Nirmatrelvir (PF-07321332)

Catalog No.C14512 Batch:C1451203

Product Datasheet

Technical Data

Formula	$C_{23}H_{32}F_3N_5O_4$					
Molecular Weight	499.53	**CAS No.**	2628280-40-8			
Solubility (25°C)*	In vitro	DMSO	100 mg/mL (200.18 mM)			
		Ethanol	100 mg/mL (200.18 mM)			
		Water	2 mg/mL (4.0 mM)			
	In vivo (Add solvents to the product individually and in order)	Oral Administration	Homogeneous suspension	CMC-NA	≥5mg/ml	Taking the 1 mL working solution as an example, add 5 mg of this product to 1 ml of CMC-Na solution, mix evenly to obtain a homogeneous suspension with a final concentration of 5 mg/ml.

* <1 mg/ml means slightly soluble or insoluble.
* Please note that Capsid Bio tests the solubility of all compounds in-house, and the actual solubility may differ slightly from published values. This is normal and is due to slight batch-to-batch variations.
* Room temperature shipping (Stability testing shows this product can be shipped at 2-8°C for storage purposes.)

Preparing Stock Solutions

Biological Activity

Description	Nirmatrelvir (PF-07321332) is an reversible covalent inhibitor of **SARS-CoV-2 main protease (M^{pro}, also referred to as 3CL protease)** with an ki of 3.11 nM. PF-07321332 binds directly to the catalytic cysteine (Cys145) residue of the enzyme.
Targets	SARS-CoV-2 Mpro [1] 3.11 nM(ki)
In vitro	Nirmatrelvir (PF-07321332) is a reversible covalent inhibitor of SARS-CoV-2 main protease (M^{pro}, also known as 3CL protease), with a ki of 3.11 nM. This compound directly binds to the catalytic cysteine (Cys145) residue of the enzyme.[1]

Protocol (from reference)

Kinase Assay:[1]

- **Enzyme kinetics assay**

  Test compounds and SARS-CoV-2 Mpro enzyme were incubated at a 1:1 molar ratio of 2 μM Nirmatrelvir (PF-07321332) and 2 μM enzyme in assay buffer for 20 minutes. The mixture was then diluted 50-fold into assay buffer followed by a transfer of 5 μl to wells of a black low volume 384-well assay plate. Enzyme activity was monitored on a BMG Pherastar at Ex/Em of 340 nm/460 nm after addition of 5 μl 60 μM peptide substrate. Final reaction conditions were 20 nM enzyme with 20 nM of this compound and 30 μM peptide substrate.

Cell Assay:[2]

- **Cell lines**

  HCoV-229E in Huh-7 cells
- **Concentrations**

  0.62 μM
- **Incubation Time**

  2 days
- **Method**

  Nirmatrelvir (PF-07321332) was evaluated in hCoV-229E experiments performed on Huh-7 cells at an MOI of 0.002, and infection was determined by in-cell ELISA 2 days later.

Animal Study:[3]

- **Animal Models**

  Female C57BL/6 Cg-Tg2Prlmn/J mice
- **Dosages**

  20 mg/kg
- **Administration**

  Oral

References

https://pubmed.ncbi.nlm.nih.gov/34726479/ https://pubmed.ncbi.nlm.nih.gov/35598779/ https://pubmed.ncbi.nlm.nih.gov/36209984/

RETURN POLICY

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SHIPPING & STORAGE

Capsid Bio products are transported at room temperature. If you receive the product at room temperature, please rest assured, the Capsid Bio Quality Inspection Department has conducted experiments to verify that the normal temperature placement of one month will not affect the biological activity of powder products. After collecting, please store the product according to the requirements described in the datasheet. Most Capsid Bio products are stable under the recommended conditions.

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EU Headquarters
Gajeva ulica 28, HR-10000 Zagreb, Croatia

US Headquarters
12222 Merit Dr STE 130 Dallas, Texas, 75251

UK Headquarters
121 ABILITY HOUSE, BROOKER ROAD, EN9 1JH, ESSEX

Orders: Sales@capsidbio.com
Enquiries: info@capsidbio.com
www.capsidbio.com