

Product Name: Mpro 13b-K

Catalog No.: 7228

Batch No.: 2

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: C₃₁H₃₉N₅O₇·1/4H₂O

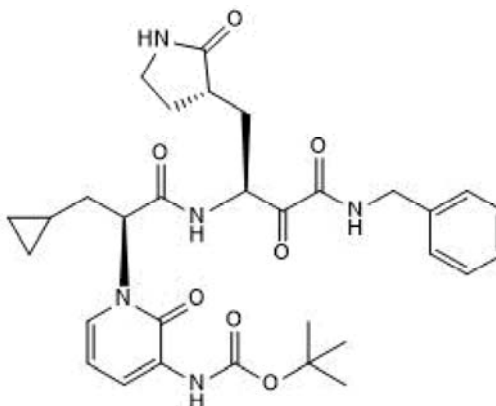
Batch Molecular Weight: 598.18

Physical Appearance: Pink solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 96.9% purity

Chiral HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.25	6.66	11.71
Found	61.96	6.64	11.69

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Description:

Mpro 13b-K is a coronavirus M^{pro} inhibitor (IC₅₀ values are 0.12, 0.58 and 0.9 μM for recombinant M^{pro} from SARS-CoV-2, MERS-CoV and SARS-CoV, respectively). Mpro 13b-K inhibits SARS-CoV-2 infection of human Calu3 cells (IC₅₀ = 2.4 μM). The compound also inhibits SARS-CoV-2 replication in A549-ACE2-TMPRSS2, VeroE6 and Huh7 cell cultures (EC₅₀ values are 0.84, 1.3 and 3.4 μM). Exhibits oral and inhalative bioavailability. Please note that this product was previously known as Mpro 13b.

Physical and Chemical Properties:

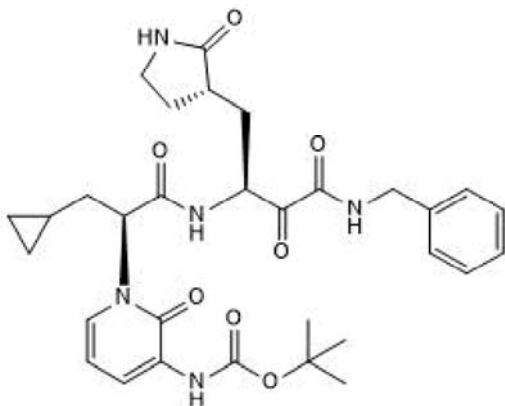
Batch Molecular Formula: C₃₁H₃₉N₅O₇·½H₂O

Batch Molecular Weight: 598.18

Physical Appearance: 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 Lübeck

References:

Cooper et al (2022) Diastereomeric resolution yields highly potent inhibitor of SARS-CoV-2 main protease. *J.Med.Chem.* **65** 13328. PMID: 36179320.

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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