

## Certificate of Analysis

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**Product Name:** AY 9944 dihydrochloride

**Catalog No.:** 1639

**Batch No.:** 2

CAS Number: 366-93-8

IUPAC Name: *trans*-*N,N*-bis[2-Chlorophenylmethyl]-1,4-cyclohexanedimethanamine dihydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>22</sub>H<sub>28</sub>Cl<sub>2</sub>N<sub>2</sub>·2HCl·¼H<sub>2</sub>O

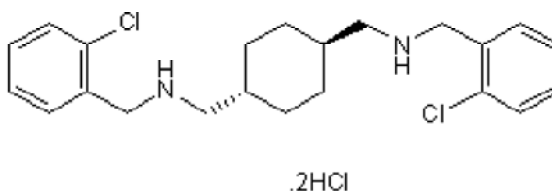
**Batch Molecular Weight:** 468.8

**Physical Appearance:** White solid

**Solubility:** water to 50 mM  
DMSO to 5 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**HPLC:** Shows 99.5% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	56.36	6.56	5.98	30.25
Found	56.27	6.66	5.94	30.61

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

**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

[www.tocris.com/distributors](http://www.tocris.com/distributors)

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**2**

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IUPAC Name: *trans*-N,N-bis[2-Chlorophenylmethyl]-1,4-cyclohexanedimethanamine dihydrochloride

**Description:**

AY 9944 dihydrochloride is an inhibitor of hedgehog (Hh) signaling, possibly via several mechanisms. Inhibits  $\Delta^7$ -dehydrocholesterol reductase ( $IC_{50}$  = 13 nM), thus reduces cholesterol biosynthesis, and also inhibits cholesterol esterification. May also directly block the cellular response to Hh proteins. Teratogenic in vivo.

**Physical and Chemical Properties:**

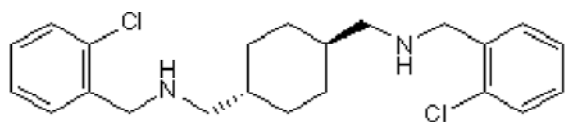
Batch Molecular Formula:  $C_{22}H_{28}Cl_2N_2 \cdot 2HCl \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 468.8

Physical Appearance: White solid

**Minimum Purity:**  $\geq 99\%$

**Batch Molecular Structure:**



.2HCl

**Storage:** Desiccate at RT

**Solubility & Usage Info:**

water to 50 mM

DMSO to 5 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:**

**Incardona and Eaton** (2000) Cholesterol in signal transduction. *Curr.Opin.Cell Biol.* **12** 193. PMID: 10712926.

**Cooper et al** (1998) Teratogen-mediated inhibition of target tissue response to Shh signaling. *Science* **280** 1603. PMID: 9616123.

**Moebius et al** (1998) Molecular cloning and expression of the human  $\Delta^7$ -sterol reductase. *Proc.Natl.Acad.Sci.U.S.A.* **95** 1899. PMID: 9465114.

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