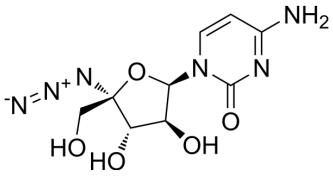
RO-9187

Cat. No.:	HY-10870
CAS No.:	876708-03-1
Molecular Formula:	$C_9H_{12}N_6O_5$
Molecular Weight:	284.23
Target:	HCV
Pathway:	Anti-infection

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (351.83 mM; Need ultrasonic)

H_2O : 5 mg/mL (17.59 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	3.5183 mL	17.5914 mL	35.1828 mL
5 mM	0.7037 mL	3.5183 mL	7.0366 mL
10 mM	0.3518 mL	1.7591 mL	3.5183 mL

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

In Vivo

1. Add each solvent one by one: PBS
   Solubility: 5.88 mg/mL (20.69 mM); Clear solution; Need ultrasonic and warming and heat to 60°C
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: 2.5 mg/mL (8.80 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (8.80 mM); Clear solution; Need ultrasonic
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (8.80 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

RO-9187 is a potent inhibitor of HCV virus replication with an IC_{50} of 171 nM. RO-9187 is a click chemistry reagent, it contains an Azide group and can undergo copper-catalyzed azide-alkyne cycloaddition reaction (CuAAc) with molecules containing Alkyne groups. Strain-promoted alkyne-azide cycloaddition (SPAAC) can also occur with molecules containing DBCO or BCN groups.

IC_{50} & Target	IC50: 171 nM (HCV)[1]
In Vitro	RO-9187 is excellent substrates for deoxycytidine kinase and is phosphorylated with efficiencies up to 3-fold higher than deoxycytidine. RO-9187 inhibits RNA synthesis by HCV polymerases from either HCV genotypes 1a and 1b or containing S96T or S282T point mutations with similar potencies, suggesting no cross-resistance with either R1479 (4′-azidocytidine) or 2′-C-methyl nucleosides. The formation of RO-9187-TP increased in a time- and dose-dependent manner. The maximal triphosphate concentration at 24 h is 87 pmol/106 cells with half-maximal triphosphate formation achieved at 12 μM RO-9187[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Plasma exposures of RO-9187 in rats increase in a dose-dependent manner between 10 and 2000 mg/kg after oral dosing. Plasma concentrations of 1.4 and 26 μM (390 and 7454 ng/mL) are achieved in rats and dogs at the 10 mg/kg dose level, respectively. Plasma concentrations up to 57 μM are achieved in rats dosed with 2000 mg/kg/day[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Animal Administration [1]	Rats: A 2-week oral range finding toxicity study is performed with RO-9187 and ribavirin in Hanover-Wistar rats. Five male and five female rats in each of five treatment groups are administered once daily doses of vehicle, 200, 600, or 2000 mg/kg RO-9187 or 200 mg/kg ribavirin by oral gavage for 14 days[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Antiviral Res. 2021 Jan;185:104968.
- Antiviral Res. 2016 Sep;133:119-29.
- J Infect Dis. 2016 Sep 1;214(5):707-11.
- J Virol. 2017 Oct 13;91(21):e01028-17.
- Antiviral Res. 2019 Oct;170:104570.

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REFERENCES

[1]. Klumpp K, et al. 2'-deoxy-4'-azido nucleoside analogs are highly potent inhibitors of hepatitis C virus replication despite the lack of 2'-alpha-hydroxyl groups. J Biol Chem. 2008 Jan 25;283(4):2167-75.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA