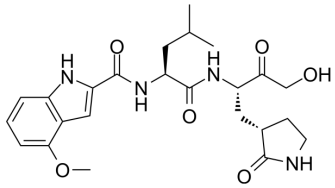
PF-00835231

Cat. No.:	HY-137048
CAS No.:	870153-29-0
Molecular Formula:	$C_{24}H_{32}N_4O_6$
Molecular Weight:	472.53
Target:	SARS-CoV
Pathway:	Anti-infection
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 250 mg/mL (529.07 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1163 mL	10.5813 mL	21.1627 mL
	5 mM	0.4233 mL	2.1163 mL	4.2325 mL
	10 mM	0.2116 mL	1.0581 mL	2.1163 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 (4.40 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (4.40 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.40 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PF-00835231 is a CoV-2 cysteine 3C-like protease ($3CL^{pro}$) inhibitor, with IC_{50}s of 0.27 nM and 4 nM for SARS CoV-2 and SARS CoV-1 $3CL^{pro}$, respectively. PF-00835231 is developed for the research of anti-SARS-CoV-2/COVID-19[1]sup>[2].

IC_{50} & Target

$3CL^{pro}$[1]

CUSTOMER VALIDATION

- J Virol. 2022 Aug 24;e0090722.

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REFERENCES

[1]. de Vries M, et al. A comparative analysis of SARS-CoV-2 antivirals in human airway models characterizes 3CLpro inhibitor PF-00835231 as a potential new treatment for COVID-19. bioRxiv [Preprint]. 2021 Feb 19:2020.08.28.272880.

[2]. Robert L Hoffman, et al. Discovery of Ketone-Based Covalent Inhibitors of Coronavirus 3CL Proteases for the Potential Therapeutic Treatment of COVID-19. J Med Chem. 2020 Nov 12;63(21):12725-12747.

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