Mpro inhibitor N3

Cat. No.: HY-136149

CAS No.: 884650-98-0

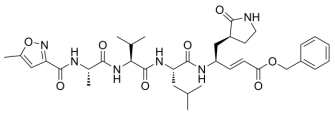
Molecular Formula: $C_{35}H_{48}N_6O_8$

Molecular Weight: 680.79

Target: SARS-CoV; Virus Protease

Pathway: Anti-infection

Storage: 4°C, sealed storage, away from moisture and light
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 20 mg/mL (29.38 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.4689 mL	7.3444 mL	14.6888 mL
	5 mM	0.2938 mL	1.4689 mL	2.9378 mL
	10 mM	0.1469 mL	0.7344 mL	1.4689 mL

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

BIOLOGICAL ACTIVITY

Description

Mpro inhibitor N3 is a potent SARS-CoV-2 MPro inhibitor with an EC_{50} value of 16.77 μM. Mpro inhibitor N3 shows antiviral activities against HCoV-229E, FIPV, IBV and MHV-A59[1][2][3].

In Vitro

Mpro inhibitor N3 (0-100 μM) shows antiviral activities with an EC_{50} value of 16.77 μM for SARS-CoV-2[1].
Mpro inhibitor N3 (0-50 μM; 14 h) inhibits the viral growth with the IC_{50} values of 4, 8.8, 2.7 μM for HCoV-229E, FIPV, IBV and MHV-A59, respectively[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

Mpro inhibitor N3 (0-0.64 μM; 3, 6 h) shows antiviral activity against IBV in chicken , embryos[3].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Chicken embryos[3]
Dosage:	0-0.64 μM
Administration:	3, 6 h with 100-EID50 titer of IBV M41 virus

Result:	Showed that N3 is able to penetrate cells to inhibit the replication of IBV viruses, probably at the beginning of infection, with the PD_{50} of 0.13 μmol for the 3-h group and 0.17 μmol for the 6-h group.

REFERENCES

[1]. Jin Z, et al. Structure of Mpro from SARS-CoV-2 and discovery of its inhibitors. Nature. 2020 Jun;582(7811):289-293.

[2]. Yang H, et al. Design of wide-spectrum inhibitors targeting coronavirus main proteases. PLoS Biol. 2005 Oct;3(10):e324.

[3]. Xue X, et al. Structures of two coronavirus main proteases: implications for substrate binding and antiviral drug design. J Virol. 2008 Mar;82(5):2515-27.

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