

Product Name: MPro N3

Catalog No.: 7230

Batch No.: 1

CAS Number: 884650-98-0

IUPAC Name: *N*-[(5-Methyl-3-isoxazolyl)carbonyl]-L-alanyl-L-valyl-*N*-[(1*S*,2*E*)-4-oxo-1-[[[(3*S*)-2-oxo-3-pyrrolidinyl]methyl]-4-(phenylmethoxy)-2-buten-1-yl]-L-leucinamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₅H₄₈N₆O₈·½H₂O

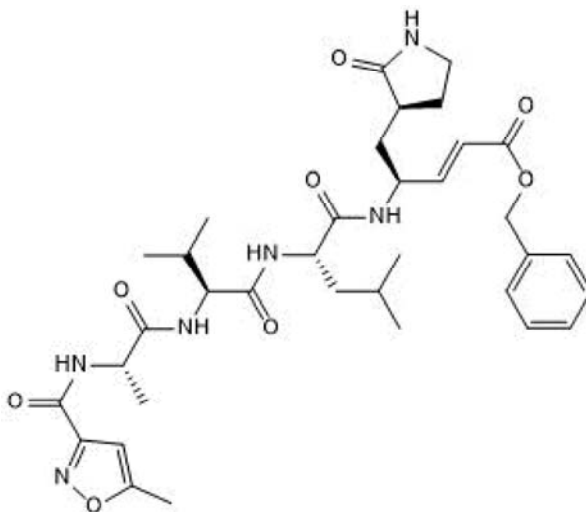
Batch Molecular Weight: 689.81

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.94	7.16	12.18
Found	60.61	7.13	12.18

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

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Description:

Coronavirus main protease (M^{pro}) inhibitor (respective IC₅₀ values are 2.7, 4 and 8.8 μM for MHV-A29, HCoV-229E and FOPV replication in vitro). Inhibits viral cell infection in an MHV plaque reduction assay. Also inhibits SARS-CoV-2 viral cell entry in a plaque reduction assay (IC₅₀ = 16.8 μM).

Physical and Chemical Properties:

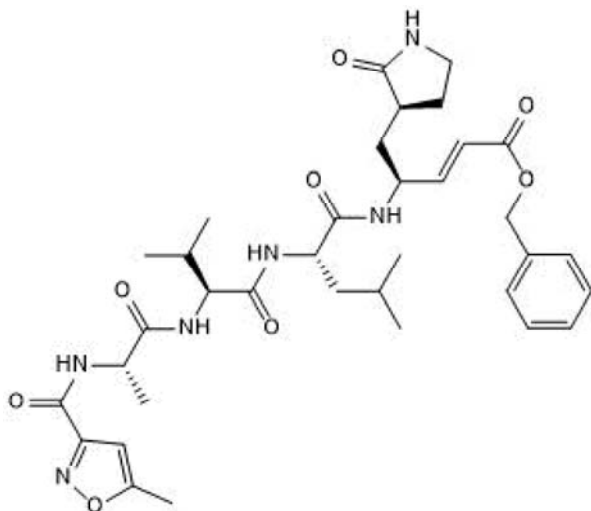
Batch Molecular Formula: C₃₅H₄₈N₆O₈·½H₂O

Batch Molecular Weight: 689.81

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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:

Jin *et al* (2020) Structure of Mpro from SARS-CoV-2 and discovery of its inhibitors. *Nature*. **582** 289. PMID: 32272481.

Yang *et al* (2005) Design of wide-spectrum inhibitors targeting coronavirus main proteases. *PLoS.One*. **10**. PMID: 16128623.

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