

**Product Name:** IB-MECA

**Catalog No.:** 1066

**Batch No.:** 3

CAS Number: 152918-18-8

IUPAC Name: 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:** C<sub>18</sub>H<sub>19</sub>IN<sub>6</sub>O<sub>4</sub>.2H<sub>2</sub>O

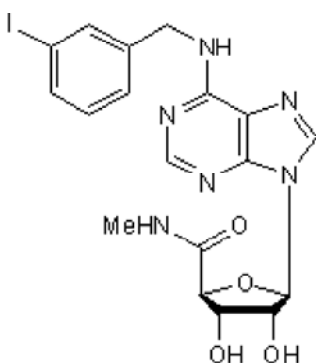
**Batch Molecular Weight:** 546.32

**Physical Appearance:** White solid

**Solubility:** DMSO to 25 mM

**Storage:** Desiccate at +4°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.35 (Dichloromethane:Methanol [10:1])

**Melting Point:** Between 175 - 177°C

**HPLC:** Shows >97.9% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	39.57	4.24	15.38
Found	39.37	3.89	15.28

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

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**Description:**

Potent and selective A<sub>3</sub> adenosine receptor agonist (K<sub>i</sub> values are 1.1, 54 and 56 nM for A<sub>3</sub>, A<sub>1</sub> and A<sub>2A</sub> receptors respectively). Cardioprotective, reduces infarct size upon reperfusion in rats.

**Physical and Chemical Properties:**

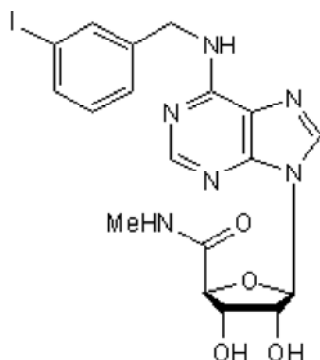
Batch Molecular Formula: C<sub>18</sub>H<sub>19</sub>IN<sub>6</sub>O<sub>4</sub>·2H<sub>2</sub>O

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.

**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°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.

**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 3β. *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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