

Product Name: KRH 3955 hydrochloride

Catalog No.: 6126

Batch No.: 2

IUPAC Name: *N*¹-[[4-[[[(1*H*-imidazol-2-yl)methyl][(1-methyl-1*H*-imidazol-2-yl)methyl]amino]methyl]phenyl]methyl]-*N*¹-methyl-*N*⁴,*N*⁴-dipropyl-1,4-butanediamine trihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₄₅N₇·3HCl·H₂O

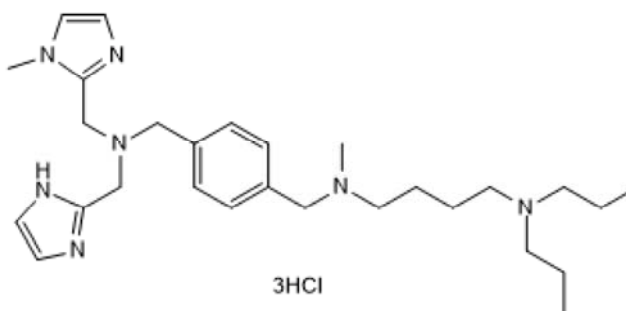
Batch Molecular Weight: 607.11

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.4	8.3	16.15
Found	55.4	8.49	15.91

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Highly potent CXCR4 antagonist (IC₅₀ = 0.61 nM). Displays selectivity for CXCR4 over a range of other CXC receptors. Inhibits replication of HIV-1 viruses in human PBMC (EC₅₀ values are 0.33 to 1.4 nM). Suppresses HIV-1 infection in mice. Orally bioavailable.

Physical and Chemical Properties:

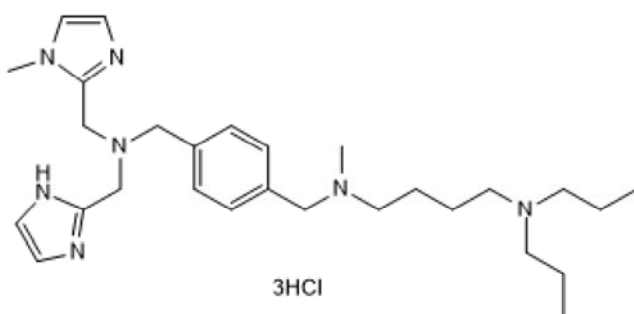
Batch Molecular Formula: C₂₈H₄₅N₇.3HCl.H₂O

Batch Molecular Weight: 607.11

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at RT. This product is packaged under an inert atmosphere.

Solubility & Usage Info:

water to 100 mM
DMSO to 100 mM

Standard retail vials are prepared by lyophilisation. The product may appear as a solid, a gel or a film. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Iwasaki et al (2009) Efficient inhibition of SDF-1α-mediated chemotaxis and HIV-1 infection by novel CXCR4 antagonists. *Cancer Sci.* **100** 778. PMID: 19245436.

Murakami et al (2009) The novel CXCR4 antagonist KRH-3955 is an orally bioavailable and extremely potent inhibitor of human immunodeficiency virus type 1 infection: comparative studies with AMD3100. *Antimicrob.Agents Chemother.* **53** 2940. PMID: 19451305.

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