

Certificate of Analysis

Product Name: AY 9944 dihydrochloride

Catalog No.: 1639

Batch No.: 1

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: C₂₂H₂₈Cl₂N₂·2HCl·¼H₂O

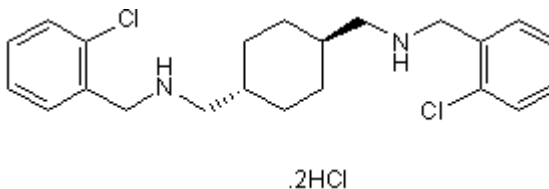
Batch Molecular Weight: 468.8

Physical Appearance: White solid

Solubility: water to 50 mM
DMSO to 5 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Dichloromethane:Methanol [95:5])

Melting Point: Between 286 - 288°C

HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure

Microanalysis:	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	56.36	6.56	5.98	30.25
Found	56.28	6.58	6.04	30.32

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

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Description:

Inhibitor of hedgehog (Hh) signaling, possibly via several mechanisms. Inhibits Δ^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:

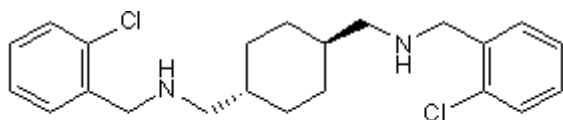
Batch Molecular Formula: $C_{22}H_{28}Cl_2N_2 \cdot 2HCl \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 468.8

Physical Appearance: White solid

Minimum Purity: >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:

Kraml et al (1964) Inhibition of the conversion of 7-dehydrocholesterol to cholesterol by AY-9944. *Biochem.Biophys.Res.Comm.* **15** 455. PMID: 4283982.

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

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

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

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