Emivirine

Cat. No.: HY-15353

CAS No.: 149950-60-7

Molecular Formula: $C_{17}H_{22}N_2O_3$

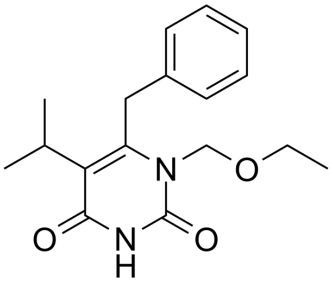
Molecular Weight: 302.37

Target: HIV

Pathway: Anti-infection

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (330.72 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.3072 mL	16.5360 mL	33.0721 mL
	5 mM	0.6614 mL	3.3072 mL	6.6144 mL
	10 mM	0.3307 mL	1.6536 mL	3.3072 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (8.27 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (8.27 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Emivirine (MKC-442) is a non-nucleoside reverse transcriptase inhibitors (NNRTIs) with K_i values of 0.20 and 0.01 μM for dTTP- and dGTP-dependent DNA or RNA polymerase activity, respectively. Emivirine displays potent and selective anti-human immunodeficiency virus type 1 (HIV-1) activity[1][2].

In Vitro

Emivirine (EMV) is also specific for HIV-1 RT and was without effect on HIV-2[2].
Emivirine (EMV) has no obvious toxicity for human healthy cells[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[2]

Cell Line:	Human bone marrow cells collected from normal healthy volunteers.
Concentration:	0, 0.1, 1, 10, or 100 μM.
Incubation Time:	14 days.
Result:	At concentrations of 0.1 to 10 μM, no effect on cell growth, lactic acid production, mitochondrial DNA synthesis, or mitochondrial structure was seen compared to what occurred with untreated HepG2 cells.

In Vivo

Tthe approximate lethal oral dose of Emivirine (EMV) for rats was ≥3 g/kg for males and 2.5 g/kg for females[2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male Sprague-Dawley rats[2].
Dosage:	50 mg/kg.
Administration:	Gavage.
Result:	The oral absorption was 68%.

REFERENCES

[1]. Panita Decha, et al. Theoretical studies on the molecular basis of HIV-1RT/NNRTIs interactions. J Enzyme Inhib Med Chem. 2011 Feb;26(1):29-36.

[2]. G M Szczech, et al. Safety assessment, in vitro and in vivo, and pharmacokinetics of emivirine, a potent and selective nonnucleoside reverse transcriptase inhibitor of human immunodeficiency virus type 1. Antimicrob Agents Chemother. 2000 Jan;44(1):123-30

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