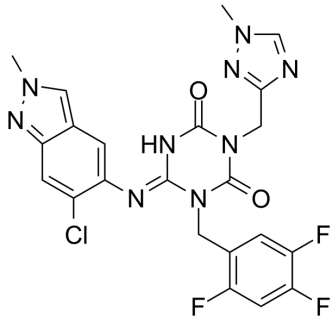
Ensitrelvir

Cat. No.:	HY-143216
CAS No.:	2647530-73-0
Molecular Formula:	$C_{22}H_{17}ClF_3N_9O_2$
Molecular Weight:	532
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 (93.98 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8797 mL	9.3985 mL	18.7970 mL
	5 mM	0.3759 mL	1.8797 mL	3.7594 mL
	10 mM	0.1880 mL	0.9398 mL	1.8797 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 (4.70 mM); Clear solution
2. 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
3. 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.
- Structure. 2023 Jun 27;S0969-2126(23)00207-1.
- J Biol Chem. 2023 Jun 2;104886.
- bioRxiv. 2023 Nov 27.
- bioRxiv. 2023 Oct 21.

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REFERENCES

[1]. McKimm-Breschkin JL, et al. COVID-19, Influenza and RSV: Surveillance-informed prevention and treatment - Meeting report from an isirv-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.

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