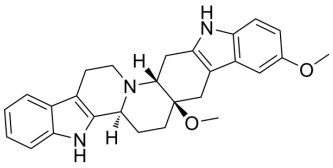
SIMR3030

Cat. No.:	HY-149940
CAS No.:	2708270-99-7
Molecular Formula:	$C_{27}H_{29}N_3O_2$
Molecular Weight:	427.54
Target:	SARS-CoV
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	SIMR3030 is a potent SARS-CoV-2 PLpro inhibitor with an IC_{50} value of 0.0399 μg/mL. SIMR3030 shows antiviral activity. SIMR3030 decreases SARS-CoV spike, ORF1b, IFN-α, IL-6 mRNA expression. SIMR3030 exhibits a satisfactory safety profile in mice[1].
IC_{50} & Target	IC_{50}: 0.0399 μg/mL (SARS-CoV-2 PLpro)[1]

In Vitro

SIMR3030 (0-100 μg/mL) shows antiviral activity with IC_{50} values of 12.1, 6.206 μg/mL for SARS-CoV-2 and MERS-CoV, respectively[1].

SIMR3030 (20 μg/mL; 1, 6, 12 h) decreases SARS-CoV spike, ORF1b, IFN-α, IL-6 mRNA expression levels in Caco-2 cells[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

RT-PCR[1]

Cell Line:	Caco-2 cells (SARS-CoV-2 RNA infected)
Concentration:	20 μg/mL
Incubation Time:	1, 6, 12 h
Result:	Decreased SARS-CoV spike and ORF1b mRNA expression levels, reduced the mRNA expression of IFN-α at 1 and 3 h , IL-6 and OAS1 at 1, 3 and 12 h.

In Vivo

SIMR3030 (25, 50, 100 mg/kg; I.p.; daily for 14 days) exhibits a satisfactory safety profile in experimental mice model[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	18-25 g, adult female Balb/c mice[1]
Dosage:	25, 50, 100 mg/kg
Administration:	I.p.; daily for 14 days
Result:	Showed no signs of toxicity or weight loss were noticed during 12.5 and 25 mg/kg multiple-dose studies for 14 days, no signs of toxicity or weight loss were noticed during 12.5 and 25 mg/kg multiple-dose studies for 14 days.

REFERENCES

[1]. Hersi F, et al. Discovery of novel papain-like protease inhibitors for potential treatment of COVID-19. Eur J Med Chem. 2023 Jun 5;254:115380.

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