

Product Name: Rupintrivir

Catalog No.: 6414

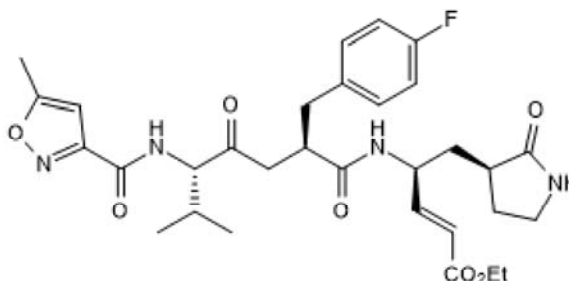
Batch No.: 1

CAS Number: 223537-30-2

IUPAC Name: Ethyl (2*E*,4*S*)-4-[[[(2*R*,5*S*)-2-[(4-fluorophenyl)methyl]-6-methyl-5-[[[(5-methyl-3-isoxazolyl)carbonyl]amino]-1,4-dioxoheptyl]amino]-5-[(3*S*)-2-oxo-3-pyrrolidinyl]-2-pentenoate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₁H₃₉FN₄O₇
Batch Molecular Weight: 598.66
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = +40.8 (Concentration = 0.5, Solvent = Chloroform)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.19	6.57	9.36
Found	62.21	6.64	9.42

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

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Description:

Potent and selective irreversible human rhinovirus (HRV) 3C protease inhibitor (EC₅₀ = 5 nM). Exhibits no significant inhibition against a variety of serine and cysteine proteases. Inhibits replication of a panel of 48 different HRV serotypes in H1-HeLA and MRC-5 cell protection assays. Tocris products are for biomedical research use only. They are not intended for human or veterinary use.

Physical and Chemical Properties:

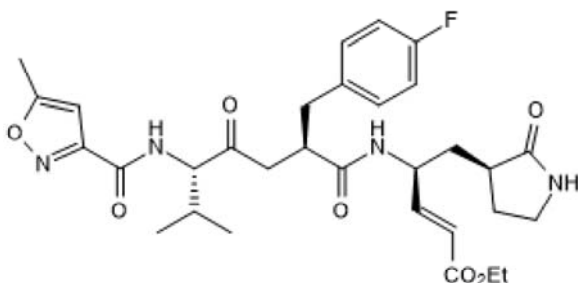
Batch Molecular Formula: C₃₁H₃₉FN₄O₇

Batch Molecular Weight: 598.66

Physical Appearance: White solid

Minimum Purity: ≥98%

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 for research purposes under agreement from Pfizer Inc.

References:

Dragovich *et al* (1999) Structure-based design, synthesis, and biological evaluation of irreversible human rhinovirus 3C protease inhibitors. 3. Structure-activity studies of ketomethylene-containing peptidomimetics. *J.Med.Chem.* **42** 1203. PMID: 10197964.

Patick *et al* (1999) In vitro antiviral activity of AG7088, a potent inhibitor of human rhinovirus 3C protease. *Antimicrob.Agents Chemother.* **43** 2444. PMID: 10508022 .

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