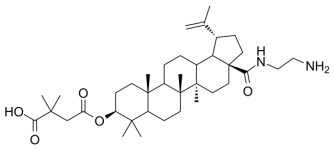
EP39

Cat. No.:	HY-150536
Molecular Formula:	$C_{38}H_{62}N_2O_5$
Molecular Weight:	626.91
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	EP39 is a potent HIV-1 maturation inhibitor. EP39 interacts with the SP1 domain of Gag. EP39 decreases the dynamics of CA-SP1 junction, by binding to the QVT motif of the SP1 domain, and perturbs the natural coil-helix equilibrium on both sides of the SP1 domain by stabilizing the transient alpha helical structure. EP39 acts by arresting maturation of HIV-1 thereby blocking its infectivity[1].
In Vitro	EP39 has binding affinity to different residues of SP1. SP1-T^{239} has the highest binding affinity (52.4 μM); SP1-S^{236}, SP1-Q^{237} and SP1-V^{238} have relatively high binding affinities (179.6 μM, 154,5 μM and 204.4 μM, respectively); SP1-E^{233}, SP1-M^{235} and NC-T^{257} have medium binding affinities (237.0 μM, 235,4 μM, 308.4 μM, respectively); CA-V^{221}, CA-L^{231} and SP1-A^{232} have weak binding affinities (669.6 μM, 678.4 μM and 691.9 μM, respectively) [1]. EP39 perturbs the natural coil-helix equilibrium on both sides of the SP1 domain by stabilizing the transient alpha helical structure[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Chen X, et, al. The HIV-1 maturation inhibitor, EP39, interferes with the dynamic helix-coil equilibrium of the CA-SP1 junction of Gag. Eur J Med Chem. 2020 Oct 15;204:112634.

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