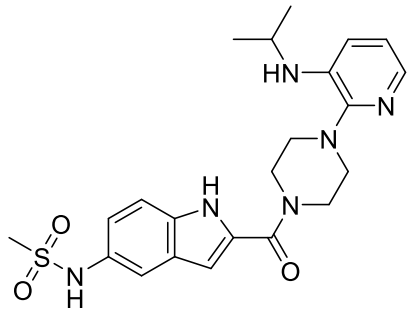
Product data sheet

MedKoo Cat#: 317587 Name: Delavirdine CAS#: 136817-59-9 (free base) Chemical Formula: $C_{22}H_{28}N_6O_3S$ Exact Mass: 456.19436 Molecular Weight: 456.56	
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:
Delavirdine is a non-nucleoside reverse transcriptase inhibitor (NNRTI). It is used as part of highly active antiretroviral therapy (HAART) for the treatment of human immunodeficiency virus (HIV) type 1. Although delavirdine was approved by the U.S. Food and Drug Administration in 1997, its efficacy is lower than other NNRTIs, especially efavirenz, and it also has an inconvenient schedule. These factors have led the U.S. DHHS not to recommend its use as part of initial therapy. (Source: https://en.wikipedia.org/wiki/Delavirdine).

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
H2O	30.0	65.71

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.19 mL	10.95 mL	21.90 mL
5 mM	0.44 mL	2.19 mL	4.38 mL
10 mM	0.22 mL	1.10 mL	2.19 mL
50 mM	0.04 mL	0.22 mL	0.44 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. Dueweke TJ, Poppe SM, Romero DL, Swaney SM, So AG, Downey KM, Althaus IW, Reusser F, Busso M, Resnick L, et al. U-90152, a potent inhibitor of human immunodeficiency virus type 1 replication. Antimicrob Agents Chemother. 1993 May;37(5):1127-31. doi: 10.1128/AAC.37.5.1127. PMID: 7685995; PMCID: PMC187915.
2. Romero MA, Mobley CB, Mumford PW, Roberson PA, Haun CT, Kephart WC, Healy JC, Beck DT, Young KC, Martin JS, Lockwood CM, Roberts MD. Acute and chronic resistance training downregulates select LINE-1 retrotransposon activity markers in human skeletal muscle. Am J Physiol Cell Physiol. 2018 Mar 1;314(3):C379-C388. doi: 10.1152/ajpcell.00192.2017. Epub 2017 Dec 20. PMID: 29351416.

In vivo study

1. Chang M, Sood VK, Wilson GJ, Kloosterman DA, Sanders PE, Hauer MJ, Zhang W, Branstetter DG. Metabolism of the HIV-1 reverse transcriptase inhibitor delavirdine in mice. Drug Metab Dispos. 1997 Jul;25(7):828-39. PMID: 9224777.

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7. Bioactivity

Biological target:

Delavirdine (U 90152) is a non-nucleoside reverse transcriptase inhibitor (NNRTI) that selectively inhibits HIV-1 reverse transcriptase (RT) (IC50=0.26 μM) over DNA polymerase α (IC50=440 μM) and polymerase δ (IC50>550 μM).

In vitro activity

A novel bisheteroarylpiperazine, U-90152 [1-(5-methanesulfonamido-1H-indol-2-yl-carbonyl)-4-[3-(1-methyl eth yl-amino)pyridinyl]piperazine] inhibited recombinant HIV-1 RT at a 50% inhibitory concentration (IC50) of 0.26 microM (compared with IC50s of > 440 microM for DNA polymerases alpha and delta). U-90152 blocked the replication in peripheral blood lymphocytes of 25 primary HIV-1 isolates, including variants that were highly resistant to 3'-azido-2',3'-dideoxythymidine (AZT) or 2',3'-dideoxyinosine, with a mean 50% effective dose of 0.066 +/- 0.137 microM. U-90152 had low cellular cytotoxicity, causing less than 8% reduction in peripheral blood lymphocyte viability at 100 microM. In experiments assessing inhibition of the spread of HIV-1IIIB in cell cultures, U-90152 was much more effective than AZT. 3 microM U-90152 totally prevented the spread of HIV-1, and death and/or dilution of the original inoculum of infected cells prevented renewed viral growth after U-90152 was removed at day 24. U-90152 drug retains significant activity against these mutant RTs (K103N and Y181C) in vitro (IC50s, approximately 8 microgramM).

Reference: Antimicrob Agents Chemother. 1993 May;37(5):1127-31. https://pubmed.ncbi.nlm.nih.gov/7685995/

In vivo activity

The excretion, disposition, brain penetration, and metabolism of delavirdine were investigated in CD-1 mice after oral administration of [14C]delavirdine mesylate at single doses of 10 and/or 250 mg/kg and multiple doses of 200 mg/kg/day. Delavirdine was absorbed and metabolized rapidly, that it constituted a minor component in circulation, that its pharmacokinetics were nonlinear, and that its metabolism to desalkyl delavirdine was capacity limited or inhibitable. Delavirdine did not significantly cross the blood-brain barrier; however, itsN-isopropylpyridinepiperazine metabolite—arising from amide bond cleavage—was present in brain at levels 2- to 3-fold higher than in plasma. The metabolism of delavirdine in the mouse was extensive and involved amide bond cleavage,N-desalkylation, hydroxylation at the C-6′ position of the pyridine ring, and pyridine ring-cleavage as determined by MS and/or1H and 13C NMR spectroscopies. N-desalkylation and amide bond cleavage were the primary metabolic pathways at low drug doses and, as the biotransformation of delavirdine to desalkyl delavirdine reached saturation or inhibition, amide bond cleavage became the predominant pathway at higher doses and after multiple doses.

Reference: . Drug Metab Dispos. 1997 Jul;25(7):828-39. https://dmd.aspetjournals.org/content/25/7/828.long