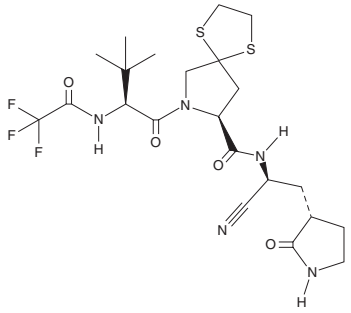
PRODUCT INFORMATION

Simnotrelvir

Item No. 46220

CAS Registry No.: 2920904-06-7
Formal Name: N-[(1S)-1-cyano-2 [(3S)-2-oxo-3-pyrrolidinyl] ethyl]-7-[(2S)-3,3-dimethyl-1-oxo-2-[(2,2,2-trifluoroacetyl)amino]butyl]-1,4-dithia-7-azaspiro[4.4]nonane-8S-carboxamide
MF: $C_{22}H_{30}F_3N_5O_4S_2$
FW: 549.6
Purity: ≥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

Simnotrelvir is supplied as a solid. A stock solution may be made by dissolving the simnotrelvir in the solvent of choice, which should be purged with an inert gas. Simnotrelvir is soluble (≥10 mg/ml) in ethanol and DMSO.

Description

Simnotrelvir is an inhibitor of the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) main protease (M^{pro}), also known as 3C-like protease ($3C^{pro}$; IC_{50} = 9 nM).[1] It is selective for M^{pro} over chymotrypsin at 20 µM, cathepsin A, D, E, and L at 100 µM, and a panel of 413 kinases at 10 µM. Simnotrelvir (200 mg/kg, p.o.) reduces lung and brain viral titers, alveolar atrophy, alveolar septal thickening, and neuron degeneration when administered with ritonavir (Item No. 13872) in a mouse model of SARS-CoV-2 infection.

Reference

1. Jiang, X., Su, H., Shang, W., *et al.* Structure-based development and preclinical evaluation of the SARS-CoV-2 3C-like protease inhibitor simnotrelvir. *Nat. Commun.* **14(1)**, 6463 (2023).

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.

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