

CCF0058981

Chemical Properties

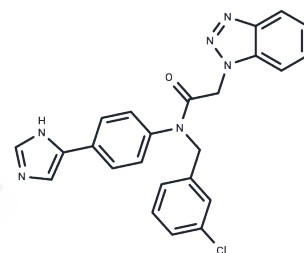
CAS No. : 2708934-53-4

Formula: C₂₄H₁₉ClN₆O

Molecular Weight: 442.9

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	CCF0058981 (CCF981) is a 3-chlorophenyl analogue, serving as a noncovalent inhibitor of SARS-CoV-2 3CL pro (SC2), demonstrating potent activity with an IC ₅₀ of 68 nM. It also exhibits inhibitory effects against SARS-CoV-1 3CL pro (SC1) with an IC ₅₀ of 19 nM, highlighting its antiviral efficacy and potential in COVID-19 research [1].
Targets(IC ₅₀)	SARS-CoV, Virus Protease
In vitro	CCF0058981 (CCF981) demonstrates inhibition of cytopathic effect (CPE) and plaque reduction in vitro viral replication, with EC ₅₀ values of 497 nM and 558 nM, respectively [1]. Additionally, its 50% cytotoxic concentration (CC ₅₀) in the CPE antiviral assay exceeds 50 μM [1]. The compound has a half-life (T _{1/2}) of 21.1 minutes and a clearance rate (CL _{int}) of 141 mL/min/kg in human liver microsomes [1].

Solubility Information

Solubility	DMSO: 1 mg/mL (2.26 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.2578 mL	11.2892 mL	22.5785 mL
5 mM	0.4516 mL	2.2578 mL	4.5157 mL
10 mM	0.2258 mL	1.1289 mL	2.2578 mL
50 mM	0.0452 mL	0.2258 mL	0.4516 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

Han SH, et al. Structure-Based Optimization of ML300-Derived, Noncovalent Inhibitors Targeting the Severe Acute Respiratory Syndrome Coronavirus 3CL Protease (SARS-CoV-2 3CLpro). J Med Chem. 2022 Feb 24;65(4):2880-2904.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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