

**Product Name:** (S)-WAY 100135 dihydrochloride

**Catalog No.:** 1253

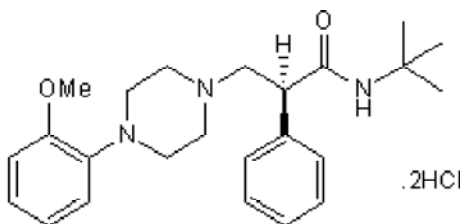
**Batch No.:** 6

CAS Number: 149007-54-5

IUPAC Name: (S)-N-tert-Butyl-3-(4-(2-methoxyphenyl)-piperazin-1-yl)-2-phenylpropanamide dihydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>24</sub>H<sub>33</sub>N<sub>3</sub>O<sub>2</sub>·2HCl·½H<sub>2</sub>O  
**Batch Molecular Weight:** 477.48  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
 water to 5 mM with gentle warming  
 water to 10 mM with sonication  
**Storage:** Desiccate at +4°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.3 (Dichloromethane)  
**HPLC:** Shows 99.5% purity  
**Chiral HPLC:** Shows 99.2% purity  
<sup>1</sup>H NMR: Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = -50 (Concentration = 1, Solvent = Methanol)  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	60.37	7.6	8.8
Found	60.41	7.43	8.76

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

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**Description:**

Potent, selective 5-HT<sub>1A</sub> receptor antagonist (IC<sub>50</sub> = 15 nM). Selective over 5-HT<sub>1B</sub>, 1C, 2, α<sub>1</sub>, α<sub>2</sub> and D<sub>2</sub> receptors (IC<sub>50</sub> > 1000 nM). Centrally active on systemic administration.

**Physical and Chemical Properties:**

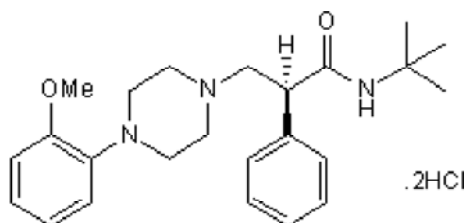
Batch Molecular Formula: C<sub>24</sub>H<sub>33</sub>N<sub>3</sub>O<sub>2</sub>·2HCl·½H<sub>2</sub>O

Batch Molecular Weight: 477.48

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Desiccate at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM

water to 5 mM with gentle warming

water to 10 mM with sonication

**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.

**Licensing Information:**

Sold with the permission of Wyeth-Ayerst Research, US Patent 4,988,814

**References:**

**Rodgers and Cole** (1994) Anxiolytic-like effect of (S)-WAY 100135, a 5-HT<sub>1A</sub> receptor antagonist, in the murine elevated plus-maze test. *Eur.J.Pharmacol.* **261** 321. PMID: 7813555.

**Cliffe et al** (1993) (S)-N-tert-Butyl-3-(4-(2-methoxyphenyl)-piperazin-1-yl)-2-phenylpropanamide [(S)-WAY-100135]: a selective antagonist at presynaptic and postsynaptic 5-HT<sub>1A</sub> receptors. *J.Med.Chem.* **36** 1509. PMID: 8496920.

**Fletcher et al** (1993) WAY100135: a novel, selective antagonist at presynaptic and postsynaptic 5-HT<sub>1A</sub> receptors. *Eur.J.Pharmacol.* **237** 283. PMID: 8365456.

**Fletcher et al** (1993) Silent 5-HT<sub>1A</sub> receptor antagonists: utility as research tools and therapeutic agents. *Trends Pharmacol.Sci.* **14** 41. PMID: 8122313.

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