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

CAS Number: 139290-65-6

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

1. PHYSICAL AND CHEMICAL PROPERTIES

   - **Batch Molecular Formula:** \(\text{C}_{22}\text{H}_{28}\text{FNO}_{3}\)
   - **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

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
   - **\(^1\)H NMR:** Consistent with structure
   - **Mass Spectrum:** Consistent with structure
   - **Optical Rotation:** \([\alpha]_D = +18\) (Concentration = 1, Solvent = Methanol)
   - **Microanalysis:**
     | Element | Theoretical | Found |
     |---------|-------------|-------|
     | C       | 70.75       | 70.86 |
     | H       | 7.56        | 7.64  |
     | N       | 3.75        | 3.76  |

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

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Product Information

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

Description:
MDL 100907 is a potent and selective 5-HT2A receptor antagonist (Kᵢ = 0.36 nM, IC₅₀ = 3.3-5.1 nM). MDL 100907 exhibits > 80-fold selectivity for 5-HT2A 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: C₂₂H₂₀FNO₃  
Batch Molecular Weight: 373.46  
Physical Appearance: White solid

Minimum Purity: ≥98%

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-piperinemethanol (M100907) attenuates impulsivity after both drug-induced disruption (dizocilpine) and enhancement (antidepressant dr J.Pharmacol.Exp.Ther. 327 891. PMID: 18772320.
