

## Certificate of Analysis

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**Product Name:** Doxepin hydrochloride

**Catalog No.:** 0508

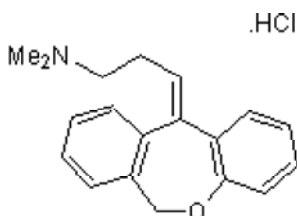
**Batch No.:** 5

**CAS Number:** 1229-29-4

**IUPAC Name:** 11-(3-dimethylaminopropylidene)-6,11-dihydrodibenz[*b,e*]oxepin hydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>19</sub>H<sub>21</sub>NO.HCl  
**Batch Molecular Weight:** 315.84  
**Physical Appearance:** White solid  
**Solubility:** water to 100 mM  
DMSO to 100 mM  
**Storage:** Store at RT  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**HPLC:** Shows 99.6% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	72.25	7.02	4.43
Found	72.4	7.05	4.48

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

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**IUPAC Name:** 11-(3-dimethylaminopropylidene)-6,11-dihydrodibenz[*b,e*]oxepin hydrochloride

**Description:**

Highly potent H<sub>1</sub> histamine receptor antagonist ( $K_d = 310$  pM) and tricyclic antidepressant. Also binds to the H<sub>4</sub> histamine receptor ( $pK_i = 6.79$ ). This compound is a mixture of E/Z isomers (ratio: 85:15).

**Physical and Chemical Properties:**

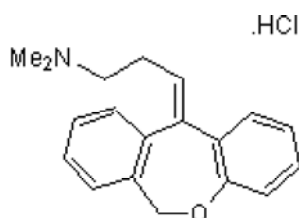
Batch Molecular Formula: C<sub>19</sub>H<sub>21</sub>NO.HCl

Batch Molecular Weight: 315.84

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Store at RT

**Solubility & Usage Info:**

water to 100 mM

DMSO to 100 mM

This compound is a mixture of E/Z isomers (ratio: 85:15)

**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:**

**Nguyen *et al*** (2001) Discovery of a novel member of the histamine receptor family. *Mol.Pharmacol.* **59** 427. PMID: 11179435.

**Lurchins** (1983) Review of clinical and animal studies comparing the cardiovascular effects of doxepin and other tricyclic antidepressants. *Am.J.Psychiatry* **140** 1006. PMID: 6346907.

**Tran *et al*** (1981) [<sup>3</sup>H]Doxepin interactions with histamine H<sub>1</sub>-receptors and other sites in guinea pig brain homogenates. *Eur.J.Pharmacol.* **70** 501. PMID: 7238574.

Merck Index **12** 3492.

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