

Ensitrelvir fumarate

Chemical Properties

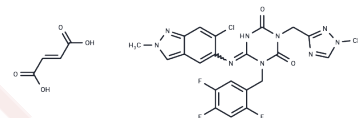
CAS No. : 2757470-18-9

Formula: C₂₆H₂₁ClF₃N₉O₆

Molecular Weight: 647.96

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) fumarate is a novel orally active inhibitor targeting the SARS-CoV-2 3CL protease (IC ₅₀ = 13 nM), demonstrating non-covalent and non-peptidic characteristics. This compound represents a pioneering advancement in the development of effective antiviral agents against the SARS-CoV-2 virus. |
| Targets(IC ₅₀) | Others,SARS-CoV,Virus Protease |
| In vitro | In a cytopathic effect (cpe)-inhibition assay on VeroE6/TMPRSS2 cells infected with SARS-CoV-2, Ensitrelvir fumarate demonstrated EC ₅₀ values of approximately 0.4 μM for the wild-type virus and the Alpha, Beta, Gamma, and Delta variants, and EC ₅₀ values of 0.21 μM and 1.4 μM for SARS-CoV and MERS-CoV, respectively[1]. |
| In vivo | Ensitrelvir fumarate effectively reduces SARS-CoV-2 replication within the lungs of mice in a dose-dependent manner[2]. |

Preparing Stock Solutions

| | 1mg | 5mg | 10mg |
|-------|-----------|-----------|------------|
| 1 mM | 1.5433 mL | 7.7165 mL | 15.4331 mL |
| 5 mM | 0.3087 mL | 1.5433 mL | 3.0866 mL |
| 10 mM | 0.1543 mL | 0.7717 mL | 1.5433 mL |
| 50 mM | 0.0309 mL | 0.1543 mL | 0.3087 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

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.

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.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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