Certificate of Analysis

Product Name: **PLpro inhibitor 19** **Catalog No.: 7505** **Batch No.: 2**

IUPAC Name: (*R*)-*N*-(3-Fluoro-5-((1-(1-(naphthalen-1-yl)ethyl)piperidine-4-carboxamido)methyl)phenyl)-4-methylpiperazine-1-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{31}H_{38}FN_5O_2.¾H_2O$

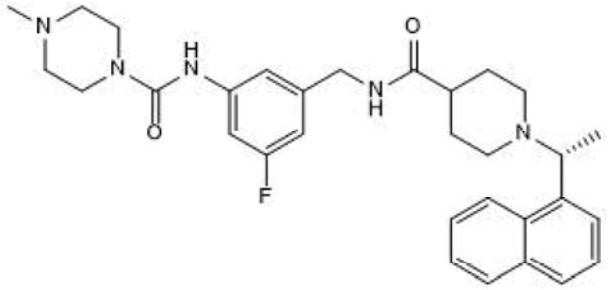
Batch Molecular Weight: 545.19

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.1% purity

Chiral HPLC: Shows 99.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.3	7.3	12.85
Found	68.03	7.14	12.84

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Description:

PLpro inhibitor 19 is a SARS-CoV-2 inhibitor that inhibits viral replication and PLpro enzymatic activity in vitro (IC_{50} values are 0.18 µM and 0.44 µM respectively). PLpro inhibitor 19 is selective for PLpro over human deubiquitinating enzymes (DUBs) and DUB-like proteases and displays no cytotoxicity at up to 10 µM.

Physical and Chemical Properties:

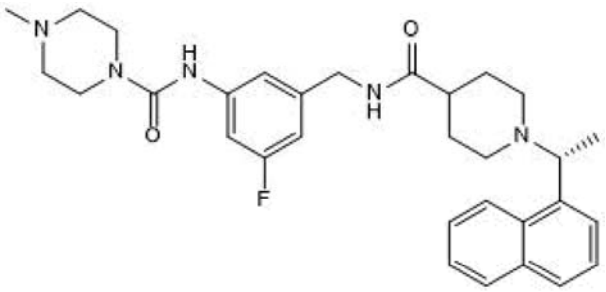
Batch Molecular Formula: $C_{31}H_{38}FN_5O_2.¾H_2O$

Batch Molecular Weight: 545.19

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Shan *et al* (2021) Development of potent and selective inhibitors targeting the papain-like protease of SARS-CoV-2. Cell Chem.Biol. ***28*** 855. PMID: 33979649.