1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{28}\text{H}_{54}\text{N}_{8}.8\text{HCl}.6\text{H}_{2}\text{O} \)

Batch Molecular Weight: 902.57

Physical Appearance: Off-white solid

Solubility: Water to 100 mM

Storage: Desiccated at -20°C

Batch Molecular Structure:

![Molecular Structure](image)

2. ANALYTICAL DATA

\(^1\text{H NMR:}\) 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>37.26</td>
<td>8.26</td>
<td>12.42</td>
</tr>
<tr>
<td>Found</td>
<td>37.04</td>
<td>8.3</td>
<td>12.25</td>
</tr>
</tbody>
</table>
**Product Name:** AMD 3100 octahydrochloride  
**Catalog No.:** 3299  
**Batch No.:** 2  
**CAS Number:** 155148-31-5  
**IUPAC Name:** 1,1’-[1,4-Phenylenebis{(methylene)}]bis{(1,4,8,11-tetraazacyclotetradecane)} octahydrochloride

**Description:**
Highly selective CXCR4 chemokine receptor antagonist (IC\(_{50}\) values are 0.02 - 0.13 and > 25 μM for CXCR4 and all other chemokine receptors respectively). Switches inflammatory responses from Th2 to Th1 type and reduces airway hyperresponsiveness in a mouse model of asthma. Potently inhibits HIV-1 and HIV-2 replication in vitro (EC\(_{50}\) = 4 - 35 nM) and mobilizes hematopoietic stem cells in vivo. Attenuates cocaine place preference and locomotor stimulation in rats. Attenuates microglial activation neurological function after ischemic stroke in mice. Inhibits tumor cell migration and proliferation in vitro and in vivo in a range of cancers... Please see product datasheet on www.tocris.com for full description.

**Physical and Chemical Properties:**
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- **Batch Molecular Weight:** 902.57
- **Physical Appearance:** Off-white solid

**Batch Molecular Structure:**

![Molecular Structure](image)

**Storage:** Desiccate at -20°C

**Solubility & Usage Info:**
- Water to 100 mM
- CAUTION - This product is hygroscopic and we recommend that it is desiccated upon arrival.

**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:**