

Certificate of Analysis

Print Date: Feb 4th 2022

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Product Name: MDL 100907 Catalog No.: 4173 Batch No.: 3

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:373.46Physical 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 (Dichloromethen:Methanol:Ammonia soln. [90:9:1])

HPLC: Shows >99.8% purity
Chiral HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = +18$ (Concentration = 1, Solvent = Methanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 70.75 7.56 3.75 Found 70.86 7.64 3.76

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



Product Information

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Description:

MDL 100907 is a potent and selective 5-HT $_{2A}$ receptor antagonist (K $_{\rm i}$ = 0.36 nM, IC $_{50}$ = 3.3-5.1 nM). MDL 100907 exhibits > 80-fold selectivity for 5-HT $_{2A}$ over other serotonergic receptor subtypes. MDL 100907 is neuroprotective; protects cultured dopaminergic neurons from MPP+ induced toxicity. 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:

Ardayfio *et al* (2008) The 5-hydroxytryptamine2A 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 dr J.Pharmacol.Exp.Ther. *327* 891. PMID: 18772320.

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.

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.