

# Certificate of Analysis

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**Product Name:** AMD 3100 octahydrochloride

**Catalog No.:** 3299

**Batch No.:** 3

CAS Number: 155148-31-5

IUPAC Name: 1,1'-[1,4-Phenylenebis-(methylene)]-bis-(1,4,8,11-tetraazacyclotetradecane) octahydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>28</sub>H<sub>54</sub>N<sub>8</sub>.8HCl.6.5H<sub>2</sub>O

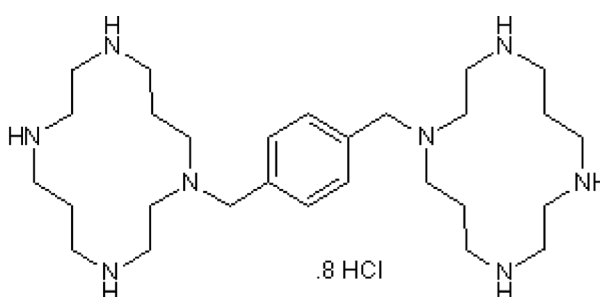
**Batch Molecular Weight:** 911.61

**Physical Appearance:** White solid

**Solubility:** water to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	36.89	8.29	12.29	31.11
Found	36.2	8.31	11.9	29.95

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

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**Description:**

AMD 3100 octahydrochloride is a highly selective CXCR4 chemokine receptor antagonist (IC<sub>50</sub> values are 0.02 - 0.13 and > 25 µM for CXCR4 and most other chemokine receptors, respectively). Also CXCR7 allosteric agonist. 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<sub>50</sub> = 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 migra... Please see product specific page on [www.tocris.com](http://www.tocris.com) for full description.

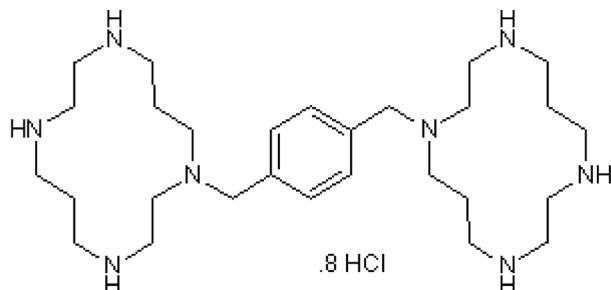
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Batch Molecular Weight: 911.61

Physical Appearance: White solid

**Batch Molecular Structure:**



**References:**

**Kim et al** (2017) Chemokines and cocaine: CXCR4 receptor antagonist AMD3100 attenuates cocaine place preference and locomotor stimulation in rats. *Brain Behav. Immun.* **62** 30. PMID: 27575003 .

**Wu et al** (2017) A novel CXCR4 antagonist CX549 induces neuroprotection in stroke brain. *Cell. Transplant.* **26** 571. PMID: 27938478 .

**Paganessi et al** (2011) Effective mobilization of hematopoietic progenitor cells in G-CSF mobilization defective CD26<sup>-/-</sup> mice through AMD3100-induced disruption of the CXCL12-CXCR4 axis. *Exp. Hematol.* **39** 384. PMID: 21168468.

**Storage:** Store at -20°C

**Solubility & Usage Info:**

water to 100 mM

This compound is hygroscopic and may absorb atmospheric moisture during prolonged storage, causing the solid to become sticky and/or collapse into a gel or glass-like form. Although purity is unaffected, it may be difficult to extract the full quantity from the vial. In such a situation, we recommend that solutions are 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. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

**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.

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