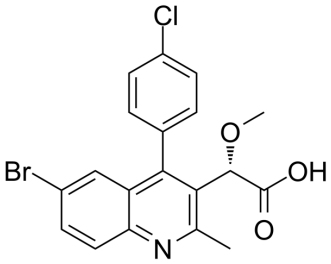
(S)-BI-1001

Cat. No.:	HY-12210
CAS No.:	957889-73-5
Molecular Formula:	$C_{19}H_{15}BrClNO_3$
Molecular Weight:	420.68
Target:	HIV Integrase
Pathway:	Metabolic Enzyme/Protease
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	(S)-BI-1001 (Compound 11) is an active S-enantiomer of BI-1001. (S)-BI-1001 exhibits antiviral potency against HIV-1 integrase with an IC_{50} of 28 nM, an EC_{50} of 450 nM and a K_d of 4.7 μM[1].
IC_{50} & Target	IC50: 28 nM (HIV-1 integrase)[1] EC50: 450 nM (HIV-1 integrase)[1] Kd: 4.7 μM (HIV-1 integrase)[1]
In Vitro	The C3 substituent is critical to the binding of (S)-BI-1001 (Compound 11) to the CCD of integrase and makes two key contacts with the protein: (a) a bivalent hydrogen bonding interaction with protein backbone at residues E170 and H171, and (b) a van der Waals contact deep in the hydrophobic pocket via the methoxyl group. The quinoline scaffold lies flat on the surface of the protein partially covering residues 124 and 125 and makes productive contact with the methyl group of A128[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Fader LD, et al. Discovery of BI 224436, a Noncatalytic Site Integrase Inhibitor (NCINI) of HIV-1. ACS Med Chem Lett. 2014 Jan 22;5(4):422-7.

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