

Product Name: ML 252

Catalog No.: 4687

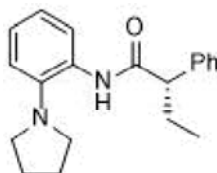
Batch No.: 1

CAS Number: 1392494-64-2

IUPAC Name: (S)-2-Phenyl-N-(2-(pyrrolidin-1-yl)phenyl)butanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₄N₂O
Batch Molecular Weight: 308.43
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity
Chiral HPLC: Shows 99.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	77.89	7.84	9.08
Found	77.63	7.94	9.18

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

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Description:

ML 252 is a potent and selective inhibitor of K_v7.2 voltage-gated potassium channels (IC₅₀ = 70 nM), which displays >40-fold selectivity for K_v7.2 over K_v7.1 channels (IC₅₀ = 2.9 μM for K_v7.1). ML 252 is the (S)-enantiomer, and is more potent than the (R)-enantiomer or racemic mixture (IC₅₀ values are 944 and 160 nM, respectively). ML 252 displays selectivity for K_v7.2 over a panel of >68 GPCRs, ion channels and transporters; inhibits melatonin MT₁ receptor 60% at 10 μM. ML 252 is brain penetrant.

Physical and Chemical Properties:

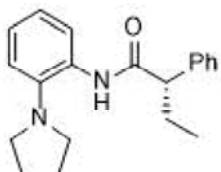
Batch Molecular Formula: C₂₀H₂₄N₂O

Batch Molecular Weight: 308.43

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Cheung et al (2012) Discovery of a series of 2-phenyl-N-(2-(pyrrolidin-1-yl)phenyl)acetamides as novel molecular switches that modulate modes of K_v7.2 (KCNQ2) channel pharmacology: identification of (S)-2-phenyl-N-(2-(pyrrolidin-1-yl)phenyl)butanamide (ML252) as a potent, brain penetrant K_v7.2 channel inhibitor. *J.Med.Chem.* **55** 6975. PMID: 22793372.

Storage: Store at -20°C

Solubility & Usage Info:

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.

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