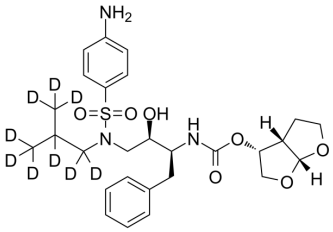
Darunavir-d9

Cat. No.:	HY-112585
CAS No.:	1133378-37-6
Molecular Formula:	$C_{27}H_{28}D_9N_3O_7S$
Molecular Weight:	556.72
Target:	HIV; HIV Protease
Pathway:	Anti-infection; Metabolic Enzyme/Protease
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Darunavir-d9 (TMC114-d9) is the deuterium labeled Darunavir. Darunavir (TMC114), an orally active next generation HIV protease inhibitor, has a similar antiviral activity against the mutant and the wild-type viruses. Darunavir (TMC114) is potent against laboratory HIV-1 strains and primary clinical isolates (IC_{50} = 0.003 μM; IC_{90} = 0.009 μM) with minimal cytotoxicity[1][2].
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]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

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

[2]. Dominique L N G Surleraux, et al. Discovery and selection of TMC114, a next generation HIV-1 protease inhibitor. J Med Chem. 2005 Mar 24;48(6):1813-22.;Yasuhiro Koh, et al. Novel bis-tetrahydrofuranylurethane-containing nonpeptidic protease inhibitor (PI) UIC-94017 (TMC114) with potent activity against multi-PI-resistant human immunodeficiency virus in vitro. Antimicrob Agents Chemother. 2003 Oct;47(10):3123-9.

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