

Product Name: MRS 2500 tetraammonium salt

Catalog No.: 2159

Batch No.: 6

CAS Number: 630103-23-0

IUPAC Name: (1*R**,2*S**)-4-[2-Iodo-6-(methylamino)-9*H*-purin-9-yl]-2-(phosphonoxy)bicyclo[3.1.0]hexane-1-methanol dihydrogen phosphate ester tetraammonium salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₁₈N₅O₈P₂·4NH₃

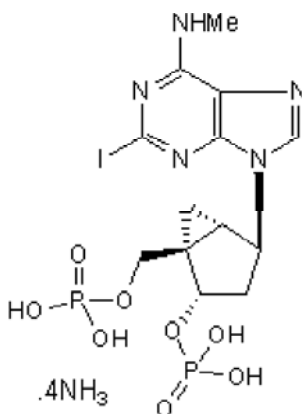
Batch Molecular Weight: 629.29

Physical Appearance: White solid

Solubility: water to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

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

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Description:

Highly potent and selective antagonist of the platelet P2Y₁ receptor (K_i = 0.78 nM). Inhibits ADP-induced aggregation of human platelets with an IC₅₀ value of 0.95 nM. Inhibits the upregulation of NTPDase1 by ATPγS. Prevents thrombus formation in vivo.

Physical and Chemical Properties:

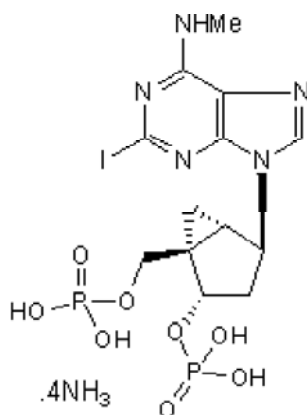
Batch Molecular Formula: C₁₃H₁₈N₅O₈P₂·4NH₃

Batch Molecular Weight: 629.29

Physical Appearance: White solid

Minimum Purity: ≥96%

Batch Molecular Structure:



Storage: Store at -20°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:

water to 20 mM

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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 under license from the NIH, US Patent 10/169975

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.

Hechler et al (2006) MRS2500 [2-iodo-N⁶-methyl-(*N*)-methanocarba-2'-deoxyadenosine-3', 5'-bisphosphate], a potent, selective, and stable antagonist of the platelet P2Y₁ receptor with strong antithrombotic activity in mice. *J.Pharmacol.Exp.Ther.* **316** 556. PMID: 16236815.

Cattaneo et al (2004) Antiaggregatory activity in human platelets of potent antagonists of the P2Y₁ receptor. *Biochem.Pharmacol.* **68** 1995. PMID: 15476670.

Kim et al (2003) 2-Substitution of adenine nucleotide analogues containing a bicyclo[3.1.0]hexane ring system locked in a northern conformation: enhanced potency as P2Y₁ receptor antagonists. *J.Med.Chem* **46** 4974. PMID: 14584948.

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