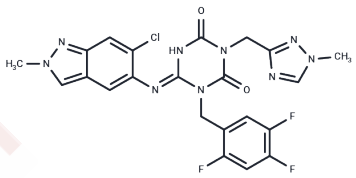
Data Sheet (Cat.No.T9716)

TargetMol

Ensitrelvir

Chemical Properties



CAS No. : 2647530-73-0

Formula: C22H17ClF3N9O2

Molecular Weight: 531.88

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Ensitrelvir (S-217622) is an orally active inhibitor of SARS-CoV-2 3CL protease with IC50 of 13 nM.
Targets(IC50)	SARS-CoV,Virus Protease
In vitro	The EC50 values for SARS-CoV and MERS-CoV were 0.21 and 1.4 μM respectively. In a cytopathic effect (cpe)-inhibition assay of SARS-CoV-2 infected VeroE6/TMPRSS2 cells, Ensitrelvir shows the EC50 values are approximately 0.4 μM for both wild-type virus and Alpha, Beta, Gamma and Delta variants[1].
In vivo	Ensitrelvir inhibits intrapulmonary replication of SARS-CoV-2 in mice in a dose-dependent manner[1].

Solubility Information

Solubility	DMSO: 75.76 mg/mL (142.44 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: < 7.58 mg/mL (14.25 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 7.58 mg/mL (14.25 mM),Solution. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.8801 mL	9.4006 mL	18.8012 mL
5 mM	0.376 mL	1.8801 mL	3.7602 mL
10 mM	0.188 mL	0.9401 mL	1.8801 mL
50 mM	0.0376 mL	0.188 mL	0.376 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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.
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.