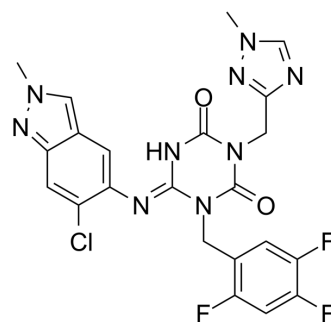


Ensitrelvir

Cat. No.:	HY-143216		
CAS No.:	2647530-73-0		
Molecular Formula:	C ₂₂ H ₁₇ ClF ₃ N ₉ O ₂		
Molecular Weight:	531.88		
Target:	SARS-CoV; Virus Protease		
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 : 50 mg/mL (94.01 mM; Need ultrasonic)			
		Solvent Concentration	Mass	
			1 mg	5 mg
			10 mg	
Preparing Stock Solutions	1 mM	1.8801 mL	9.4006 mL	18.8012 mL
	5 mM	0.3760 mL	1.8801 mL	3.7602 mL
	10 mM	0.1880 mL	0.9401 mL	1.8801 mL
Please refer to the solubility information to select the appropriate solvent.				
In Vivo	<ol style="list-style-type: none"> Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (4.70 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (4.70 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (4.70 mM); Clear solution 			

BIOLOGICAL ACTIVITY

Description	Ensitrelvir (S-217622) is the first orally active non-covalent, non-peptidic, SARS-CoV-2 3CL protease inhibitor (IC ₅₀ =13 nM) ^[1] [2].
In Vitro	In a cytopathic effect (cpe)-inhibition assay of SARS-CoV-2 infected VeroE6/TMPRSS2 cells, Ensitrelvir shows the EC ₅₀ values are approximately 0.4 μM for both wild-type virus and Alpha, Beta, Gamma and Delta variants. EC ₅₀ values for SARS-CoV and MERS-CoV were 0.21 and 1.4 μM respectively ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

Ensitrelvir dose-dependently inhibits intrapulmonary replication of SARS-CoV-2 in mice^[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Nat Commun. 2023 Feb 25;14(1):1076.
- J Biol Chem. 2023 Jun 2;104886.
- bioRxiv. 2023 Feb 27.

See more customer validations on www.MedChemExpress.com

REFERENCES

[1]. McKimm-Breschkin JL, et al. COVID-19, Influenza and RSV: Surveillance-informed prevention and treatment - Meeting report from an isiv-WHO virtual conference. Antiviral Res. 2022;197:105227.

[2]. Yuto Unoh, et al. Discovery of S-217622, a Non-Covalent Oral SARS-CoV-2 3CL Protease Inhibitor Clinical Candidate for Treating COVID-19. bioRxiv 2022.01.26.477782.

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

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