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### Print Date: Oct 7th 2024

# **Certificate of Analysis**

# www.tocris.com

Batch No.: 3

Catalog No.: 1066

## Product Name: IB-MECA

CAS Number: 152918-18-8

1-Deoxy-1-[6-[[(3-iodophenyl)methyl]amino]-9H-purin-9-yl]-N-methyl-β-D-ribofuranuronamide

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight:

Physical Appearance:

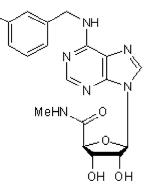
Solubility:

Storage:

**IUPAC Name:** 

**Batch Molecular Structure:** 

 $\begin{array}{l} C_{18}H_{19}IN_6O_4.2H_2O\\ \\546.32\\ \\White \ solid\\ \\DMSO \ to \ 25 \ mM\\ \\Desiccate \ at \ +4^\circ C \end{array}$ 



## 2. ANALYTICAL DATA

TLC: Melting Point: HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis: Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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IUPAC Name: 1-Deoxy-1-[6-[[(3-iodophenyl)methyl]amino]-9*H*-purin-9-yl]-*N*-methyl-β-D-ribofuranuronamide

#### **Description:**

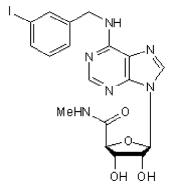
IB-MECA is a potent and selective  $A_3$  adenosine receptor agonist (K<sub>i</sub> values are 1.1, 54 and 56 nM for  $A_3$ ,  $A_1$  and  $A_{2A}$  receptors respectively). Cardioprotective, reduces infarct size upon reperfusion in rats.

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

Batch Molecular Formula: C<sub>18</sub>H<sub>19</sub>IN<sub>6</sub>O<sub>4</sub>.2H<sub>2</sub>O Batch Molecular Weight: 546.32 Physical Appearance: White solid

#### Minimum Purity: ≥97%

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



#### Storage: Desiccate at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Catalog No.: 1066

#### Solubility & Usage Info:

DMSO to 25 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  $45-60^{\circ}C$  water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

#### Licensing Information:

Sold with the permission of the NIH, US Patent 08/091,109

#### **References:**

**Park** *et al* (2006) N<sup>6</sup>-(3-iodobenzyl)-adenosine-5'-N-methylcarboxamide confers cardioprotection at reperfusion by inhibiting mitochondrial permeability transition pore opening via glycogen synthase kinase  $3\beta$ . J.Pharmacol.Exp.Ther. **318** 124. PMID: 16611852.

Klotz (2000) Adenosine receptors and their ligands. Naunyn Schmiedebergs Arch.Pharmacol. 362 382. PMID: 11111832.

**Gallo-Rodriguez** *et al* (1994) Structure-activity relationships of N<sup>6</sup>-benzyladenosine-5'-uronamides as A<sub>3</sub>-selective adenosine agonists. J.Med.Chem. **37** 636. PMID: 8126704.

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