



Certificate of Analysis

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Product Name: MDL 100907 Catalog No.: 4173 Batch No.: 1

CAS Number: 139290-65-6

IUPAC Name: (R)-(+)- α -(2,3-Dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-4-piperinemethanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{28}FNO_3$

Batch Molecular Weight: 373.46

Physical Appearance: White solid

Solubility: 1eq. HCl to 50 mM

DMSO to 100 mM ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.4$ (Chloroform:Methanol:NH4OH. [90:9:1])

HPLC: Shows >98.8% purity
Chiral HPLC: Shows >99.4% purity

1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = +23.2$ (Concentration = 2.14, Solvent = Methanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 70.75 7.56 3.75 Found 70.57 7.53 3.9

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





Product Information

Print Date: Feb 13th 2014

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CAS Number: 139290-65-6

IUPAC Name: $(R)-(+)-\alpha-(2,3-Dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-4-piperinemethanol$

Description:

Potent and selective 5-HT_{2A} receptor antagonist ($K_i = 0.36$ nM). Exhibits > 80-fold selectivity for 5-HT_{2A} over other serotonergic receptor subtypes. Antipsychotic agent in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₂H₂₈FNO₃ Batch Molecular Weight: 373.46 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

1eq. HCl to 50 mM DMSO to 100 mM ethanol 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:

Sorensen *et al* (1993) Characterization of the 5-HT2 receptor antagonist MDL 100907 as a putative atypical antipsychotic: behavioral, electrophysiological and neurochemical studies. J.Pharmacol.Exp.Ther. **266** 684. PMID: 8102646.

Kehne *et al* (1996) Preclinical characterization of the potential of the putative atypical antipsychotic MDL 100,907 as a potent 5-HT2A antagonist with a favorable CNS safety profile. J.Pharmacol. **277** 968. PMID: 8627580.

Ardayfio *et al* (2008) The 5-hydroxytryptamine_{2A} receptor antagonist R-(+)-alpha-(2,3-dimethoxyphenyl)-1-[2-(4-fluorophenyl) ethyl-4-piperidinemethanol (M100907) attenuates impulsivity after both drug-induced disruption (dizocilpine) and enhancement (antidepressant drugs) of differential-reinforcement-of-low-rate 72-s behavior in the rat. J.Pharmacol.Exp.Ther. **327** 891. PMID: 18772320.

