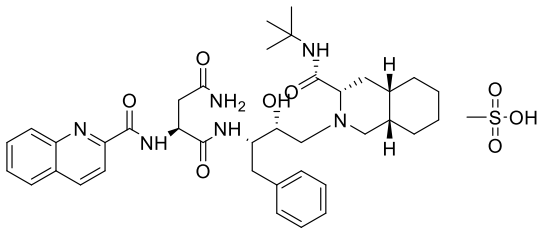
Product data sheet

MedKoo Cat#: 326756 Name: Saquinavir mesylate CAS#: 149845-06-7 (mesylate) Chemical Formula: $C_{39}H_{54}N_6O_8S$ Molecular Weight: 766.96	
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:

Saquinavir, also known as Ro 31-8959, is an antiretroviral drug used together with other medications to treat or prevent HIV/AIDS. Typically it is used with ritonavir or lopinavir/ritonavir to increase its affect. It is in the protease inhibitor class and works by blocking the HIV protease. Saquinavir was first sold in 1995.

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	38.35	50

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.30 mL	6.52 mL	13.04 mL
5 mM	0.26 mL	1.30 mL	2.61 mL
10 mM	0.13 mL	0.65 mL	1.30 mL
50 mM	0.03 mL	0.13 mL	0.26 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

1. Yao K, Wang Z, Peng C, Wang Y, Xue B, Tang Y, Wang Z, Xu H. HIV protease inhibitor saquinavir inhibits toll-like receptor 4 activation by targeting receptor dimerization. Immunopharmacol Immunotoxicol. 2023 Aug 7:1-7. doi: 10.1080/08923973.2023.2239488. Epub ahead of print. PMID: 37485845.
2. Park S, Auyeung A, Lee DL, Lambert PF, Carchman EH, Sherer NM. HIV-1 Protease Inhibitors Slow HPV16-Driven Cell Proliferation through Targeted Depletion of Viral E6 and E7 Oncoproteins. Cancers (Basel). 2021 Feb 24;13(5):949. doi: 10.3390/cancers13050949. PMID: 33668328; PMCID: PMC7956332.

In vivo study

1. Elgammal Y, Salama EA, Seleem MN. Saquinavir potentiates itraconazole's antifungal activity against multidrug-resistant Candida auris in vitro andin vivo. Med Mycol. 2023 Sep 4;61(9):myad081. doi: 10.1093/mmy/myad081. PMID: 37558393.
2. Liu H, Shen Y, Zhao B, Poon EH, Qi S, Ker DFE, Billiar TR, Cooper GM, Xu Y, Wang D. Short-Term Administration of HIV Protease Inhibitor Saquinavir Improves Skull Bone Healing with Enhanced Osteoclastogenesis. Plast Reconstr Surg. 2022 Dec 1;150(6):1264e-1274e. doi: 10.1097/PRS.0000000000009734. Epub 2022 Sep 19. PMID: 36112847; PMCID: PMC9698106.

7. Bioactivity

Biological target:

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Saquinavir is an HIV protease inhibitor (Kis = 0.12 and <0.1 nM for HIV-1 and HIV-2 protease, respectively). Saquinavir inhibits replication of clinical isolates of HIV-1 in a variety of cell-based assays and has antiviral activity against HIV-1 in infected C8166 cells (IC50 = 2 nM). It also inhibits the activity of the severe acute respiratory coronavirus 2 (SARS-CoV-2) main protease (Mpro), also known as 3C-like protease (3CLpro), with an IC50 value of 9.92 μM.

In vitro activity

In this study, saquinavir could modulate TLR4-mediated immune responses and consequent risk for uncontrolled inflammation. Saquinavir suppressed both MyD88- and TRIF-dependent pathways in response to LPS, leading to downregulation of NF-κB and IRF3. Saquinavir did not suppress MyD88-dependent pathway triggered by Pam3csk4. Saquinavir did not alleviate IRF3 phosphorylation induced by Poly(I:C). Saquinavir decreased dimerization of TLR4 following LPS or HMGB1 stimulation.

Reference: Immunopharmacol Immunotoxicol. 2023 Aug 7:1-7. https://pubmed.ncbi.nlm.nih.gov/37485845/

In vivo activity

Short term saquinavir application improved skull bone healing in a mouse calvarial defect model.Saquinavir may have potential for skeletal repair. It enhanced osteoclast and M2 macrophage infiltration, elevated gene expression related to bone healing, and promoted osteoclastic differentiation. However, high concentrations inhibited cell viability.

Reference: Plast Reconstr Surg. 2022 Dec 1;150(6):1264e-1274e. https://pubmed.ncbi.nlm.nih.gov/36112847/

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.