

Product Name: MPro 13b

Catalog No.: 7228

Batch No.: 1

CAS Number: 2412965-59-2

IUPAC Name: *tert*-Butyl (1-((S)-1-(((S)-4-(benzylamino)-3,4-dioxo-1-((S)-2-oxopyrrolidin-3-yl)butan-2-yl)amino)-3-cyclopropyl-1-oxopropan-2-yl)-2-oxo-1,2-dihydropyridin-3-yl)carbamate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₁H₃₉N₅O₇·½H₂O

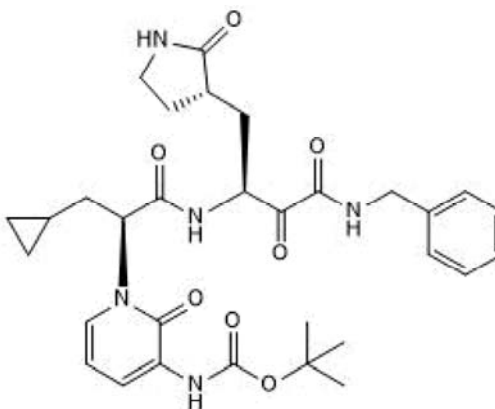
Batch Molecular Weight: 602.69

Physical Appearance: Pale pink solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.78	6.69	11.62
Found	61.57	6.56	11.5

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Description:

Coronavirus M^{Pro} inhibitor (IC₅₀ values are 0.58, 0.9 and 0.67 μM for recombinant M^{Pro} from MERS-CoV, SARS-CoV and SARS-CoV-2, respectively). Inhibits SARS-CoV-2 infection of human Calu3 cells (IC₅₀ = 4-5 μM). Please note, unpublished data suggest MPro 13b is 2-fold more potent than published data.

Physical and Chemical Properties:

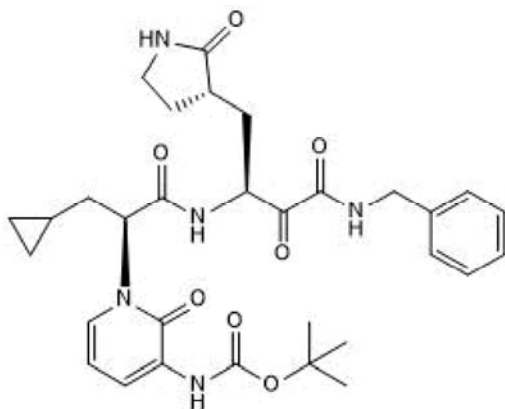
Batch Molecular Formula: C₃₁H₃₉N₅O₇·½H₂O

Batch Molecular Weight: 602.69

Physical Appearance: Pale pink solid

Minimum Purity: ≥97%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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.

Licensing Information:

Sold under license from the University of Luebeck

References:

Zhang *et al* (2020) Crystal structure of SARS-CoV-2 main protease provides a basis for design of improved α-ketoamide inhibitors. *Science*. **368** 409. PMID: 32198291.

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