

PRODUCT INFORMATION



Ensitrelvir (fumarate)

Item No. 35844

CAS Registry No.: 2757470-18-9

Formal Name: (6E)-6-[(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, (2E)-2-butenedioate

Synonym: S-217622

MF: $C_{22}H_{17}ClF_3N_9O_2 \cdot C_4H_4O_4$

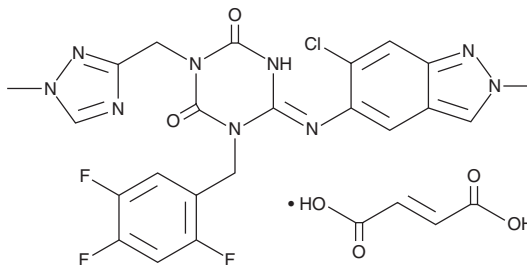
FW: 647.9

Purity: $\geq 98\%$

Supplied as: A 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 (fumarate) is supplied as a solid. A stock solution may be made by dissolving the ensitrelvir (fumarate) in the solvent of choice, which should be purged with an inert gas. Ensitrelvir (fumarate) is soluble in organic solvents such as DMSO and dimethyl formamide. The solubility of ensitrelvir (fumarate) in these solvents is approximately 10 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 IC_{50} value of $0.013 \mu\text{M}$.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 (IC_{50} s = $>100 \mu\text{M}$ for all). Ensitrelvir reduces the cytopathic effects of SARS-CoV-2 clinical isolates, including 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; EC_{50} s = $0.29\text{--}1.4 \mu\text{M}$). 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

Buyer agrees to purchase the material subject to Cayman's Terms and Conditions. Complete Terms and Conditions including Warranty and Limitation of Liability information can be found on our website.

Copyright Cayman Chemical Company, 04/16/2024

CAYMAN CHEMICAL

1180 EAST ELLSWORTH RD
ANN ARBOR, MI 48108 · USA

PHONE: [800] 364-9897
[734] 971-3335

FAX: [734] 971-3640

CUSTSERV@CAYMANCHEM.COM
WWW.CAYMANCHEM.COM