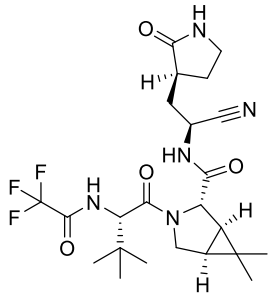
Product data sheet

MedKoo Cat#: 555985 Name: PF-07321332 CAS#: 2628280-40-8 Chemical Formula: $C_{23}H_{32}F_3N_5O_4$ Exact Mass: 499.2406 Molecular Weight: 499.5352	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:

PF-07321332 is an orally bioavailable 3C-like protease (3CLPRO) inhibitor. This drug is being investigated for safety, tolerability, and pharmacokinetics before moving on to studies of efficacy in the treatment or prophylaxis of COVID-19. 3CLPRO is responsible for cleaving polyproteins 1a and 1ab of SARS-CoV-2. PF-07321332 is an oral COVID-19 antiviral clinical candidate. By inhibiting the main protease, PF-07321332 prevents the virus from cleaving long protein chains into the parts it needs to reproduce itself.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	2.08	4.16

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.00 mL	10.01 mL	20.02 mL
5 mM	0.40 mL	2.00 mL	4.00 mL
10 mM	0.20 mL	1.00 mL	2.00 mL
50 mM	0.04 mL	0.20 mL	0.40 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

Pavan M, Bolcato G, Bassani D, Sturlese M, Moro S. Supervised Molecular Dynamics (SuMD) Insights into the mechanism of action of SARS-CoV-2 main protease inhibitor PF-07321332. J Enzyme Inhib Med Chem. 2021 Dec;36(1):1646-1650. doi: 10.1080/14756366.2021.1954919. PMID: 34289752.

In vivo study

Schooley RT, Carlin AF, Beadle JR, Valiaeva N, Zhang XQ, Clark AE, McMillan RE, Leibel SL, McVicar RN, Xie J, Garretson AF, Smith VI, Murphy J, Hostetler KY. Rethinking Remdesivir: Synthesis, Antiviral Activity and Pharmacokinetics of Oral Lipid Prodrugs. Antimicrob Agents Chemother. 2021 Jul 26:AAC0115521. doi: 10.1128/AAC.01155-21. Epub ahead of print. PMID: 34310217.

7. Bioactivity

Biological target:

Targets to the SARS-CoV-2 virus and can be used for COVID-19 reseacrch. IC50: 3CLPRO

Product data sheet

In vitro activity

The structural insights provided by SuMD will hopefully be able to inspire the rational discovery of other potent and selective protease inhibitors.

Reference: Pavan M, Bolcato G, Bassani D, Sturlese M, Moro S. Supervised Molecular Dynamics (SuMD) Insights into the mechanism of action of SARS-CoV-2 main protease inhibitor PF-07321332. J Enzyme Inhib Med Chem. 2021 Dec;36(1):1646-1650. doi: 10.1080/14756366.2021.1954919. PMID: 34289752.

In vivo activity

In addition to high oral bioavailability, stability in plasma and simpler metabolic activation, new oral lipid prodrugs of RVn had submicromolar anti-SARS-CoV-2 activity in a variety of cell types including Vero E6, Calu-3, Caco-2, human pluripotent stem cell (PSC)-derived lung cells and Huh7.5 cells. In Syrian hamsters oral treatment with ODBG-P-RVn was well tolerated and achieved therapeutic levels in plasma above the EC90 for SARS-CoV-2. The results suggest further evaluation as an early oral treatment for SARS-CoV-2 infection to minimize severe disease and reduce hospitalizations.

Reference: Schooley RT, Carlin AF, Beadle JR, Valiaeva N, Zhang XQ, Clark AE, McMillan RE, Leibel SL, McVicar RN, Xie J, Garretson AF, Smith VI, Murphy J, Hostetler KY. Rethinking Remdesivir: Synthesis, Antiviral Activity and Pharmacokinetics of Oral Lipid Prodrugs. Antimicrob Agents Chemother. 2021 Jul 26:AAC0115521. doi: 10.1128/AAC.01155-21. Epub ahead of print. PMID: 34310217.

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.