

Certificate of Analysis

Print Date: Oct 12th 2022

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Product Name: 2-CI-IB-MECA Catalog No.: 1104 Batch No.: 9

CAS Number: 163042-96-4

IUPAC Name: 1-[2-Chloro-6-[[(3-iodophenyl)methyl]amino]-9*H*-purin-9-yl]-1-deoxy-*N*-methyl-β-D-ribofuranuronamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{18}CIIN_6O_4$

Batch Molecular Weight: 544.74

Physical Appearance: White solid

Solubility: DMSO to 100 mM
Storage: Desiccate at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.35$ (Chloroform:Methanol [9:1])

HPLC: Shows 99.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 39.69 3.33 15.43 Found 39.57 3.32 15.3

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



Product Information

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Description:

2-CI-IB-MECA is a high affinity and extremely selective A_3 adenosine receptor agonist ($K_i = 0.33$ nM). Displays 2500- and 1400-fold selectivity over A_1 and A_{2A} receptors respectively. Exhibits high selectivity over the Na+-independent adenosine transporter.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₁₈ClIN₆O₄

Batch Molecular Weight: 544.74 Physical Appearance: White solid

Minimum Purity: ≥98%

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 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.

Licensing Information:

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

References:

Jacobson (1998) Adenosine A₃ receptors: novel ligands and paradoxical effects. TiPS 19 184. PMID: 9652191.

Schaick *et al* (1996) Hemodynamic effects of histamine release elicited by the selective adenosine A₃ receptor agonist 2-CI-IB-MECA in conscious rats. Eur.J.Pharmacol. *308* 311. PMID: 8858305.

Kim et al (1994) 2-Substitution of N^6 -benzyladenosine-5'-uronamides enhances selectivity for A_3 adenosine receptors. J.Med.Chem. **37** 3614. PMID: 7932588.

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