

**Product Name:** Lopinavir

**Catalog No.:** 7052

**Batch No.:** 2

CAS Number: 192725-17-0

IUPAC Name: ( $\alpha$ S)-N-[(1S,3S,4S)-4-[[2-(2,6-Dimethylphenoxy)acetyl]amino]-3-hydroxy-5-phenyl-1-(phenylmethyl)pentyl] tetrahydro- $\alpha$ -(1-methylethyl)-2-oxo-1(2H)-pyrimidineacetamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>37</sub>H<sub>48</sub>N<sub>4</sub>O<sub>5</sub> · 1<sup>3</sup>/<sub>4</sub>H<sub>2</sub>O

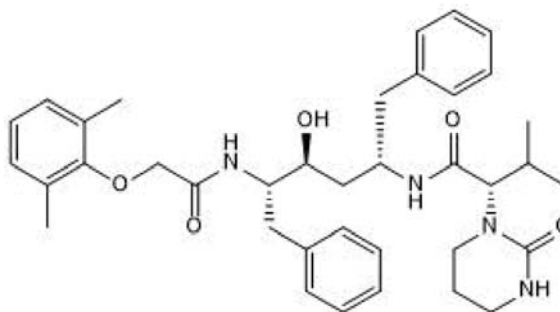
**Batch Molecular Weight:** 660.32

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
ethanol to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 99.8% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub> = -28.3 (Concentration = 0.4, Solvent = Methanol)

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	67.3	7.86	8.48
Found	67.13	7.88	8.6

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

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**Description:**

Highly potent and selective HIV-1 protease inhibitor ( $IC_{50}$  = 6.5 nM, HIV cultured in peripheral blood mononuclear cells;  $K_i$  = 1.3  $\mu$ M). Displays  $>10^5$ -fold selectivity for HIV-1 protease over mammalian proteases including renin and cathepsin D and E. Inhibits HIV-1 protease in patient HIV isolates displaying mutations that confer resistance to ritonavir (Cat. No. 5856) ( $IC_{50}$  values in 5 - 50 nM range). Also inhibits SARS-CoV-2 replication *in vitro* ( $IC_{50}$  = 26  $\mu$ M)

**Physical and Chemical Properties:**

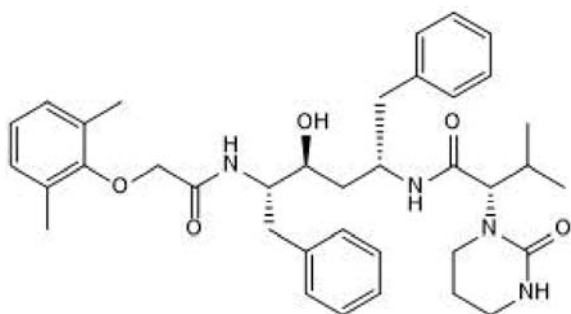
Batch Molecular Formula:  $C_{37}H_{48}N_4O_5 \cdot 1\frac{3}{4}H_2O$

Batch Molecular Weight: 660.32

Physical Appearance: White solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**References:**

**Choy et al** (2020) Remdesivir, lopinavir, emetine, and homoharringtonine inhibit SARS-CoV-2 replication *in vitro*. *Antiviral Res.* **178**. PMID: 32251767.

**Carrillo et al** (1998) *In vitro* selection and characterization of human immunodeficiency virus type 1 variants with increased resistance to ABT-378, a novel protease inhibitor. *J.Virol.* **72** 7532. PMID: 9696850.

**Sham et al** (1998) ABT-378, a highly potent inhibitor of the human immunodeficiency virus protease. *Antimicrob.Agents Chemother.* **42** 3218. PMID: 9835517.

**Storage:** Store at  $-20^{\circ}C$

**Solubility & Usage Info:**

DMSO to 100 mM  
ethanol 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  $45-60^{\circ}C$  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  $-20^{\circ}C$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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