1. PHYSICAL AND CHEMICAL PROPERTIES

   **Batch Molecular Formula:** \( \text{C}_{23}\text{H}_{33}\text{NO}_2\cdot\text{HCl} \)
   
   **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:**
   
   ![Molecular Structure Image]

2. ANALYTICAL DATA

   **TLC:**
   
   \( R_f = 0.21 \) (Ethyl acetate:Petroleum ether [1:1])
   
   **HPLC:**
   
   Shows 99.8% purity
   
   **\(^1\)H NMR:**
   
   Consistent with structure
   
   **Mass Spectrum:**
   
   Consistent with structure
   
   **Microanalysis:**
   
<table>
<thead>
<tr>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
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<td>70.48</td>
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<td>8.62</td>
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Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Information

**Product Name:** NE 100 hydrochloride

**CAS Number:** 149409-57-4

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

**Catalog No.:** 3133

**Batch No.:** 3

**Description:**
Potent and selective $\sigma_1$ receptor antagonist ($K_i = 0.86$ nM) that displays > 55-fold selectivity over $\sigma_2$ 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%
- **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:**

- Chaki et al (1994) NE-100, a novel potent $\sigma$ ligand, preferentially binds to $\sigma1$ binding sites in guinea pig brain. Eur.J.Pharmacol. 251 R1. PMID: 8137864.