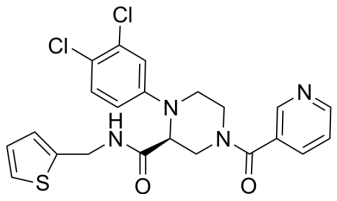
SARS-CoV-2 Mpro-IN-2

Cat. No.:	HY-151482
CAS No.:	2768834-39-3
Molecular Formula:	$C_{22}H_{20}Cl_2N_4O_2S$
Molecular Weight:	475.39
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 Mpro-IN-2 (compound GC-14) is a selective, low cytotoxic and non-covalent M^{pro} inhibitor (IC_{50}=0.40 μM) with good anti-SARS-CoV-2 activity (EC_{50}=1.1 μM). SARS-CoV-2 Mpro-IN-2 can be used in COVID-19 studies[1].

IC_{50} & Target

Mpro
0.40 μM (IC_{50})

In Vitro

SARS-CoV-2 Mpro-IN-2 (0.01-100 μM; 4 h) shows low cytotoxicity in Vero E6 cells[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Cytotoxicity Assay[1]

Cell Line:	Vero E6 cells
Concentration:	0.01-100 μM
Incubation Time:	4 h
Result:	Exhibited low cytotoxicity with a CC_{50} value of more than 100 μM.

In Vivo

SARS-CoV-2 Mpro-IN-2 (2 mg/kg; i.v.; single) exhibits clearance rate (CL), mean residence time (MRT), and half-life ($t_{1/2}$) are 3140 mL/h/kg, 0.40 h, and 0.36 h, respectively[1].
SARS-CoV-2 Mpro-IN-2 (10 mg/kg; p.o.; single) is rapidly absorbed, with a time-to-maximum concentration (T_{max}) of 0.5 h, and shows a moderate pharmacokinetic profile including a favorable $t_{1/2}$ (1.73 h), a maximum concentration (C_{max}) 74.6 ng/mL, and an area under curve (AUC_{0-t}) of 235 ng h/mL[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male Sprague-Dawley rats[1].
Dosage:	2 mg/kg (for i.v.); 10 mg/kg (for p.o.).
Administration:	Intravenous injection or oral administration; single.
Result:	Pharmacokinetic Parameters of SARS-CoV-2 Mpro-IN-2 in Male Sprague-Dawley rats[1].

	IV (2 mg/kg)	PO (10 mg/kg)
$t_{1/2}$ (h)	0.36	1.73
T_{max} (h)	0.08	0.5
C_{max} (ng/mL)	1310	74.6
C_0 (ng/mL)	1760	-
AUC_{0-t} (ng/mL•h)	627	235
$AUC_{0-\infty}$ (ng/mL•h)	637	230
$MRT_{0-\infty}$ (h)	0.40	2.45
CL (mL/h/kg)	3140	-
F (%)	-	7.2

REFERENCES

[1]. Gao S, et al. Discovery and Crystallographic Studies of Trisubstituted Piperazine Derivatives as Non-Covalent SARS-CoV-2 Main Protease Inhibitors with High Target Specificity and Low Toxicity. J Med Chem. 2022 Sep 15:acs.jmedchem.2c01146.

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