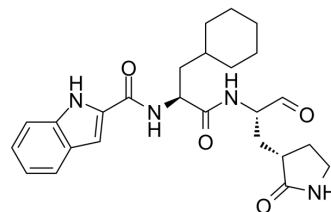


Bofutrelvir

Cat. No.:	HY-133894
CAS No.:	2103278-86-8
Molecular Formula:	C ₂₅ H ₃₂ N ₄ O ₄
Molecular Weight:	452.55
Target:	SARS-CoV
Pathway:	Anti-infection
Storage:	-20°C, protect from light, stored under nitrogen * In solvent : -80°C, 6 months; -20°C, 1 month (protect from light, stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro	DMSO : 100 mg/mL (220.97 mM; Need ultrasonic)					
		Solvent Concentration	Mass			
	Preparing Stock Solutions			1 mg	5 mg	10 mg
		1 mM		2.2097 mL	11.0485 mL	22.0970 mL
		5 mM		0.4419 mL	2.2097 mL	4.4194 mL
	10 mM		0.2210 mL	1.1049 mL	2.2097 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 (5.52 mM); Clear solution					
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: 2.5 mg/mL (5.52 mM); Suspended solution; Need ultrasonic					
	3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (5.52 mM); Clear solution					

BIOLOGICAL ACTIVITY

Description	Bofutrelvir (FB2001) is a SARS-CoV-2 main protease M ^{pro} inhibitor with an IC ₅₀ value of 53 nM and an EC ₅₀ value of 0.53 μM. Bofutrelvir exhibits potent antiviral efficacy against several current SARS-CoV-2 variants with EC ₅₀ values of 0.26-0.42 μM. Bofutrelvir has an additive antiviral effect when combined with Remdesivir (HY-104077) ^{[1][2]} .
IC₅₀ & Target	IC ₅₀ : 53 nM (M ^{pro}) ^[1]
In Vitro	Bofutrelvir (24 h) shows in vitro activity against SARS-CoV-2 and its variants with EC ₅₀ values of 0.42, 0.39, 0.28, 0.27 and 0.26 μM for SARS-CoV-2, SARS-CoV-2 (Alpha), SARS-CoV-2 (Beta), SARS-CoV-2 (Delta) and SARS-CoV-2 (Omicron), respectively ^[2] .

Bofutrelvir inhibits SARS-CoV-2 replication in vero E6 cells in the presence of human serum (1.1-2.4 μ M) even at the dose of EC₅₀ values^[2].

Bofutrelvir exhibits an additive effect against SARS-CoV-2 in vitro when combined treatment with remdesivi^[2].

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

In Vivo

Bofutrelvir (100 and 200 mg/kg; i.p. once daily on day 0 and twice daily on day 1, 2 and 3 for 4 consecutive days) effectively against SARS-CoV-2 delta variant infection in vivo^[2].

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

Animal Model:	K18-hACE2 mice with SARS-CoV-2 delta variant infection ^[2]
Dosage:	100 and 200 mg/kg
Administration:	Intraperitoneal injection; 100 and 200 mg/kg once daily on day 0 and twice daily on day 1, 2 and 3 for 4 consecutive days
Result:	Showed a dose-dependent efficacy to virus titers of lung. Effectively reduces the lung viral loads. Dose-dependently showed antiviral activity against the SARS-CoV-2 Delta variant and significantly reduced viral load in mouse lung and brain.

REFERENCES

[1]. Ullrich S, Nitsche C. The SARS-CoV-2 main protease as drug target. *Bioorg Med Chem Lett*. 2020 Sep 1;30(17):127377.

[2]. Shang W, et al. In vitro and in vivo evaluation of the main protease inhibitor FB2001 against SARS-CoV-2. *Antiviral Res*. 2022 Dec;208:105450.

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

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