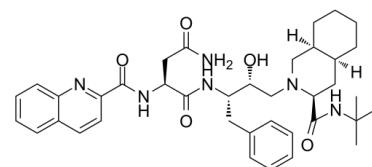


Data Sheet

Product Name:	Saquinavir
Cat. No.:	CS-1180
CAS No.:	127779-20-8
Molecular Formula:	C ₃₈ H ₅₀ N ₆ O ₅
Molecular Weight:	670.84
Target:	HIV; HIV Protease
Pathway:	Anti-infection; Metabolic Enzyme/Protease
Solubility:	DMSO : 100 mg/mL (149.07 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Saquinavir(Ro 31-8959) is an HIV Protease inhibitor used in antiretroviral therapy. IC₅₀ Value: Target: HIV Protease Saquinavir is a protease inhibitor. Proteases are enzymes that cleave protein molecules into smaller fragments. HIV protease is vital for both viral replication within the cell and release of mature viral particles from an infected cell. Saquinavir binds to the active site of the viral protease and prevents cleavage of viral polyproteins, preventing maturation of the virus. Saquinavir inhibits both HIV-1 and HIV-2 proteases. Studies have also looked at Saquinavir as a possible anti-cancer agent.

References:

- [1]. Marco Donia, Danijela Maksimovic-Ivanic, Sanja Mijatovic, et al. In vitro and in vivo anticancer action of Saquinavir-NO, a novel nitric oxide-derivative of the protease inhibitor saquinavir, on hormone resistant prostate cancer cells. *Cell cycle*. 2011, 10(3): 492 - 499.
- [2]. Walmsley Sharon, Avihingsanon Anchalee, Slim Jihad et al. Gemini: A Noninferiority Study of Saquinavir/Ritonavir Versus Lopinavir/Ritonavir as Initial HIV-1 Therapy in Adults. *JAIDS Journal of Acquired Immune Deficiency Syndromes*. 2009,50 (4) :367-374.
- [3]. Saquinavir
- [4]. Barillari Giovanna, Iovane Andréa, Bacigalupo Ilariaa, et al. Ritonavir or saquinavir impairs the invasion of cervical intraepithelial neoplasia cells via a reduction of MMP expression and activity. *AIDS*. 2012, 26 (8): 909-919.
- [5]. Martha Stefanidou, Carolina Herrera, Naomi Armanasco et al. Saquinavir Inhibits Early Events Associated with Establishment of HIV-1 Infection: Potential Role for Protease Inhibitors in Prevention. *Antimicrob. Agents Chemother*. 2012, 56 (8): 4381-4390.

CAIndexNames:

Butanediamide, N1-[(1S,2R)-3-[(3S,4aS,8aS)-3-[[[(1,1-dimethylethyl)amino]carbonyl]octahydro-2(1H)-isoquinolinyl]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)-

SMILES:

O=C(N[C@@H](CC(N)=O)C(N[C@@H](CC1=CC=CC=C1)[C@H](O)CN2[C@H](C(NC(C)(C)C)=O)[C@@](CCCC3)([H])[C@@]3([H])C2=O)C4=NC5=CC=CC=C5C=C4

Caution: Product has not been fully validated for medical applications. For research use only.

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