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## DATASHEET

AMD 3100 octahydrochloride

### Product overview

|                   |   |
|-------------------|---|
| Name              | AMD 3100 octahydrochloride  |
| Cat No            | HB2739  |
| Alternative names | Plerixafor   JM3100   |
| Biological action | Antagonist  |
| Description       | Potent, selective CXCR4 antagonist. Mobilizes hematopoietic stem cells. |

### Biological Data

|                        |  |
|------------------------|--|
| Biological description | Potent and selective CXCR4 antagonist ( $IC_{50}$ values are 0.79 and 0.18 at CXCR4 and CCR2 respectively). Blocks the route of HIV entry into T-cells. Shows potent anti-HIV activity <i>in vitro</i> and <i>in vivo</i> . Also mobilizes hematopoietic stem cells. |
|------------------------|--|

### Solubility & Handling

|                      |   |
|----------------------|---|
| Storage instructions | -20°C (desiccate)   |
| Solubility overview  | Soluble in water (100mM)  |
| Important            | This product is for RESEARCH USE ONLY and is not intended for therapeutic or diagnostic use. Not for human or veterinary use. |

### Chemical Data

|                    |   |
|--------------------|---|
| Chemical name      | 1,1'-[1,4-Phenylenebis-(methylene)]- bis-(1,4,8,11-tetraazacyclotetradecane) octahydrochloride  |
| Molecular Weight   | 794.48  |
| Chemical structure | The chemical structure shows a central phenylene ring linked via two methylene groups to two 1,4,8,11-tetraazacyclotetradecane (cyclam) macrocycles. The macrocycles are nitrogen-containing macrocyclic polyamines with four nitrogen atoms per macrocycle. The entire molecule is labeled with a dot and "8HCl (H<sub>2</sub>O)" indicating its octahydrate form. |
| Molecular Formula  | C<sub>28</sub>H<sub>54</sub>N<sub>8</sub>·8HCl  |
| CAS Number         | 155148-31-5   |
| PubChem identifier | 65014   |
| SMILES             | C1(CN3CCCNCNCCNCC3)=CC=C(CN2CCCNCNCCNCC2)C=C1.C1.C1.C1.C1.C1.C1.C1  |
| InChIKey           | UEUPDYPUTTUXLJ-UHFFFAOYSA-N   |

### References

**Synthesis and structure-activity relationships of phenylenebis(methylene)-linked bis-tetraazamacrocycles that inhibit HIV replication. Effects of macrocyclic ring size and substituents on the aromatic linker.**

Bridge et al (1995) J Med Chem 38(2)

PubMedID [7830280](#)

**Characterization of the molecular pharmacology of AMD3100: a specific antagonist of the G-protein coupled chemokine receptor, CXCR4.**

**Effective mobilization of hematopoietic progenitor cells in G-CSF mobilization defective CD26-/- mice through AMD3100-induced disruption of the CXCL12-CXCR4 axis.**

Paganessi (2011) Exp Hematol 39(3)

PubMedID

21168468

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