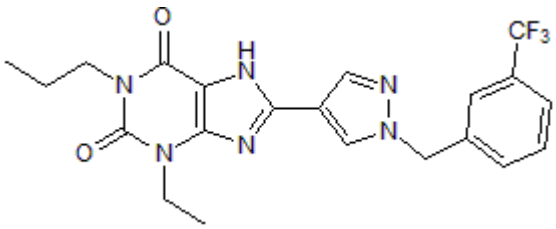
Batch Molecular Weight: 455.44

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 >99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.38	4.87	18.45
Found	55.47	4.66	18.5

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

Product Information

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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: $C_{21}H_{21}F_3N_6O_2.½H_2O$

Batch Molecular Weight: 455.44

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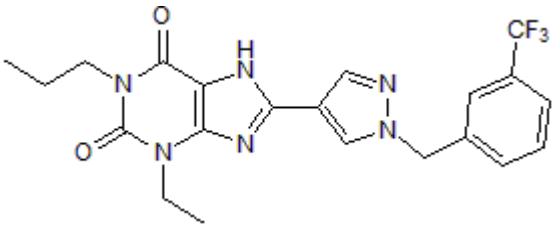
Minimum Purity: >99%

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:

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.

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.

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.

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
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