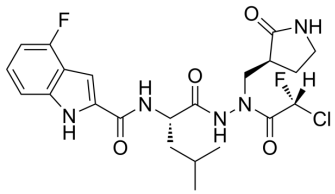
SARS-CoV-2 3CLpro-IN-5

Cat. No.:	HY-151535
CAS No.:	2913186-57-7
Molecular Formula:	$C_{22}H_{26}ClF_2N_5O_4$
Molecular Weight:	497.92
Target:	SARS-CoV
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	SARS-CoV-2 3CLpro-IN-5 is a covalent inhibitor of 3C-like protease ($3CL^{pro}$). SARS-CoV-2 3CLpro-IN-5 has inhibitory activity for $3CL^{pro}$ with an IC_{50} value of 3.8 nM. SARS-CoV-2 3CLpro-IN-5 has 9.0% oral bioavailability (BA). SARS-CoV-2 3CLpro-IN-5 can be used for the research of coronavirus disease 2019 (COVID-19)[1].
IC_{50} & Target	IC50: 3.8 nM ($3CL^{pro}$)[1]. EC50 for SARS-CoV-2 strains: 13.8 nM (α), 7.57 nM (δ), 9.01 nM (Om BA.1) and 17.1 nM (Om BA.2) [1]. EC50: 59.3 nM (SARS-CoV in 293TAT cells); 4.72 nM (MERS-CoV in 293TDPP4 cells); 1.67 nM (HCoV-OC43 in 293TAT cells)[1].
In Vitro	SARS-CoV-2 3CLpro-IN-5 has inhibitory activity for $3CL^{pro}$ with an IC_{50} value of 3.8 nM[1]. SARS-CoV-2 3CLpro-IN-5 has antiviral activity in 293TAT cells againsts various SARS-CoV-2 strains α, δ, Om BA.1 and Om BA.2 with EC_{50} values of 13.8 nM, 7.57 nM, 9.01 nM and 17.1 nM, respectively[1]. SARS-CoV-2 3CLpro-IN-5 has antiviral activity against various coronaviruses SARS-CoV (293TAT cells), MERS-CoV (293TDPP4 cells) and HCoV-OC43 (293TAT cells) with EC_{50} values of 59.3 nM, 4.72 nM and 1.67 nM, respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	SARS-CoV-2 3CLpro-IN-5 (oral, i.v.; 10, 100 mg/kg) has strong antiviral activity and favorable pharmacokinetic properties[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	mice[1]
Dosage:	10, 100 mg/kg
Administration:	oral (100 mg/kg) and intravenous (10 mg/kg) administration
Result:	Showed the plasma concentration was 15.2 μM after 1 h and decreased to 0.40 μM over 6 h after oral administration (100 mg/kg) . Showed the plasma concentration reached 9.3 μM after 1 h and decreased to 0.33 μM after 6 h in intravenous administration (10 mg/kg) . Had approximately 9.0% estimated bioavailability (BA).

REFERENCES

[1]. Yuya Hirose, et al. Discovery of Chlorofluoroacetamide-Based Covalent Inhibitors for Severe Acute Respiratory Syndrome Coronavirus 2 3CL Protease. J Med Chem

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