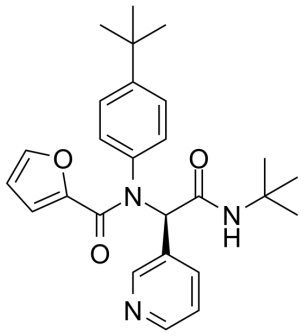
ML188

Cat. No.:	HY-136259
CAS No.:	1417700-13-0
Molecular Formula:	$C_{26}H_{31}N_3O_3$
Molecular Weight:	433.54
Target:	SARS-CoV; Virus Protease
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 : 250 mg/mL (576.65 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3066 mL	11.5330 mL	23.0659 mL
	5 mM	0.4613 mL	2.3066 mL	4.6132 mL
	10 mM	0.2307 mL	1.1533 mL	2.3066 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: ≥ 6.25 mg/mL (14.42 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 6.25 mg/mL (14.42 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 6.25 mg/mL (14.42 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ML188, a first in class probe, is a selective non-covalent SARS-CoV 3CLpro inhibitor with an IC_{50} of 1.5 μM. Antiviral activity[1].

In Vitro

ML188 (0-30 μM; 48 hours) effectively inhibit SARS-CoV replication in cell culture[1].
Probe ML188 is a modest molecular weight SARS-CoV 3CLpro inhibitor with demonstrated antiviral activity and a non-covalent mechanism of action. ML188 yields an antiviral EC_{50} value ranging from 12.9 to 13.4 μM in mock-infected and SARS-CoV infected cells[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[1]

Cell Line:	Vero E6 cells (mock-infected or infected with SARS-CoV)
Concentration:	3, 4, 5, 8,10, 15, 20, 30 μM
Incubation Time:	48 hour
Result:	Against mock-infected and SARS-CoV infected cells.

CUSTOMER VALIDATION

- Nucleic Acids Res. 2021 Jan 8;49(D1):D1113-D1121.
- Sci Rep. 2021 Mar 8;11(1):5433.
- Viruses. 2021 Jan 25;13(2):174.
- bioRxiv. 2020 Jul.

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REFERENCES

[1]. Jacobs J, et al. Discovery, synthesis, and structure-based optimization of a series of N-(tert-butyl)-2-(N-arylamido)-2-(pyridin-3-yl) acetamides (ML188) as potent noncovalent small molecule inhibitors of the severe acute respiratory syndrome coronavirus (SARS-CoV) 3CL protease. J Med Chem. 2013 Jan 24;56(2):534-46.

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