

Certificate of Analysis

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Product Name: NE 100 hydrochloride

Catalog No.: 3133

Batch No.: 3

CAS Number: 149409-57-4

IUPAC Name: 4-Methoxy-3-(2-phenylethoxy)-*N,N*-dipropylbenzeneethanamine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₃₃NO₂.HCl

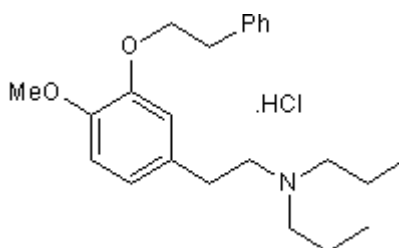
Batch Molecular Weight: 391.97

Physical Appearance: White solid

Solubility: water to 25 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.21 (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	70.48	8.74	3.57
Found	70.26	8.62	3.84

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

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Description:

Potent and selective σ_1 receptor antagonist ($K_i = 0.86$ nM) that displays > 55-fold selectivity over σ_2 receptors and > 6000-fold selectivity over D_1 , D_2 , 5-HT_{1A}, 5-HT₂ and PCP receptors. Exhibits reversible binding ($K_d = 1.2$ nM) and displays antipsychotic activity in vivo. Orally active.

Physical and Chemical Properties:

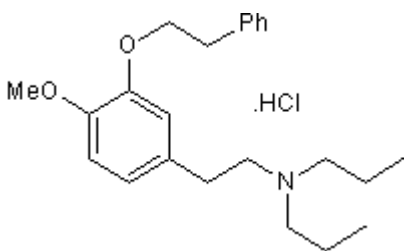
Batch Molecular Formula: C₂₃H₃₃NO₂.HCl

Batch Molecular Weight: 391.97

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 25 mM
DMSO 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:

Okuyama et al (1993) NE-100, a novel sigma receptor ligand: in vivo tests. *Pharmacol.Letts.* **53** PL285.

Chaki et al (1994) NE-100, a novel potent σ ligand, preferentially binds to σ_1 binding sites in guinea pig brain. *Eur.J.Pharmacol.* **251** R1. PMID: 8137864.

Tanaka et al (1995) Characteristics of binding of [³H]NE-100, a novel sigma-receptor ligand, to guinea-pig brain membranes. *Naunyn Schmied.Arch.Pharmacol.* **351** 244.

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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
Tel: +1 612 379 2956