

Product Name: BMS 986094

Catalog No.: 6974

Batch No.: 1

CAS Number: 1234490-83-5

IUPAC Name: Neopentyl [[[(2*R*,3*R*,4*R*,5*R*)-5-(2-amino-6-methoxy-9*H*-purin-9-yl)-3,4-dihydroxy-4-methyltetrahydrofuran-2-yl]methoxy](naphthalen-1-yloxy)phosphoryl]-L-alaninate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₀H₃₉N₆O₉P.¾H₂O

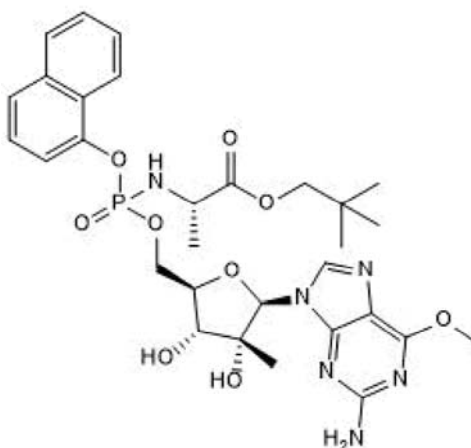
Batch Molecular Weight: 672.16

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.61	6.07	12.5
Found	53.56	5.85	12.43

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

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Description:

Potent hepatitis C virus (HCV) replication inhibitor ($EC_{50} = 35$ nM). Is rapidly metabolized in primary human hepatocytes to 2'-C-methyl guanosine triphosphate, an inhibitor of HCV RNA-dependent RNA polymerase NS5b. Displays 10-fold reduction in potency in S282T mutant-expressing versus wild-type replicons. Exhibits synergy with Ribavirin (Cat. No. 4501). Orally bioavailable.

Physical and Chemical Properties:

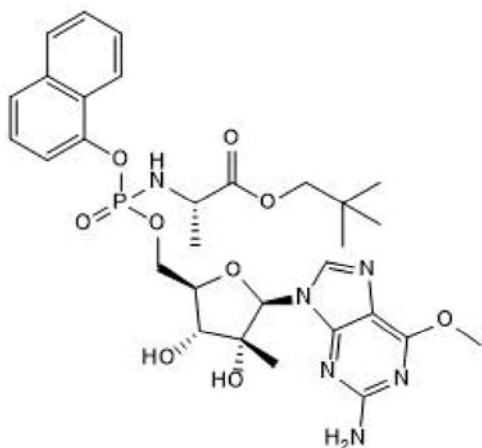
Batch Molecular Formula: $C_{30}H_{39}N_6O_9P \cdot \frac{3}{4}H_2O$

Batch Molecular Weight: 672.16

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Vernachio et al (2011) INX-08189, a phosphoramidate prodrug of 6-O-methyl-2'-C-methyl guanosine, is a potent inhibitor of hepatitis C virus replication with excellent pharmacokinetic and pharmacodynamic properties. *Antimicrob.Agents Chemother.* **55** 1843. PMID: 21357300.

McGuigan et al (2010) Design, synthesis and evaluation of a novel double pro-drug: INX-08189. A new clinical candidate for hepatitis C virus. *Bioorg.Med.Chem.Lett.* **20** 4850. PMID: 20637609.

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