# **Product data sheet**



MedKoo Cat#: 330115		
Name: Nelfinavir free base		
CAS: 159989-64-7 (free base)		
Chemical Formula: C <sub>32</sub> H <sub>45</sub> N <sub>3</sub> O <sub>4</sub> S		
Exact Mass: 567.3131		o s o NH
Molecular Weight: 567.789		
Product supplied as:	Powder	
Purity (by HPLC):	≥ 98%	] " Он 🔎"
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:

Nelfinavir, also known as AG-1343, is an antiretroviral drug used in the treatment of the human immunodeficiency virus (HIV). It belongs to the class of drugs known as protease inhibitors (PIs) and like other PIs is almost always used in combination with other antiretroviral drugs.

## 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

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Solvent	Max Conc. mg/mL	Max Conc. mM		
DMF	20.0	35.22		
DMSO	57.0	100.39		
Ethanol	20.0	35.22		
Ethanol:PBS (pH 7.2)	0.33	0.58		
(1:2)				

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.76 mL	8.81 mL	17.61 mL
5 mM	0.35 mL	1.76 mL	3.52 mL
10 mM	0.18 mL	0.88 mL	1.76 mL
50 mM	0.04 mL	0.18 mL	0.35 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. Mondal D, Liu K, Hamblin M, Lasky JA, Agrawal KC. Nelfinavir suppresses insulin signaling and nitric oxide production by human aortic endothelial cells: protective effects of thiazolidinediones. Ochsner J. 2013 Spring;13(1):76-90. PMID: 23533049; PMCID: PMC3603192.
- 2. Kaldor SW, Kalish VJ, Davies JF 2nd, Shetty BV, Fritz JE, Appelt K, Burgess JA, Campanale KM, Chirgadze NY, Clawson DK, Dressman BA, Hatch SD, Khalil DA, Kosa MB, Lubbehusen PP, Muesing MA, Patick AK, Reich SH, Su KS, Tatlock JH. Viracept (nelfinavir mesylate, AG1343): a potent, orally bioavailable inhibitor of HIV-1 protease. J Med Chem. 1997 Nov 21;40(24):3979-85. doi: 10.1021/jm9704098. PMID: 9397180.

#### In vivo study

1. Shim JS, Rao R, Beebe K, Neckers L, Han I, Nahta R, Liu JO. Selective inhibition of HER2-positive breast cancer cells by the HIV protease inhibitor nelfinavir. J Natl Cancer Inst. 2012 Oct 17;104(20):1576-90. doi: 10.1093/jnci/djs396. Epub 2012 Oct 5. PMID: 23042933; PMCID: PMC3472971.

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2. Gills JJ, Lopiccolo J, Tsurutani J, Shoemaker RH, Best CJ, Abu-Asab MS, Borojerdi J, Warfel NA, Gardner ER, Danish M, Hollander MC, Kawabata S, Tsokos M, Figg WD, Steeg PS, Dennis PA. Nelfinavir, A lead HIV protease inhibitor, is a broad-spectrum, anticancer agent that induces endoplasmic reticulum stress, autophagy, and apoptosis in vitro and in vivo. Clin Cancer Res. 2007 Sep 1;13(17):5183-94. doi: 10.1158/1078-0432.CCR-07-0161. PMID: 17785575.

### 7. Bioactivity

Biological target:

Nelfinavir (AG-1341) is a potent and orally bioavailable HIV-1 protease inhibitor (Ki=2 nM) for HIV infection.

### In vitro activity

In vitro exposure (72 hours) of HAECs to NEL (nelfinavir) (0.25-2  $\mu$ g/mL) decreased both basal (2.5-fold) and insulin-induced NO production (4- to 5-fold). NEL suppressed insulin-induced phosphorylation of both Akt and eNOS at serine residues 473 and 1177, respectively. NEL decreased tyrosine phosphorylation of IR- $\beta$ , IRS-1, and PI3K.

Reference: Ochsner J. 2013 Spring;13(1):76-90. https://pubmed.ncbi.nlm.nih.gov/23533049/

#### In vivo activity

This study evaluated antitumor activity of nelfinavir with xenografts in athymic nude mouse models (n = 4-6 per group) of human breast cancer and repeated mixed-effects regression analysis. All statistical tests were two-sided. In vivo, nelfinavir selectively inhibited the growth of HER2-positive breast cancer cells (tumor volume index of HCC1954 cells on day 29, vehicle vs nelfinavir, mean = 14.42 vs 5.16, difference = 9.25, 95% confidence interval [CI] = 5.93 to 12.56, P < .001; tumor volume index of BT474 cells on day 26, vehicle vs nelfinavir, mean = 2.21 vs 0.90, difference = 1.31, 95% CI = 0.83 to 1.78, P < .001).

Reference: J Natl Cancer Inst. 2012 Oct 17;104(20):1576-90. https://pubmed.ncbi.nlm.nih.gov/23042933/

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.