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SZABO-SCANDIC HandelsgmbH

Quellenstraße 110, A-1100 Wien

T. +43(0)1 489 3961-0

F. +43(0)1 489 3961-7

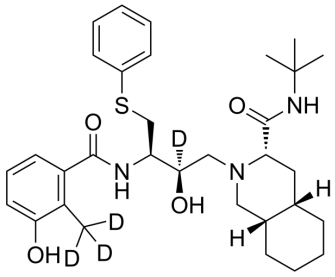
mail@szabo-scandic.com

www.szabo-scandic.com

linkedin.com/company/szaboscandic

Nelfinavir-d_4

Cat. No.:	HY-15287S1
Molecular Formula:	$C_{32}H_{41}D_4N_3O_4S$
Molecular Weight:	571.81
Target:	HIV; HIV Protease; Isotope-Labeled Compounds
Pathway:	Anti-infection; Metabolic Enzyme/Protease; Others
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Nelfinavir-d_4 is deuterated labeled Nelfinavir (HY-15287). Nelfinavir (AG-1341) is a potent and orally bioavailable HIV-1 protease inhibitor (K_i=2 nM) for HIV infection. Nelfinavir is a broad-spectrum, anticancer agent[1][2][3].
In Vitro	Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs[1]. Nelfinavir (AG1341) (1-10 μM; 48 hours) inhibits the proliferation of multiple myeloma cells[5]. Nelfinavir inhibits 26S chymotrypsin-like proteasome activity, impairs proliferation and triggers apoptosis of the myeloma cell lines and fresh plasma cells[5]. Nelfinavir (1-10 μM; 17 hours) induces apoptosis of multiple myeloma cell lines[5]. Nelfinavir (5 μM; 0-24 hours) decreases the phosphorylation of AKT[5]. Nelfinavir activates the cleavage of caspase-3, decreases the phosphorylation of AKT, STAT-3, ERK1/2, and activates the pro-apoptotic pathway of the unfolded protein response system[5]. Nelfinavir is also a SARS-CoV $3CL^{pro}$ inhibitor with an IC_{50} of 35.93 μM[6]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Nelfinavir (AG1341) (75 mg/kg; i.p.; 5 days a week for 21 days) decreases multiple myeloma cell growth in NOD/SCID mice[5]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

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[2]. Mondal D, et al. Nelfinavir suppresses signaling and nitric oxide production by human aortic endothelial cells: protective effects of thiazolidinediones. Ochsner J. 2013 Spring;13(1):76-90.

[3]. Qi Sun, et al. Bardoxolone and bardoxolone methyl, two Nrf2 activators in clinical trials, inhibit SARS-CoV-2 replication and its 3C-like protease. Signal Transduct Target Ther. 2021 May 29;6(1):212.

[4]. Gills JJ, et al. Nelfinavir, A lead HIV protease inhibitor, is a broad-spectrum, anticancer agent that inducesendoplasmic reticulum stress, autophagy, and apoptosis in vitro and in vivo. Clin Cancer Res. 2007 Sep 1;13(17):5183-94.

[5]. Kaldor SW, et al. Nelfinavir mesylate (AG1343): a potent, orally bioavailable inhibitor of HIV-1 protease. J Med Chem. 1997 Nov 21;40(24):3979-85.

[6]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019 Feb;53(2):211-216.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA