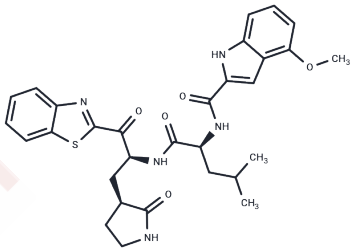
Data Sheet (Cat.No.T9686)

TargetMol

YH-53

Chemical Properties



CAS No. : 1471484-62-4

Formula: C30H33N5O5S

Molecular Weight: 575.68

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	YH-53 is a potent peptidomimetic 3CLpro inhibitor featuring a unique benzothiazolyl ketone pharmacophore that displays low-nanomolar inhibition of SARS-CoV-1 and SARS-CoV-2 main proteases and effectively blocks SARS-CoV-2 replication, thereby providing a structurally distinctive and mechanistically validated compound for antiviral and COVID-19 research.
Targets(IC50)	SARS-CoV
In vitro	In enzymatic assays, YH-53 inhibited SARS-CoV-1 and SARS-CoV-2 3CLpro with Ki values of 6.3 nM and 34.7 nM respectively. In VeroE6/TMPRSS2 cells, it dose-dependently reduced viral RNA copies and inhibited proliferation (10 μM), showing moderate inhibition of CYP2C8/2D6/1A2 but no effect on CYP2C9/3A4 [1].
In vivo	YH-53, administered to rats, demonstrates varied pharmacokinetic properties based on the route of administration. Intravenously at 0.1 mg/kg, YH-53 shows a half-life (T 1/2) of 2.97 hours, an area under the curve (AUC 0-∞) of 19.7 ng·h/mL, and a distribution volume (V d) of 3.51 L/kg. When given orally at 0.5 mg/kg, it exhibits a T 1/2 of 9.64 hours, an AUC 0-∞ of 3.49 ng·h/mL, and a maximum concentration (C max) of 1.08 ng/mL in rats. These findings provide useful insights into the compound's pharmacokinetics, indicating significant differences in half-life, distribution, and absorption rates between intravenous and oral administration in this animal model [1].

Solubility Information

Solubility	DMSO: 40 mg/mL (69.48 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
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
50 mM	0.0347 mL	0.1737 mL	0.3474 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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.

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.