Print Date: Jul 26th 2022

Certificate of Analysis

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Product Name: **Entecavir** **Catalog No.: 6234** **Batch No.: 1**

CAS Number: 142217-69-4

IUPAC Name: 2-Amino-1,9-dihydro-9-[(1*S*,3*R*,4*S*)-4-hydroxy-3-(hydroxymethyl)-2-methylenecyclopentyl]-6*H*-purin-6-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{12}H_{15}N_5O_3.H_2O$

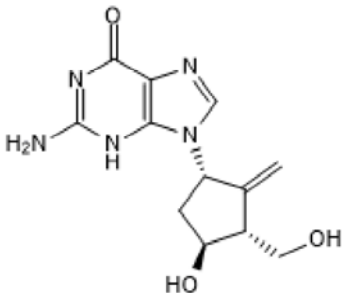
Batch Molecular Weight: 295.3

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	48.81	5.8	23.72
Found	48.97	5.76	23.71

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

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Description:

Entecavir is a potent and selective hepatitis B virus reverse transcriptase inhibitor (EC_{50} = 3 nM); guanine analog. Inhibits hepatitis B virus replication in HepG2.2.15 cells. Displays selectively over HCMV, HSV-1, VZV, HIV and influenza (EC_{50} values are 15, 32, 30-60, >10 and >80 µM respectively). Orally bioavailable.

Physical and Chemical Properties:

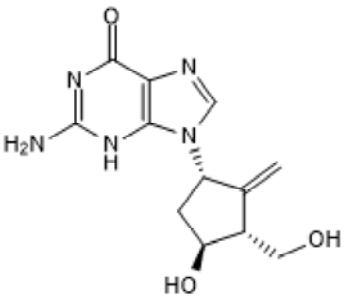
Batch Molecular Formula: $C_{12}H_{15}N_5O_3.H_2O$

Batch Molecular Weight: 295.3

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

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:

Bisacchi *et al* (1997) BMS-200475, a novel carbocyclic 2'-deoxyguanosine analog with potent and selective anti-hepatitis B virus activity *in vitro* Bioorganic & Medicinal Chemistry Letters ***7*** 127.

Innaimo *et al* (1997) Identification of BMS-200475 as a potent and selective inhibitor of hepatitis B virus. Antimicrob. Agents Chemother. ***41*** 1444. PMID: 9210663.