

Certificate of Analysis

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Product Name: MRS 2179 tetrasodium salt Catalog No.: 0900 Batch No.: 8

CAS Number: 1454889-37-2

IUPAC Name: 2'-Deoxy-N⁶-methyladenosine 3',5'-bisphosphate tetrasodium salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{11}H_{13}N_5O_9P_2Na_4.31/2H_2O$

Batch Molecular Weight: 576.21

Physical Appearance: White solid

Solubility: water to 100 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 22.93 3.5 12.15 Found 22.88 3.76 11.97



Product Information

Print Date: Dec 16th 2013

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IUPAC Name: 2'-Deoxy-N⁶-methyladenosine 3',5'-bisphosphate tetrasodium salt

Description:

A competitive antagonist at P2Y $_1$ receptors (K $_B$ = 100 nM). Selective over P2X $_1$ (IC $_{50}$ = 1.15 μ M), P2X $_3$ (IC $_{50}$ = 12.9 μ M), P2X $_2$, P2X $_4$, P2Y $_2$, P2Y $_4$ and P2Y $_6$ receptors. Inhibits the upregulation of NTPDase1 by ATPyS.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₁H₁₃N₅O₉P₂Na₄.3½H₂O

Batch Molecular Weight: 576.21 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Desiccate at -20°C

Solubility & Usage Info:

water 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:

Boyer *et al* (1998) Competitive and selective antagonism of $P2Y_1$ receptors by N^6 -methyl 2'-deoxyadenosine 3',5'-bisphosphate. Br.J.Pharmacol. **124** 1. PMID: 9630335.

Nandanan *et al* (2000) Synthesis, biological activity, and molecular modeling of ribose-modified deoxyadenosine bisphosphate analogues as P2Y₁ receptor ligands. J.Med.Chem. *43* 829. PMID: 10715151.

Brown *et al* (2000) Activity of novel adenine nucleotide derivatives as agonists and antagonists at recombinant rat P2X receptors. Drug Dev.Res. *49* 253.

Lu *et al* (2007) Stimulation of the P2Y₁ receptor up-regulates nucleoside-triphosphate diphosphohydrolase-1 in human retinal pigment epithelial cells. J.Pharmacol.Exp.Ther. **323** 157. PMID: 17626796.

