Certificate of Analysis

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Print Date: Sep 22nd 2022

MRS 2179 tetrasodium salt Product Name:

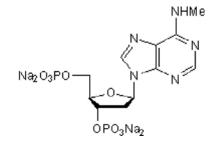
CAS Number: 1454889-37-2

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: **Batch Molecular Structure:**

 $C_{11}H_{13}N_5O_9P_2Na_4.3.75H_2O$ 580.72 White solid water to 50 mM Store at -20°C



2. ANALYTICAL DATA

Mass Spectrum: **Microanalysis:**

Shows 99.6% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Sodium

Theoretical	22.75	3.56	12.06
Found	23.02	4.07	12.02

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

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Catalog No.: 0900

Batch No.: 10



IUPAC Name:

HPLC: ¹H NMR:



Product Information

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Product Name: MRS 2179 tetrasodium salt

CAS Number: 1454889-37-2

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

Description:

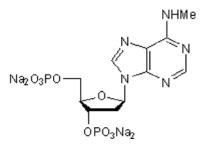
MRS 2179 tetrasodium salt is a competitive antagonist at P2Y₁ receptors (K_B = 100 nM). Selective over P2X₁ (IC₅₀ = 1.15 μ M), P2X₃ (IC₅₀ = 12.9 μ M), P2X₂, P2X₄, P2Y₂, P2Y₄ and P2Y₆ receptors. Inhibits the upregulation of NTPDase1 by ATP_YS.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{11}H_{13}N_5O_9P_2Na_4.3.75H_2O$ Batch Molecular Weight: 580.72 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C. This product is packaged under an inert atmosphere.

Catalog No.: 0900

Solubility & Usage Info:

water to 50 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. 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:

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.

Brown et al (2000) Activity of novel adenine nucleotide derivatives as agonists and antagonists at recombinant rat P2X receptors. Drug Dev.Res. 49 253. PMID: 22791931.

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.

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