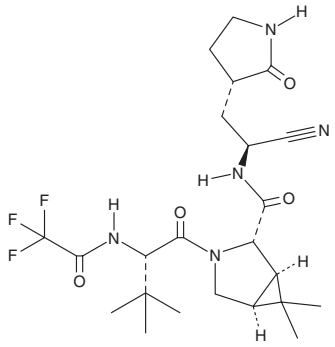
PRODUCT INFORMATION

PF-07321332

Item No. 35257

CAS Registry No.:	2628280-40-8
Formal Name:	(1R,2S,5S)-N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrrolidinyl]ethyl]-3-[(2S)-3,3-dimethyl-1-oxo-2-[(2,2,2-trifluoroacetyl)amino]butyl]-6,6-dimethyl-3-azabicyclo[3.1.0]hexane-2-carboxamide
Synonym:	Nirmatrelvir
MF:	$C_{23}H_{32}F_3N_5O_4$
FW:	499.5
Purity:	≥95%
Supplied as:	A solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

PF-07321332 is supplied as a solid. A stock solution may be made by dissolving the PF-07321332 in the solvent of choice, which should be purged with an inert gas. PF-07321332 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of PF-07321332 in these solvents is approximately 15, 5, and 2 mg/ml, respectively.

Description

PF-07321332 is an orally bioavailable inhibitor of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) main protease (M^{pro}), also known as 3C-like protease ($3CL^{pro}$), with a K_i value of 3.11 nM.[1] It also inhibits M^{pro} from other members of the *Betacoronavirus* genus, including SARS-CoV-1, HKU1-CoV, OC43-CoV, and MERS-CoV (K_is = 4.94, 189, 36.4, and 187 nM, respectively), as well as M^{pro} from NL-63-CoV and 229E CoV (K_is = 226 and 44.4 nM, respectively), which are members of the *Alphacoronavirus* genus. PF-07321332 is selective for these enzymes over several other proteases, including human and HIV-1 proteases (IC_{50}s = >100 µM for all), as well as a panel of G protein-coupled receptors, kinases, and transporters (IC_{50}s = ≥100 µM for all). It inhibits SARS-CoV-2 replication in A549 cells (EC_{50} = 77.9 nM) and reduces the cytopathic effect of SARS-CoV-2 in infected Vero E6 cells (EC_{50} = 74.5 nM) with a 50% cytotoxic concentration (CC_{50}) value of greater than 100 µM. PF-07321332 (300 and 1,000 mg/kg) reduces lung viral titers and the severity of pulmonary lesions in mice infected with the mouse-adapted SARS-CoV-2 MA10 variant. Formulations containing PF-07321332 have been used in the treatment of COVID-19.

Reference

1. Owen, D.R., Allerton, C.M.N., Anderson, A.S., *et al.* An oral SARS-CoV-2 M^{pro} inhibitor clinical candidate for the treatment of COVID-19. *Science* **374(6575)**, 1586-1593 (2021).

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