

Print Date: Oct 28th 2022

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Product Name: SCH 442416 Catalog No.: 2463 Batch No.: 7

CAS Number: 316173-57-6

IUPAC Name: 2-(2-Furanyl)-7-[3-(4-methoxyphenyl)propyl]-7*H*-pyrazolo[4,3-e][1,2,4]triazolo[1,5-c]pyrimidin-5-amine

### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{19}N_7O_2$ Batch Molecular Weight:389.42Physical Appearance:White solid

Solubility: DMSO to 100 mM

Storage: Store at RT

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

**HPLC:** Shows 99.8% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 61.69 4.92 25.18 Found 61.74 4.93 25.31



# **Product Information**

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#### **Description:**

SCH 442416 is a selective adenosine  $A_{2A}$  receptor antagonist; binds to human and rat  $A_{2A}$  receptors with high affinity ( $K_i$  values are 0.048 and 0.5 nM respectively). Displays > 23000-fold selectivity for  $hA_{2A}$  over  $hA_1$  in vitro with minimal affinity for  $hA_{2B}$  and  $hA_3$  receptors ( $IC_{50}$  > 10  $\mu$ M). Blocks the cytoprotective effect of  $A_{2A}$  agonist CGS-21680 (Cat.No. 1063).

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>20</sub>H<sub>19</sub>N<sub>7</sub>O<sub>2</sub> Batch Molecular Weight: 389.42 Physical Appearance: White solid

Minimum Purity: ≥99%

#### **Batch Molecular Structure:**

Storage: Store at RT

## Solubility & Usage Info:

DMSO to 100 mM

When purched as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

## 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:

**Zheng** et al (2007) Protective roles of adenosine  $A_1$ ,  $A_2$ , and  $A_3$  receptors in skeletal muscle ischemia and reperfusion injury. Am.J.Physiol.Heart Circ.Physiol. **293** 3685.

**Todde** *et al* (2000) Design, radiosynthesis, and biodistribution of a new potent and selective ligand for in vivo imaging of the adenosine A<sub>2A</sub> receptor system using positron emission tomography. J.Med.Chem. *43* 4359. PMID: 11087559.

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use