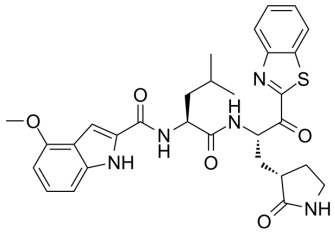
YH-53

Cat. No.:	HY-139311
CAS No.:	1471484-62-4
Molecular Formula:	$C_{30}H_{33}N_5O_5S$
Molecular Weight:	575.68
Target:	SARS-CoV
Pathway:	Anti-infection
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (86.85 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.7371 mL	8.6854 mL	17.3708 mL
	5 mM	0.3474 mL	1.7371 mL	3.4742 mL
	10 mM	0.1737 mL	0.8685 mL	1.7371 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (3.61 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.08 mg/mL (3.61 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (3.61 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

YH-53 is a potent $3CL^{pro}$ inhibitor with K_i values of 6.3 nM, 34.7 nM for SARS-CoV-1 $3CL^{pro}$ and SARS-CoV-2 $3CL^{pro}$, respectively. YH-53 strongly blocks the SARS-CoV-2 replication. YH-53 is a peptidomimetic compound with a unique benzothiazolyl ketone. YH-53 has the potential for COVID-19 research[1][2].

IC_{50} & Target

Ki: 6.3 nM (SARS-CoV-1 $3CL^{pro}$) and 34.7 nM (SARS-CoV-2 $3CL^{pro}$)[1]

In Vitro

YH-53 (1-25 μM; for 24 h) efficiently reduces copies of total RNA with increased concentrations in VeroE6/TMPRSS2 cells[1].

? ?YH-53 (1, 5, 10, 15, 20, 25 μM; for 48 h) with 10 μM completely blocks the viral proliferation against SARS-CoV-2 were examined by a cytopathic effect (CPE) assay in Vero cells[1].
? ?YH-53 (10, 100 μM; for 24 h) has no cytotoxicity with a CC_{50} value of >100 μM in vero cells[1].
? ?YH-53 (10 μM) moderately inhibits CYP1A2, CYP2D6, and CYP2C8 (26.6%, 38.0%, 66.4%, respectively). YH-53 has no inhibition on CYP2C9 and CYP3A4[1].
? ?YH-53 inhibits SARS-CoV $3CL^{pro}$ with an IC_{50} of 0.74 μM.
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

RT-PCR[1]

Cell Line:	VeroE6/TMPRSS2 cells
Concentration:	1, 5, 10, 15, 20, 25 μM
Incubation Time:	24 hours
Result:	Efficiently reduced copies of total RNA.

In Vivo

YH-53 (0.1 mg/kg; iv) has a $T_{1/2}$ of 2.97 hours, an $AUC_{0-\infty}$ of 19.7 ng?h/mL, a V_d of 3.51 L/kg in rats[1].
? ?YH-53 (0.5 mg/kg; oral) has a $T_{1/2}$ of 9.64 hours, an $AUC_{0-\infty}$ of 3.49 ng?h/mL, a C_{max} of 1.08 ng/mL in rats[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Rats[1]
Dosage:	0.1 mg/kg (Pharmacokinetic Analysis)
Administration:	IV
Result:	Had a $T_{1/2}$ of 2.97 hours, an $AUC_{0-\infty}$ of 19.7 ng•h/mL, a V_d of 3.51 L/kg.

REFERENCES

[1]. Sho Konno, et al. 3CL Protease Inhibitors with an Electrophilic Arylketone Moiety as Anti-SARS-CoV-2 Agents. J Med Chem. 2021 Jul27;acs.jmedchem.1c00665.

[2]. Pillaiyar Thanigaimalai, et al. Development of potent dipeptide-type SARS-CoV 3CL protease inhibitors with novel P3 scaffolds: design, synthesis, biological evaluation, and docking studies. Eur J Med Chem. 2013 Oct;68:372-84.

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