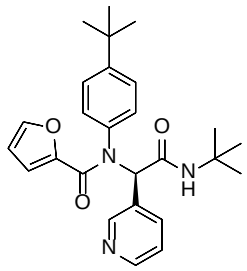
Product data sheet

MedKoo Cat#: 555785 Name: ML188 CAS: 1417700-13-0 (R-isomer) Chemical Formula: $C_{26}H_{31}N_3O_3$ Exact Mass: 433.2365 Molecular Weight: 433.552	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
ML188 is a Potent Noncovalent Small Molecule Inhibitor of the Severe Acute Respiratory Syndrome Coronavirus (SARS-CoV) 3CL Protease. The X-ray structure of SARS-CoV 3CLpro bound with ML188 was instrumental in guiding subsequent rounds of chemistry optimization. ML188 provides an excellent starting point for the further design and refinement of 3CLpro inhibitors that act by a noncovalent mechanism of action.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	168.5	388.65
Ethanol	87.0	200.67

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	2.31 mL	11.53 mL	23.07 mL
5 mM	0.46 mL	2.31 mL	4.61 mL
10 mM	0.23 mL	1.15 mL	2.31 mL
50 mM	0.05 mL	0.23 mL	0.46 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Lockbaum GJ, Reyes AC, Lee JM, Tilvawala R, Nalivaika EA, Ali A, Kurt Yilmaz N, Thompson PR, Schiffer CA. Crystal Structure of SARS-CoV-2 Main Protease in Complex with the Non-Covalent Inhibitor ML188. Viruses. 2021 Jan 25;13(2):174. doi: 10.3390/v13020174. PMID: 33503819; PMCID: PMC7911568.
2. Jacobs J, Grum-Tokars V, Zhou Y, Turlington M, Saldanha SA, Chase P, Eggler A, Dawson ES, Baez-Santos YM, Tomar S, Mielech AM, Baker SC, Lindsley CW, Hodder P, Mesecar A, Stauffer SR. 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. doi: 10.1021/jm301580n. Epub 2013 Jan 3. PMID: 23231439; PMCID: PMC3569073.

In vivo study
TBD

7. Bioactivity
Biological target:

Product data sheet

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

In vitro activity

A high-throughput screen of the NIH molecular libraries sample collection and subsequent optimization of a lead dipeptide-like series of severe acute respiratory syndrome (SARS) main protease (3CLpro) inhibitors led to the identification of probe compound ML188 (16-(R), (R)-N-(4-(tert-butyl)phenyl)-N-(2-(tert-butylamino)-2-oxo-1-(pyridin-3-yl)ethyl)furan-2-carboxamide, Pubchem CID: 46897844). Unlike the majority of reported coronavirus 3CLpro inhibitors that act via covalent modification of the enzyme, 16-(R) is a noncovalent SARS-CoV 3CLpro inhibitor with moderate MW and good enzyme and antiviral inhibitory activity. 16-(R) provides an excellent starting point for the further design and refinement of 3CLpro inhibitors that act by a noncovalent mechanism of action.

Reference: J Med Chem. 2013 Jan 24;56(2):534-46. https://pubmed.ncbi.nlm.nih.gov/23231439/

In vivo activity

TBD

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.