bio-techne
TOCRIS

Print Date: Apr 6th 2023

# Certificate of Analysis

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**Product Name:** **KRH 3955 hydrochloride** **Catalog No.: 6126** **Batch No.: 2**

CAS Number: 2253744-59-9

IUPAC Name: $N^1$-[[4-[[(1*H*-Imidazol-2-ylmethyl)[(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:** $C_{28}H_{45}N_7.3HCl.H_2O$

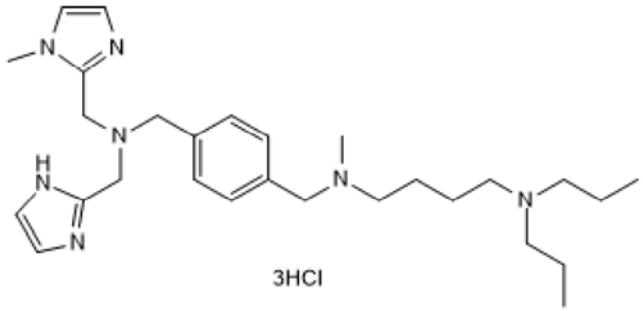
**Batch Molecular Weight:** 607.11

**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

**$^1$H 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 |



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**Description:**

KRH 3955 hydrochloride is a highly potent CXCR4 antagonist ($IC_{50}$ = 0.61 nM). Displays selectivity for CXCR4 over a range of other CXC receptors. Inhibits replication of HIV-1 viruses in human PBMC ($EC_{50}$ values are 0.33 to 1.4 nM). Supresses HIV-1 infection in mice. Orally bioavailable.

**Physical and Chemical Properties:**

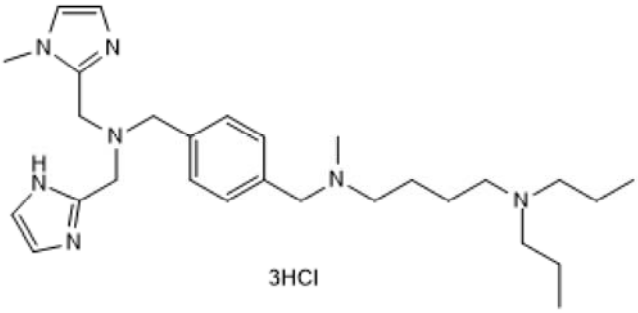
Batch Molecular Formula: $C_{28}H_{45}N_7.3HCl.H_2O$

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.