



Certificate of Analysis

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Product Name: Ambenonium dichloride Catalog No.: 0388 Batch No.: 1

CAS Number: 115-79-7

IUPAC Name: N,N-[(1,2-Dioxo-1,2-ethanediyl)bis(imino-2,1-ethanediyl)]bis(2-chloro-N,N-diethylbenzenemethaminium) dichloride

Store at RT

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{42}CI_4N_4O_2.4H_2O$

Batch Molecular Weight: 680.54

Physical Appearance: White solid

Solubility: water to 100 mM

Batch Molecular Structure:

Storage:

2. ANALYTICAL DATA

TLC: $R_f = 0.56$ (Dichloromethane:Methanol:Ammonia soln. [9:1:0.1])

Melting Point: At 205°C

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 49.42 7.41 8.23 Found 49.14 7.22 8.19



Product Information

Print Date: Jan 15th 2016

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Description:

Extremely potent, selective and rapidly reversible inhibitor of acetylcholinesterase (AChE) (IC $_{50}$ values are 0.000698 and 8.20 μ M at AChE and BChE respectively).

Physical and Chemical Properties:

Batch Molecular Formula: C₂₈H₄₂Cl₄N₄O₂.4H₂O

Batch Molecular Weight: 680.54 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

water to 100 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:

Lands et al (1958) An investigation of the structure-activity correlations within a series of ambenonium analogs. J.Pharmacol.Exp.Ther. 123 121 PMID: 13550066

Web (1965) Affinity for benzoquinonium, and ambenonium derivatives for the acetylcholine receptor, tested on the electroplax, and for acetylcholinesterase in solution. Biochim.Biophys.Acta. **102** 172. PMID: 5833399.

Hodge et al (1992) Ambenonium is a rapidly reversible noncovalent inhibitor of acetylcholinesterase, with one of the highest known affinities. Mol.Pharmacol. **41** 937. PMID: 1588924.

Bolognesi et al (2003) Design, synthesis and biological evaluation of ambenonium derivatives as AChE inhibitors. Farmaco **58** 917. PMID: 13679187.