

Product Name: Mpro 13b-H

Catalog No.: 7853

Batch No.: 1

CAS Number: 3031351-76-2

IUPAC Name: *tert*-Butyl (1-((*R*)-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

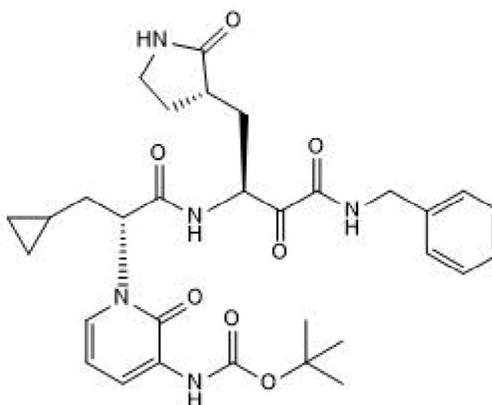
Batch Molecular Weight: 598.18

Physical Appearance: White solid

Solubility: DMSO to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.25	6.66	11.71
Found	61.48	6.48	11.46

Diastereometric Purity: 98.7%

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Mpro 13b-H is a negative control for the coronavirus Mpro inhibitor, Mpro 13b-K (Cat. No. 7228).

Physical and Chemical Properties:

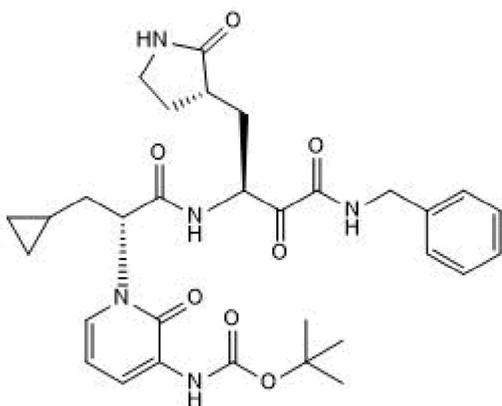
Batch Molecular Formula: C₃₁H₃₉N₅O₇·¼H₂O

Batch Molecular Weight: 598.18

Physical Appearance: White solid

Minimum Purity: ≥97%

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Cooper *et al* (2022) Diastereomeric resolution yields highly potent inhibitor of SARS-CoV-2 main protease. *J.Med.Chem.* **68** 13328. PMID: 36179320.

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