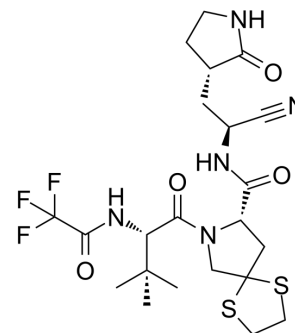


Simnotrelvir

Cat. No.:	HY-154965		
CAS No.:	2920904-06-7		
Molecular Formula:	C ₂₂ H ₃₀ F ₃ N ₅ O ₄ S ₂		
Molecular Weight:	549.63		
Target:	SARS-CoV		
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 (181.94 mM; Need ultrasonic)

Concentration	Solvent	Mass	1 mg	5 mg	10 mg
			1 mg	5 mg	10 mg
Preparing Stock Solutions	1 mM		1.8194 mL	9.0970 mL	18.1941 mL
	5 mM		0.3639 mL	1.8194 mL	3.6388 mL
	10 mM		0.1819 mL	0.9097 mL	1.8194 mL

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

In Vivo

- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
Solubility: 2.5 mg/mL (4.55 mM); Clear solution; Need ultrasonic
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
Solubility: 2.5 mg/mL (4.55 mM); Clear solution; Need ultrasonic
- Add each solvent one by one: 10% DMSO >> 90% corn oil
Solubility: 2.5 mg/mL (4.55 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

SARS-CoV-2-IN-41 (compound 2) is a potent SARS-CoV-2 3CL^{Pro} inhibitor with an IC₅₀ value of 0.022 μM. SARS-CoV-2-IN-41 shows antiviral effect^[1].

IC₅₀ & Target

IC₅₀: 0.022 μM (SARS-CoV-2 3CL^{Pro})^[1]

In Vivo

SARS-CoV-2-IN-41 (50, 200 mg/kg; I.p.) antiviral effect in SARS-CoV-2 infected mice^[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	7-8 weeks, hACE2-K18 transgenic mice (infected with the delta strain of SARS-CoV-2 by intranasal drops) ^[1]
Dosage:	50, 200 mg/kg (combined with 50 mg/kg cytochrome P450 inhibitor ritonavir)
Administration:	I.p.; dose on day 0 1 time, 2 times on the 1st day, 1 time on the 2nd day
Result:	Significantly reduced the viral load in the lungs, after 4 days of infection, a sustained inhibitory effect of compound 2 on viral copy number was observed.

REFERENCES

[1]. XiangRui et al. Cyano compound, and preparation method therefor and use thereof. WO2023051657A1.

Caution: Product has not been fully validated for medical applications. For research use only.

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