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TOCRIS

Print Date: Mar 5th 2024

Certificate of Analysis

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Product Name: **MRS 2279** **Catalog No.: 2158** **Batch No.: 1**

CAS Number: 2387505-47-5

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{13}H_{18}ClN_5O_8P_2.2NH_3.2H_2O$

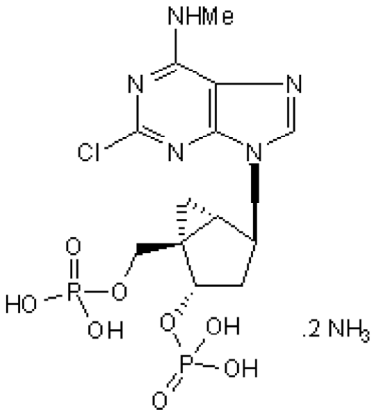
Batch Molecular Weight: 539.81

Physical Appearance: Beige solid

Solubility: water to 100 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.58 (Isopropanol:Water:Ammonia [6:3:1])

HPLC: Shows >98% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	28.93	5.23	18.16
Found	28.29	5.11	18.53

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

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Description:

MRS 2279 is a selective, high affinity competitive antagonist of the $P2Y_1$ receptor (K_i = 2.5 nM; IC_{50} = 51.6 nM). Fails to block nucleotide signaling at most other P2Y receptors ($P2Y_2$, $P2Y_4$, $P2Y_6$, $P2Y_{11}$ and $P2Y_{12}$) and potently inhibits ADP-induced aggregation of human blood platelets in vitro (pK_B = 8.05).

Physical and Chemical Properties:

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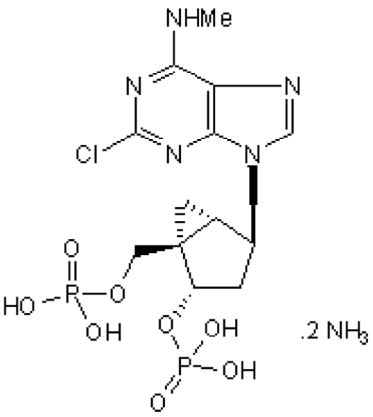
Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at -20°C

Solubility & Usage Info:

water to 100 mM

This product is supplied in lyophilized form. It may appear as a solid, gel or film and 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. *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.

Licensing Information:

Sold under license from the NIH, US Patent 10/169975

References:

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 $P2Y_1$ receptor antagonists. J.Med.Chem ***46*** 4974. PMID: 14584948.

Boyer *et al* (2002) 2-Chloro N^6-methyl-(N)-methanocarba-2'-deoxyadenosine-3',5'-bisphosphate is a selective high affinity $P2Y_1$ receptor antagonist. Br.J.Pharmacol. ***135*** 2004. PMID: 11959804.

Nandanan *et al* (2000) Synthesis, biological activity, and molecular modeling of ribose-modified deoxyadenosine bisphosphate analogues as $P2Y_1$ receptor ligands. J.Med.Chem. ***43*** 829. PMID: 10715151.