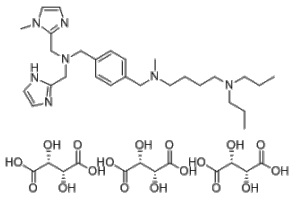
Product Name	:	KRH-3955
Synonyms	:	KRH 3955;KRH3955
Cat No.	:	M10376
CAS Number	:	1097732-62-1
Molecular Formula	:	C40H63N7O18
Formula Weight	:	929.98
Chemical Name	:	N1-(4-((((1H-imidazol-2-yl)methyl)((1-methyl-1H-imidazol-2-yl)methyl)amino)methyl)benzyl)-N1-methyl-N4,N4-dipropylbutane-1,4-diamine, (2R,3R)-2,3-dihydroxybutanedioate (1:3)
Description	:	A potent, selective, orally bioavailable inhibitor of CXCR4 that efficiently inhibits SDF-1α binding to CXCR4 with IC50 of 0.61 nM; inhibits the replication of both X4 and R5X4 HIV-1 in activated PBMCs with EC50 of 0.3 to 1.0 nM but does not affect R5 HIV-1 replication, also inhibits the replication of clinical isolates of X4 HIV-1 (92HT599) and R5X4 HIV-1 (92HT593) (EC50=4.0-4.2 nM) in activated PBMCs; exhibits inhibition of Ca2+ signaling through CXCR4, blocks X4 HIV-1 replication in human PBL/SCID mice.
Pathway	:	GPCR/G Protein
Target	:	Chemokine Receptor
Receptor	:	Chemokine Receptor
Solubility	:	——
SMILES	:	CCCN(CCC)CCCCN(CC1=CC=C(CN(CC2=NC=CN2)CC3=NC=CN3C)C=C1)C.O=C(O)[C@H](O)[C@@H](O)C(O)=O.O=C(O)[C@H](O)[C@@H](O)C(O)=O.O=C(O)[C@H](O)[C@@H](O)C(O)=O
Storage	:	(-20℃)
Stability	:	≥ 2 years
Reference	:	



1. Murakami T, et al. Antimicrob Agents Chemother. 2009 Jul;53(7):2940-8.| 2. Iwasaki Y, et al. Cancer Sci. 2009 Apr;100(4):778-81.| 3. Nakasone T, et al. Med Microbiol Immunol. 2013 Apr;202(2):175-82.| 4. Hikichi Y, et al. J Gen Virol. 2016 Sep;97(9):2427-40.