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

2. ANALYTICAL DATA

HPLC: Shows 98.3% purity
\(^1\)H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>55.4</td>
<td>8.3</td>
<td>16.15</td>
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<tr>
<td>Found</td>
<td>55.4</td>
<td>8.49</td>
<td>15.91</td>
</tr>
</tbody>
</table>
Product Name: KRH 3955 hydrochloride
Catalog No.: 6126 Batch No.: 2

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

Description:
Highly potent CXCR4 antagonist \((I_C^{50} = 0.61 \text{ nM})\). 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). Suppresses HIV-1 infection in mice. Orally bioavailable.

Physical and Chemical Properties:
- Batch Molecular Formula: \( C_{38}H_{49}N_{7} \cdot 3HCl \cdot H_2O \)
- 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

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: