

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₅₄N₈.8HCl.6H₂O

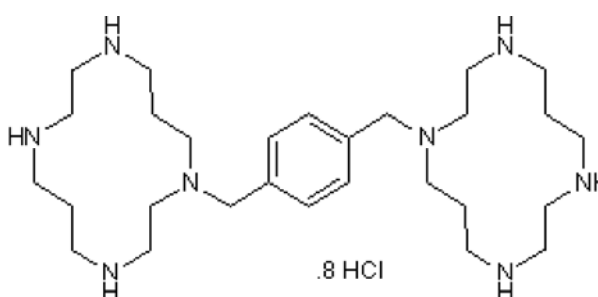
Batch Molecular Weight: 902.57

Physical Appearance: Off-white solid

Solubility: water to 100 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	37.26	8.26	12.42
Found	37.04	8.3	12.25

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

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Description:

Highly selective CXCR4 chemokine receptor antagonist (IC₅₀ 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 (EC₅₀ = 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 ... Please see product datasheet on www.tocris.com for full description.

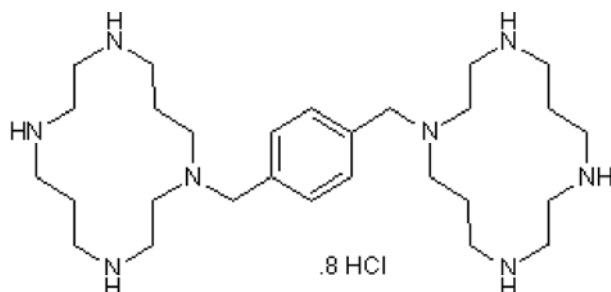
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References:

- 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^{-/-} mice through AMD3100-induced disruption of the CXCL12-CXCR4 axis. *Exp.Hematol.* **39** 384. PMID: 21168468.
- Burger and Peled et al** (2009) CXCR4 antagonists: targeting the microenvironment in leukemia and other cancers. *Leukemia* **23** 43. PMID: 18987663.
- Kalatskaya et al** (2009) MD3100 Is a CXCR7 ligand with allosteric agonist properties. *Mol.Pharmacol.* **75** 1240. PMID: 19255243.
- Hogaboam et al** (2005) The therapeutic potential in targeting CCR5 and CXCR4 receptors in infectious and allergic pulmonary disease. *Pharmacol.Ther.* **107** 314. PMID: 16009428.
- Hatse et al** (2002) Chemokine receptor inhibition by AMD3100 is strictly confined to CXCR4. *FEBS Letts.* **527** 255. PMID: 12220670.
- Bridger et al** (1995) Synthesis and structure-activity relationships of phenylenebis(methylene)-linked bis-tetraazamacrocycles that inhibits HIV replication. Effects of macrocyclic ring size and substituents on the aromatic linker. *J.Med.Chem.* **38** 366. PMID: 7830280.

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.

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