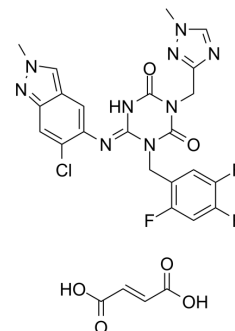


Ensitrelvir fumarate

Cat. No.:	HY-143216A
CAS No.:	2757470-18-9
Molecular Formula:	C ₂₆ H ₂₁ ClF ₃ N ₉ O ₆
Molecular Weight:	647.95
Target:	SARS-CoV; Virus Protease
Pathway:	Anti-infection
Storage:	4°C, sealed storage, away from moisture * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro	DMSO : 50 mg/mL (77.17 mM; Need ultrasonic)					
	Preparing Stock Solutions	Solvent Concentration	Mass	1 mg	5 mg	10 mg
		1 mM		1.5433 mL	7.7166 mL	15.4333 mL
		5 mM		0.3087 mL	1.5433 mL	3.0867 mL
		10 mM		0.1543 mL	0.7717 mL	1.5433 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 (3.86 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: 2.5 mg/mL (3.86 mM); Suspended solution; Need ultrasonic Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (3.86 mM); Clear solution 					

BIOLOGICAL ACTIVITY

Description	Ensitrelvir (S-217622) fumarate 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 fumarate 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 fumarate 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.

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

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