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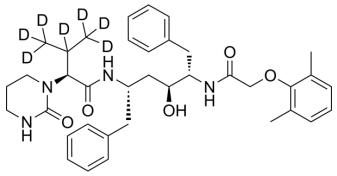
Lopinavir-d_7

Cat. No.:	HY-14588S2
CAS No.:	1432060-78-0
Molecular Formula:	$C_{37}H_{41}D_7N_4O_5$
Molecular Weight:	635.84
Target:	HIV; SARS-CoV; 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	Lopinavir-d_7 is deuterated labeled Lopinavir (HY-14588). Lopinavir (ABT-378) is a highly potent, selective peptidomimetic inhibitor of the HIV-1 protease, with K_is of 1.3 to 3.6 pM for wild-type and mutant HIV protease. Lopinavir acts by arresting maturation of HIV-1 thereby blocking its infectivity[1][2]. Lopinavir is also a SARS-CoV $3CL^{pro}$ inhibitor with an IC_{50} of 14.2 μM [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]. HIV-1 protease is an essential enzyme for production of mature, infective virus[2]. Lopinavir potently inhibits wild-type and mutant HIV protease (K_i= 1.3 to 3.6 pM), blocks the replication HIV type 1 (EC_{50} =0.006 to 0.017 μM), and maintains high potency against mutant HIV selected by Ritonavir in vivo (EC_{50}=≤0.06 μM)[3]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Coadministration with low-dose Ritonavir significantly improves the pharmacokinetic properties and hence the activity of Lopinavir against HIV-1 protease[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Cvetkovic RS, et al. Lopinavir/ritonavir: a review of its use in the management of HIV infection. Drugs. 2003;63(8):769-802.

[2]. 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.

[3]. Sham HL, et al. ABT-378, a highly potent inhibitor of the human immunodeficiency virus protease. Antimicrob Agents Chemother. 1998;42(12):3218-3224.

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

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

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