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Data Sheet

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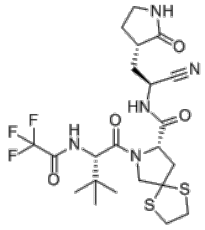
Product Name	:	Simnotrelvir
Cat. No.	:	PC-21243
CAS No.	:	2920904-06-7
Molecular Formula	:	$C_{22}H_{30}F_3N_5O_4S_2$
Molecular Weight	:	549.63
Target	:	SARS-CoV-2 Inhibitors
Solubility	:	10 mM in DMSO



CAS: 2920904-06-7

Biological Activity

Simnotrelvir (SSD8432, SIM0417) is a potent, selective, covalent and orally bioavailable SARS-CoV-2 3C-like protease (**3CLpro**) inhibitor with IC50 of 9 nM in enzymatic inhibition assays.
Simnotrelvir (SSD8432, SIM0417) shows binding Kd of 302 nM against C145G mutant 3CLpro in ITC assays.
Simnotrelvir (SSD8432, SIM0417) exhibits robust in vitro antiviral activity with nanomolar or low micromolar EC50CP and EC50 values in Vero E6 cells in the presence and absence of the P-glycoprotein inhibitor CP-100356 respectively.
Simnotrelvir (SSD8432, SIM0417) shows EC50CP values of 26, 34, and 43 nM against the SARS-CoV-2 WIV04, Delta and Omicron strains, respectively, with negligible cytotoxicity (CC50 > 500 μM).
Simnotrelvir (SSD8432, SIM0417) forms a reversible covalent bond to the catalytic C145.
Simnotrelvir (SSD8432, SIM0417) shows high specific for 3CLpro with weak inhibition on cathepsin B (IC50=7194 nM), no inhibitory effects on the 47 targets that are well-known contributors to clinical adverse drug reactions (ADRs).
Simnotrelvir (SSD8432, SIM0417) displays high potency (IC50: 8-13 nM) against six mutated 3CLpros (G15S, T21I, L89F, K90R, P132H, and L205V) that have been found in newly emerged SARS-CoV-2 variants, such as 3CLpro (P132H) in the Omicron variant.
Simnotrelvir (SSD8432, SIM0417) is a pan-CoV 3CLpro inhibitor, effectively inhibited the activity of 3CLpro from six human CoVs including SARS-CoV (IC50: 24 nM), MERS-CoV (IC50: 60 nM), HKU1-CoV (IC50: 10 nM), OC43-CoV (IC50: 5 nM), H229E-CoV (IC50: 129 nM), and NL63-CoV (IC50: 849 nM).
Simnotrelvir (SSD8432, SIM0417) (200 mg/kg, oral) demonstrates robust in vivo antiviral activity protects lung and brain tissues from lesions in K18-hACE2 mice infected with the SARS-CoV-2 Delta strain experiment, significantly reduces lung viral loads but also eliminates the virus from brains.

References

Xiangrui Jiang, et al. ***Nat Commun.*** 2023 Oct 13;14(1):6463.

Caution: Product has not been fully validated for medical applications. Lab Use Only!

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