ABT-072 potassium trihydrate

Cat. No.: HY-101634A

CAS No.: 1132940-31-8

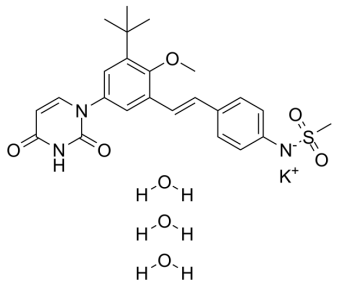
Molecular Formula: $C_{24}H_{32}KN_3O_8S$

Molecular Weight: 561.69

Target: HCV

Pathway: Anti-infection

Storage: 4°C, sealed storage, away from moisture and light
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (89.02 mM; Need ultrasonic)

H_2O : < 0.1 mg/mL (ultrasonic;warming;heat to 60°C) (insoluble)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.7803 mL	8.9017 mL	17.8034 mL
	5 mM	0.3561 mL	1.7803 mL	3.5607 mL
	10 mM	0.1780 mL	0.8902 mL	1.7803 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: ≥ 5 mg/mL (8.90 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 5 mg/mL (8.90 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ABT-072 (potassium trihydrate) 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 (potassium trihydrate) 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.) (potassium trihydrate) shows good PK properties[3].

ABT-072 (2.5 and/or 30 mg/kg; i.v. or p.o.) (potassium trihydrate) 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.

[3]. Randolph JT, et al. Synthesis and Biological Characterization of Aryl Uracil Inhibitors of Hepatitis C Virus NS5B Polymerase: Discovery of ABT-072, a trans-Stilbene Analog with Good Oral Bioavailability. J Med Chem. 2018;61(3):1153-1163.

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