

Certificate of Analysis

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Product Name: (S)-WAY 100135 dihydrochloride

Catalog No.: 1253

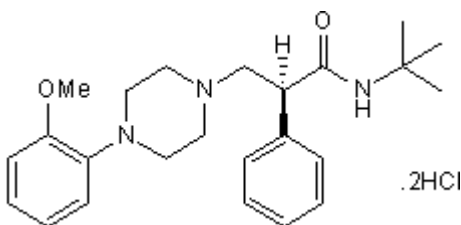
Batch No.: 6

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: C₂₄H₃₃N₃O₂·2HCl·½H₂O
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_f = 0.3 (Dichloromethane)
HPLC: Shows 99.5% purity
Chiral HPLC: Shows 99.2% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = -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_{1A} receptor antagonist (IC₅₀ = 15 nM). Selective over 5-HT_{1B}, 1C, 2, α₁, α₂ and D₂ receptors (IC₅₀ > 1000 nM). Centrally active on systemic administration.

Physical and Chemical Properties:

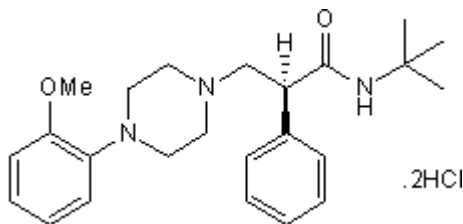
Batch Molecular Formula: C₂₄H₃₃N₃O₂·2HCl·½H₂O

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.

References:

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_{1A} receptors. *J.Med.Chem.* **36** 1509. PMID: 8496920.

Fletcher et al (1993) WAY100135: a novel, selective antagonist at presynaptic and postsynaptic 5-HT_{1A} receptors. *Eur.J.Pharmacol.* **237** 283. PMID: 8365456.

Fletcher et al (1993) Silent 5-HT_{1A} receptor antagonists: utility as research tools and therapeutic agents. *Trends Pharmacol.Sci.* **14** 41. PMID: 8122313.

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

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