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Print Date: Jan 14th 2016

Certificate of Analysis

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Product Name: **TC-G 1004** **Catalog No.: 4407** **Batch No.: 1**

CAS Number: 1061747-72-5

IUPAC Name: *N*-[2-(3,5-Dimethyl-1*H*-pyrazol-1-yl)-6-[6-(4-methoxy-1-piperidinyl)-2-pyridinyl]-4-pyrimidinyl]acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{27}N_7O_2.½H_2O$

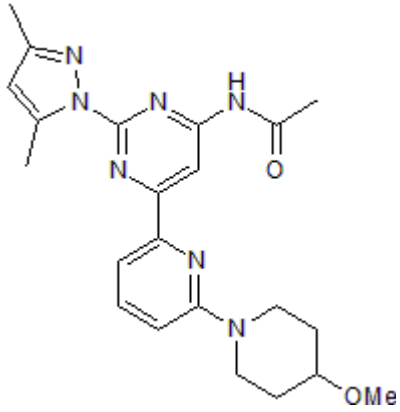
Batch Molecular Weight: 430.51

Physical Appearance: Yellow solid

Solubility: 1eq. HCl to 100 mM
DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.55 (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.3% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.38	6.56	22.77
Found	61.7	6.52	22.94

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Product Information

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Description:

Potent antagonist of adenosine A_{2A} receptors; displays >100-fold selectivity for A_{2A} over A_1 receptors (K_i values are 0.44 and 85 nM respectively). Potentiates L-DOPA-induced rotational behavior in 6-OHDA-lesioned rats.

Physical and Chemical Properties:

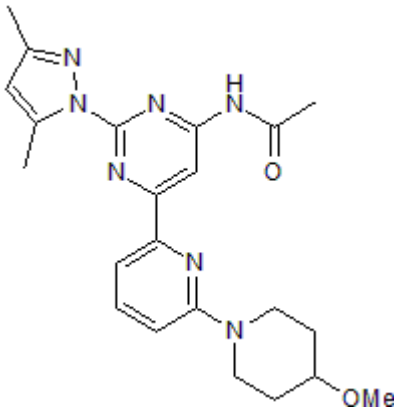
Batch Molecular Formula: $C_{22}H_{27}N_7O_2.½H_2O$

Batch Molecular Weight: 430.51

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

1eq. HCl to 100 mM
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:

Zhang *et al* (2008) Lead optimization of 4-acetylamino-2-(3,5-dimethylpyrazol-1-yl)-6-pyridylpyrimidines as A_{2A} adenosine receptor antagonists for the treatment of Parkinson's disease. J.Med.Chem. ***51*** 7099. PMID: 18947224.

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