

Product Name	: KRH-1636
Synonyms	: KRH1636;KRH 1636
Cat No.	: M15068
CAS Number	: 568526-77-2
Molecular Formula	: C32H37N7O2
Formula Weight	: 551.70
Chemical Name	: N-((S)-5-guanidino-1-(((S)-1-(naphthalen-1-yl)ethyl)amino)-1-oxopentan-2-yl)-4-(((pyridin-2-yl)methyl)amino)methyl)benzamide
Description	A potent, selective inhibitor of CXCR4 with IC50 of 13 nM, has no effect on CXCR1, CCR3, CCR4, or CCR5; completely inhibits X4 HIV-1 (IIIB strain) replication in MT-4 cells with EC50 of 19.3 nM and EC90 of 47.8 nM, without cytotoxic concentration (CC50>400 uM), also has effectivity against HTLV-IIIB and three clinical isolates in PBMCs including YU-6 (EC50=46 nM), but not R5 HIV-1, YU-1, YU-2; selectively blocks CXCR4-mediated Ca2+ signaling, blocks X4 HIV-1 replication in human PBL/SCID mice.
Pathway	: GPCR/G Protein
Target	: Chemokine Receptor
Receptor	: Chemokine Receptor
Solubility	: —
SMILES	: <chem>NC(NCCC[C@@H](C(N[C@H](C1=CC=CC=CC2=CC=C1)C)=O)NC(C3=CC=C(C=C3)CNCC4=NC=CC=C4)=O)=N</chem>
Storage	: (-20°C)
Stability	: ≥ 2 years
Reference	:

1. Ichiyama K, et al. Proc Natl Acad Sci U S A. 2003 Apr 1;100(7):4185-90. 2. Murakami T, et al. Antimicrob Agents Chemother. 2009 Jul;53(7):2940-8. 3. Zachariassen ZG, et al. J Med Chem. 2015 Oct 22;58(20):8141-53.