

Certificate of Analysis

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Product Name: RO 5263397 hydrochloride

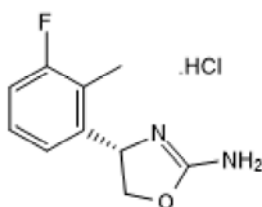
Catalog No.: 6833

Batch No.: 2

IUPAC Name: (4S)-4-(3-Fluoro-2-methylphenyl)-4,5-dihydro-2-oxazolamine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

| | |
|-----------------------------------|---|
| Batch Molecular Formula: | C ₁₀ H ₁₁ FN ₂ O.HCl |
| Batch Molecular Weight: | 230.67 |
| Physical Appearance: | White solid |
| Solubility: | DMSO to 100 mM water to 100 mM |
| Storage: | Store at -20°C |
| Batch Molecular Structure: | |



2. ANALYTICAL DATA

| | |
|---------------------------|---------------------------|
| HPLC: | Shows 99.8% purity |
| Chiral HPLC: | Shows 100.0% purity |
| ¹H NMR: | Consistent with structure |
| Mass Spectrum: | Consistent with structure |
| Microanalysis: | |
| | Carbon Hydrogen Nitrogen |
| Theoretical | 52.07 5.24 12.14 |
| Found | 52.57 5.17 11.99 |

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

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Catalog No.: 6833

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IUPAC Name: (4S)-4-(3-Fluoro-2-methylphenyl)-4,5-dihydro-2-oxazolamine hydrochloride

Description:

RO 5263397 hydrochloride is a potent trace amine 1 (TA₁) receptor agonist (EC₅₀ values are 0.12, 35 and 17-85 nM for mouse, rat and human receptors, respectively). Increases wakefulness and reduces REM and NREM sleep duration in wild type mice. Inhibits spontaneous locomotor activity in dopamine transport (DAT) knockout mice.

Physical and Chemical Properties:

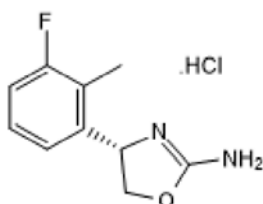
Batch Molecular Formula: C₁₀H₁₁FN₂O.HCl

Batch Molecular Weight: 230.67

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Espinoza et al (2018) Biochemical and functional characterization of the trace amine-associated receptor 1 (TAAR1) agonist RO5263397. *Front.Pharmacol.* **9** 645. PMID: 29977204.

Schwartz et al (2017) Trace amine-associated receptor 1 regulates wakefulness and EEG spectral composition. *Neuropsychopharmacology.* **42** 1305. PMID: 27658486.

Galley et al (2015) Discovery and characterization of 2-aminoxazolines as highly potent, selective, and orally active TAAR1 agonists. *ACS.Med.Chem.Letts.* **7** 192. PMID: 26985297.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

water 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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