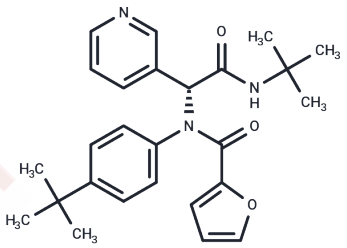
Data Sheet (Cat.No.T8371)

TargetMol

ML188

Chemical Properties



CAS No. : 1417700-13-0

Formula: C26H31N3O3

Molecular Weight: 433.54

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	ML188 is a selective noncovalent SARS-CoV 3CLpro inhibitor(IC50 : 1.5 μM), with moderate MW and good enzyme and antiviral inhibitory activity.
Targets(IC50)	SARS-CoV,Virus Protease
In vitro	Probe 16-(R) (ML188) is a modest molecular weight SARS-CoV 3CLpro inhibitor with demonstrated antiviral activity and a non-covalent mechanism of action[1].

Solubility Information

Solubility	DMSO: 4.34 mg/mL (10.01 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 1 mg/mL (2.31 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.3066 mL	11.533 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
50 mM	0.0461 mL	0.2307 mL	0.4613 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

Jacobs J , Grum-Tokars V , Zhou Y , 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]. Journal of Medicinal Chemistry, 2013, 56(2):534-546.

Michael Berry, Burtram Fielding , Junaid Gamieldien.Human Coronavirus OC43 3CL Protease and the Potential of ML188 as a Broad-Spectrum Lead Compound: Homology Modelling and Molecular Dynamic Studies[J].BMC Struct Biol. 2015 Apr 28;15:8.