1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{13}\text{H}_{18}\text{N}_{5}\text{O}_{8}\text{P}_{2}\cdot 4\text{NH}_{3} \)

Batch Molecular Weight: 629.29

Physical Appearance: Beige solid

Solubility: water to 100 mM

Storage: Store at -20°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.39 \) (Isopropanol:Ammonia solution:Water [6:3:1])

HPLC: Shows 97.6% purity

\(^1\text{H} \text{NMR:} \) Consistent with structure

Mass Spectrum: Consistent with structure
Product Name: MRS 2500 tetraammonium salt
CAS Number: 630103-23-0
IUPAC Name: (1R*,2S*)-4-[2-Iodo-6-(methylamino)-9H-purin-9-yl]-2-(phosphonooxy)bicyclo[3.1.0]hexane-1-methanol dihydrogen phosphate ester tetraammonium salt

Description:
Highly potent and selective antagonist of the platelet P2Y₁ receptor (Kᵢ = 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: C₁₃H₁₈N₄O₅P₂J₄NH₄₃
Batch Molecular Weight: 629.29
Physical Appearance: Beige solid
Minimum Purity: >96%

Solubility & Usage Info:
Water to 100 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: