bio-techne
TOCRIS

Print Date: Sep 23rd 2024

Certificate of Analysis

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Product Name: **NE 100 hydrochloride** **Catalog No.: 3133** **Batch No.: 4**

CAS Number: 149409-57-4

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{33}NO_2.HCl$

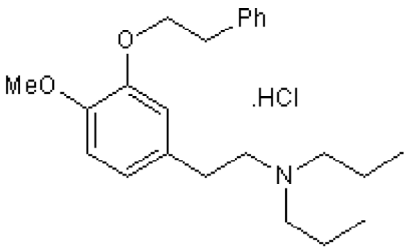
Batch Molecular Weight: 391.97

Physical Appearance: White solid

Solubility: water to 5 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	70.48	8.74	3.57
Found	70.55	8.69	3.56

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

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CAS Number: 149409-57-4

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

Description:

NE 100 hydrochloride is a 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-HT_2 and PCP receptors. Exhibits reversible binding (K_d = 1.2 nM) and displays antipsychotic activity in vivo. Orally active.

Physical and Chemical Properties:

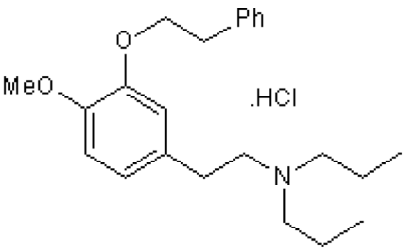
Batch Molecular Formula: $C_{23}H_{33}NO_2$.HCl

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 5 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

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

Chaki *et al* (1994) NE-100, a novel potent σ ligand, preferentially binds to σ1 binding sites in guinea pig brain. Eur.J.Pharmacol. ***251*** R1. PMID: 8137864.

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