Print Date: Apr 26th 2018

Certificate of Analysis

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Product Name: **PSB 36** **Catalog No.: 2019** **Batch No.: 1**

CAS Number: 524944-72-7

IUPAC Name: 1-Butyl-8-(hexahydro-2,5-methanopentalen-3a(1*H*)-yl)-3,7-dihydro-3-(3-hydroxypropyl)-1*H*-purine-2,6-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{30}N_4O_3$

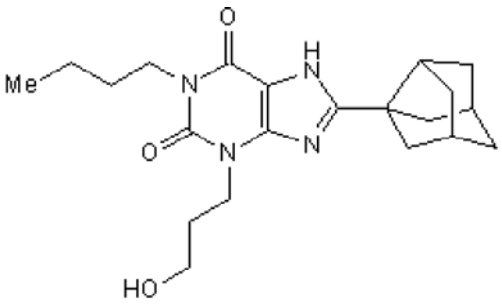
Batch Molecular Weight: 386.49

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.54 (Ethyl acetate)

HPLC: Shows 99.1% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.26	7.82	14.5
Found	65.23	7.86	14.57

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Product Information

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Description:

Potent and selective A_1 adenosine receptor antagonist. Displays binding affinities of 0.12, 187, 552, 6500 and 2300 nM for rA_1, hA_{2B}, rA_{2A}, rA_3 and hA_3 receptors respectively. Demonstrates greater selectivity than DPCPX (Cat. No. 0439).

Physical and Chemical Properties:

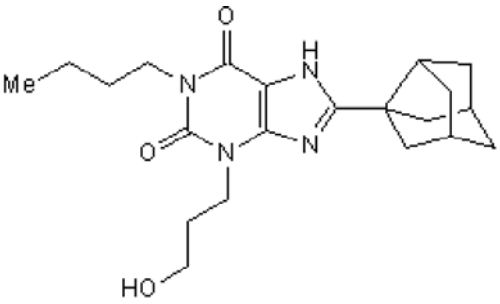
Batch Molecular Formula: $C_{21}H_{30}N_4O_3$

Batch Molecular Weight: 386.49

Physical Appearance: Pale yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 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:

Weyler *et al* (2006) Improving potency, selectivity, and water solubility of adenosine A_1 receptor antagonists: xanthines modified at position 3 and related pyrimido[1,2,3-*cd*]purinediones. Chem.Med.Chem. ***1*** 891.

Abo-Salem *et al* (2004) Antinociceptive effects of novel A_{2B} adenosine receptor antagonists. J.Pharmacol.Exp.Ther ***308*** 358. PMID: 14563788.

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