

Certificate of Analysis

Product Name: Abacavir hemisulfate

Catalog No.: 4148

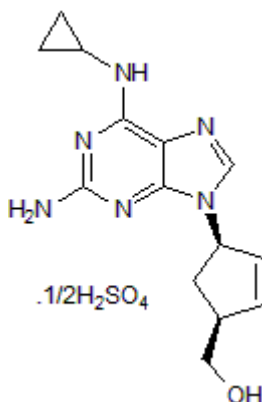
Batch No.: 1

CAS Number: 188062-50-2

IUPAC Name: (1*S*,4*R*)-4-[2-Amino-6-(cyclopropylamino)-9*H*-purin-9-yl]-2-cyclopentene-1-methanol hemisulfate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	$C_{14}H_{18}N_6O \cdot 1/2H_2SO_4 \cdot 1/4H_2O$
Batch Molecular Weight:	339.87
Physical Appearance:	Off White solid
Solubility:	water to 100 mM DMSO to 50 mM
Storage:	Store at +4°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 99.8% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	49.48	5.78	24.73
Found	49.48	5.59	24.9

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

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Description:

Competitive reverse transcriptase inhibitor; inhibits HIV replication. Orally active and brain penetrant. Antiretroviral agent.

Physical and Chemical Properties:

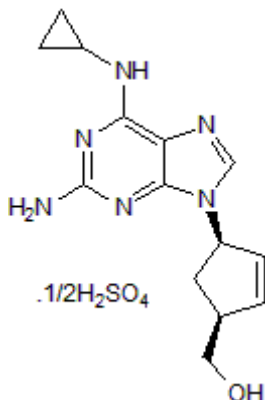
Batch Molecular Formula: C₁₄H₁₈N₆O.1/2H₂SO₄.¼H₂O

Batch Molecular Weight: 339.87

Physical Appearance: Off White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

water to 100 mM

DMSO 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. 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:

Daluge et al (1997) 1592U89, a novel carbocyclic nucleoside analog with potent, selective anti-human immunodeficiency virus activity. *Antimicrob Agents Chemother.* **41** 1082. PMID: 9145874.

Harrigan et al (2000) Resistance profile of the human immunodeficiency virus type 1 reverse transcriptase inhibitor abacavir (1592U89) after monotherapy and combination therapy. *CNA2001 Investigative Group. J.Infect.Dis.* **181** 912. PMID: 10720512.

Charneira et al (2012) N-terminal valine adduct from the anti-HIV drug abacavir in rat haemoglobin as evidence for abacavir metabolism to a reactive aldehyde in vivo. *Br.J.Pharmacol.* **167** 1353. PMID: 22725138.

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