ABT-072

Cat. No.: HY-101634 CAS No.: 1132936-00-5 Molecular Formula: $C_{24}H_{27}N_3O_5S$ Molecular Weight: 469.55 Target: HCV

Pathway: Anti-infection

Storage: Powder -20°C 3 years

4°C 2 years

In solvent -80°C 6 months

> -20°C 1 month

Product Data Sheet

SOLVENT & SOLUBILITY

In Vitro

DMSO: 80 mg/mL (170.38 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.1297 mL	10.6485 mL	21.2970 mL
	5 mM	0.4259 mL	2.1297 mL	4.2594 mL
	10 mM	0.2130 mL	1.0648 mL	2.1297 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: ≥ 4 mg/mL (8.52 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE- β -CD in saline) Solubility: ≥ 4 mg/mL (8.52 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: 4 mg/mL (8.52 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description	ABT-072 is an orally active and potent non-nucleoside HCV NS5B polymerase inhibitor (HCV GT1a EC ₅₀ =1 nM; HCV GT1b EC ₅₀ =0.3 nM) $^{[1][2][3]}$.
IC ₅₀ & Target	NS5B polymerase $^{[1]}$
In Vitro	ABT-072 is a non-nucleoside NS5B polymerase inhibitor with nanomolar potency in vitro against genotype 1a and 1b hepatitis C virus polymerases ^[1] .

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.		
In Vivo	ABT-072 (5 and/or 30 mg/kg; i.v. or p.o.) shows good PK properties ^[3] . ABT-072 (2.5 and/or 30 mg/kg; i.v. or p.o.) shows low plasma clearance and high oral bioavailability ^[3] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.		
	Animal Model:	Rats ^[3]	
	Dosage:	5 and/or 30 mg/kg (Pharmacokinetic Analysis)	
	Administration:	I.v. or p.o.	
	Result:	Showed good PK properties.	
	Animal Model:	Dog ^[3]	
	Dosage:	2.5 or 30 mg/kg (Pharmacokinetic Analysis)	
	Administration:	I.v. or p.o.	
	Result:	Showed low plasma clearance and high oral bioavailability.	

REFERENCES

[1]. Lawitz E, et al. A phase 2a trial of 12-week interferon-free therapy with two direct-acting antivirals (ABT-450/r, ABT-072) and ribavirin in IL28B C/C patients with chronic hepatitis C genotype 1. J Hepatol. 2013;59(1):18-23.

[2]. Shi Y, et al. Assessing Supersaturation and Its Impact on In Vivo Bioavailability of a Low-Solubility Compound ABT-072 With a Dual pH, Two-Phase Dissolution Method. J Pharm Sci. 2016;105(9):2886-2895.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

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