Print Date: Jul 14th 2022

Certificate of Analysis

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Product Name: **MPro 61** **Catalog No.: 7695** **Batch No.: 2**

CAS Number: 2679814-93-6

IUPAC Name: 5-[5-[3-Chloro-5-[(2-chlorophenyl)methoxy]-4-fluorophenyl]-6-oxo[1(6*H*),3'-bipyridin]-3-yl]-1-methyl-2,4(1*H*,3*H*)-pyrimidinedione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{19}Cl_2FN_4O_4.H_2O$

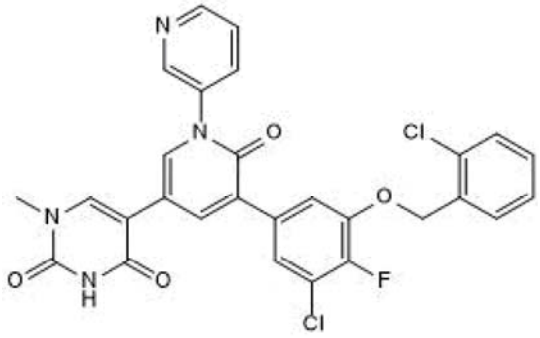
Batch Molecular Weight: 583.4

Physical Appearance: Off White solid

Solubility: DMSO to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.65	3.63	9.6
Found	57.55	3.5	9.39

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Description:

Mpro 61 is a potent non-covalent inhibitor of SARS-CoV-2 main protease (IC_{50} = 44 nM, EC_{50} = 0.175 µM in the replicon assay and EC_{50} = 0.08 µM in the infectious SARS-CoV-2 assay); it is cell permable and exhibits no apparent cytotoxicity.

Physical and Chemical Properties:

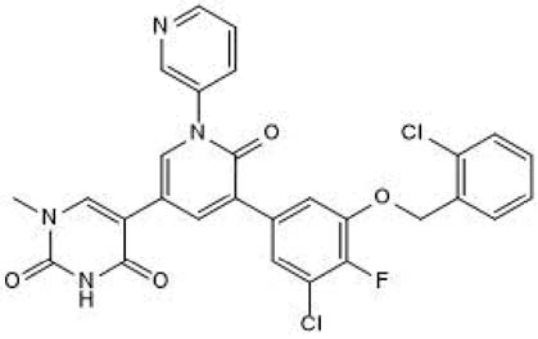
Batch Molecular Formula: $C_{28}H_{19}Cl_2FN_4O_4.H_2O$

Batch Molecular Weight: 583.4

Physical Appearance: Off White solid

Minimum Purity: ≥95%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 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.

Licensing Information:

Sold under license from Yale University. U.S. patent application number 63/135,062.

References:

Zhang *et al* (2021) Optimization of triarylpyridinone inhibitors of the main protease of SARS-CoV-2 to low-nanomolar antiviral potency. ACS Med.Chem.Lett. ***12*** 1325. PMID: 34408808.