

Certificate of Analysis

Product Name: HEMADO

Catalog No.: 1579

Batch No.: 1

CAS Number: 403842-38-6

IUPAC Name: 2-(1-Hexynyl)-*N*-methyladenosine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{23}N_5O_4 \cdot \frac{3}{4}H_2O$

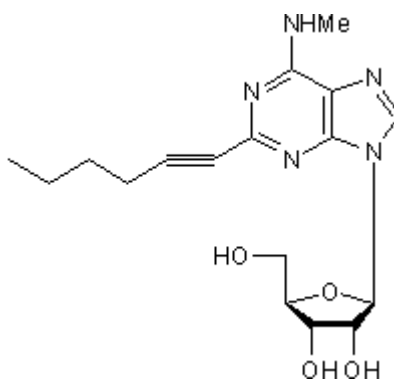
Batch Molecular Weight: 374.91

Physical Appearance: White solid

Solubility: ethanol to 100 mM
DMSO to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.18$ (Dichloromethane:Methanol:Ammonia soln. [9:1:0.1])

Melting Point: At 160°C

HPLC: Shows >99.8% purity

¹H NMR: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.46	6.59	18.68
Found	54.67	6.24	18.52

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

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IUPAC Name: 2-(1-Hexynyl)-N-methyladenosine

Description:

High affinity and selective adenosine A₃ receptor agonist (K_i values are 1.1, 327, 1230 and > 30,000 nM for human A₃, A₁, A_{2A} and A_{2B} receptors respectively).

Physical and Chemical Properties:

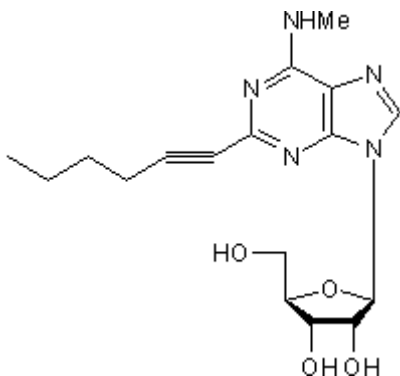
Batch Molecular Formula: C₁₇H₂₃N₅O₄·¾H₂O

Batch Molecular Weight: 374.91

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

ethanol to 100 mM

DMSO to 100 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. 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:

Volpini et al (2002) N⁶-Alkyl-2-alkynyl derivatives of adenosine as potent and selective agonists at the human adenosine A₃ receptor and a starting point for searching A_{2B} ligands *J.Med.Chem.* **45** 3271. PMID: 12109910.

Klotz et al (2006) [³H]HEMADO- a novel tritiated agonist selective for the human adenosine A₃-receptor. *Eur.J.Pharmacol.* **556** 14. PMID: 17126322.

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