

# Certificate of Analysis

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**Product Name:** MRS 2179 tetrasodium salt

**Catalog No.:** 0900

**Batch No.:** 10

**CAS Number:** 1454889-37-2

**IUPAC Name:** 2'-Deoxy-*N*<sup>6</sup>-methyladenosine 3',5'-bisphosphate tetrasodium salt

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>11</sub>H<sub>13</sub>N<sub>5</sub>O<sub>9</sub>P<sub>2</sub>Na<sub>4</sub>·3.75H<sub>2</sub>O

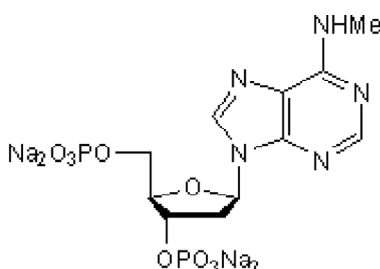
**Batch Molecular Weight:** 580.72

**Physical Appearance:** White solid

**Solubility:** water to 50 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 98.7% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen	Sodium
Theoretical	22.75	3.56	12.06	
Found	23.02	4.07	12.02	

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**Description:**

MRS 2179 tetrasodium salt is a competitive antagonist at P2Y<sub>1</sub> receptors ( $K_B$  = 100 nM). Selective over P2X<sub>1</sub> ( $IC_{50}$  = 1.15  $\mu$ M), P2X<sub>3</sub> ( $IC_{50}$  = 12.9  $\mu$ M), P2X<sub>2</sub>, P2X<sub>4</sub>, P2Y<sub>2</sub>, P2Y<sub>4</sub> and P2Y<sub>6</sub> receptors. Inhibits the upregulation of NTPDase1 by ATP $\gamma$ S.

**Physical and Chemical Properties:**

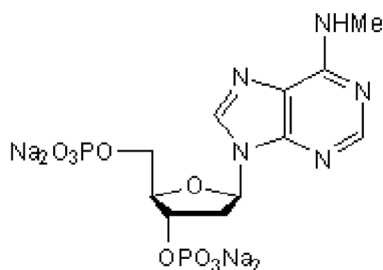
Batch Molecular Formula: C<sub>11</sub>H<sub>13</sub>N<sub>5</sub>O<sub>9</sub>P<sub>2</sub>Na<sub>4</sub>·3.75H<sub>2</sub>O

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.

**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°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.

**References:**

**Lu *et al*** (2007) Stimulation of the P2Y<sub>1</sub> 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 P2Y<sub>1</sub> receptor ligands. *J.Med.Chem.* **43** 829. PMID: 10715151.

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