

PRODUCT INFORMATION

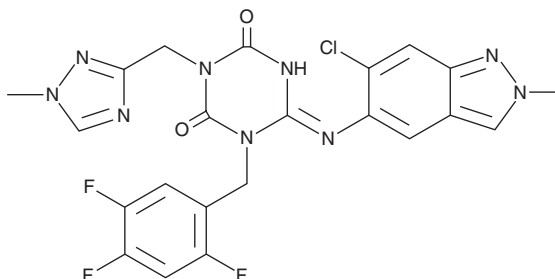


Ensitrelvir

Item No. 37945

CAS Registry No.: 2647530-73-0
Formal Name: 6E-[(6-chloro-2-methyl-2H-indazol-5-yl)imino]dihydro-3-[(1-methyl-1H-1,2,4-triazol-3-yl)methyl]-1-[(2,4,5-trifluorophenyl)methyl]-1,3,5-triazine-2,4(1H,3H)-dione

Synonym: S-217622
MF: C₂₂H₁₇ClF₃N₉O₂
FW: 531.9
Purity: ≥95%
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Ensitrelvir is supplied as a crystalline solid. A stock solution may be made by dissolving the ensitrelvir in the solvent of choice, which should be purged with an inert gas. Ensitrelvir is soluble in organic solvents such as ethanol and DMSO. The solubility of ensitrelvir in these solvents is approximately 1 mg/ml.

Description

Ensitrelvir is an orally bioavailable inhibitor of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) main protease (M^{pro}), also known as 3C-like protease (3CL^{pro}), with an IC₅₀ value of 0.013 μM.¹ It is selective for M^{pro} over HIV-1 protease and the human proteases caspase-2, chymotrypsin, thrombin, and cathepsin B, -D, -G, and -L (IC₅₀s = >100 μM for all). Ensitrelvir reduces the cytopathic effects of SARS-CoV-2 clinical isolates, including the Alpha, Beta, Gamma, Delta, and Omicron strains, SARS-CoV, and Middle East respiratory syndrome coronavirus (MERS-CoV), in Vero E6 cells expressing human transmembrane serine protease 2 (TMPRSS2; EC₅₀s = 0.29-1.4 μM). Oral administration of ensitrelvir decreases lung viral titers in a mouse model of SARS-CoV-2 Gamma variant infection when administered at doses ranging from 2 to 32 mg/kg at the time of, and 12 hours after, infection.

Reference

1. Unoh, Y., Uehara, S., Nakahara, K., *et al.* Discovery of S-217622, a noncovalent oral SARS-CoV-2 3CL protease inhibitor clinical candidate for treating COVID-19. *J. Med. Chem.* **65**(9), 6499-6512 (2022).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

WARRANTY AND LIMITATION OF REMEDY

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