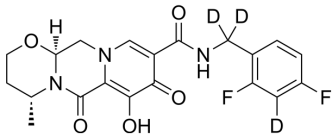
Dolutegravir-d_3

Cat. No.:	HY-13238S1
Molecular Formula:	$C_{20}H_{16}D_3F_2N_3O_5$
Molecular Weight:	422.4
Target:	HIV Integrase; HIV; Isotope-Labeled Compounds
Pathway:	Metabolic Enzyme/Protease; Anti-infection; Others
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Dolutegravir-d_3 is the deuterium labeled Dolutegravir. Dolutegravir (S/GSK1349572) is a highly potent and orally bioavailable HIV integrase strand transfer inhibitor with an IC50 of 2.7 nM for HIV-1 integrase-catalyzed strand transfer. Dolutegravir (S/GSK1349572) inhibits HIV-1 viral replication with an IC50 of 0.51 nM in peripheral blood mononuclear cells. Dolutegravir retains a high potency against the HIV-1 Y143R, N155H, and G140S/Q148H mutants (EC50=3.6-5.8 nM)[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]. Kobayashi M, et al. In Vitro antiretroviral properties of S/GSK1349572, a next-generation HIV integrase inhibitor. Antimicrob Agents Chemother. 2011 Feb;55(2):813-21.

[3]. Hare S, et al. Structural and functional analyses of the second-generation integrase strand transfer inhibitor dolutegravir (S/GSK1349572). Mol Pharmacol. 2011 Oct;80(4):565-72.

[4]. Moss L, et al. The comparative disposition and metabolism of dolutegravir, a potent HIV-1 integrase inhibitor, in mice, rats, and monkeys. Xenobiotica. 2015 Jan;45(1):60-70.

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