TOCRIS
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Print Date: Dec 16th 2020

# Certificate of Analysis

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**Product Name:** **R 568 hydrochloride** **Catalog No.: 3815** **Batch No.: 2**

CAS Number: 177172-49-5

IUPAC Name: 2-Chloro-*N*-[(1*R*)-1-(3-methoxyphenyl)ethyl]-benzenepropanamine hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{18}H_{22}ClNO.HCl$

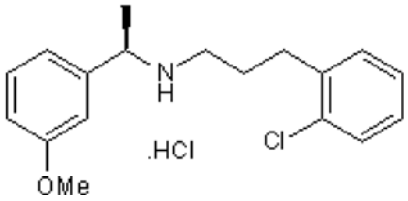
**Batch Molecular Weight:** 340.29

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM
ethanol to 100 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**HPLC:** Shows 100.0% purity

**Chiral HPLC:** Shows 100.0% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 63.53 | 6.81 | 4.12 |
| Found | 63.34 | 6.9 | 4.11 |



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IUPAC Name: 2-Chloro-*N*-[(1*R*)-1-(3-methoxyphenyl)ethyl]-benzenepropanamine hydrochloride

**Description:**

Positive allosteric modulator and allosteric agonist of the human calcium-sensing receptor (hCaSR). Exhibits calcimimetic activity. Has the ability to restore function to hCaSR mutants that cause familial hypocalciuric hypercalcemia (FHH) and neonatal severe hyperparathyroidism (NSHPT). Exerts a suppressive effect on parathyroid (PT) hormone secretion; inhibits PT cell proliferation in rats with renal insufficiency.

**Physical and Chemical Properties:**

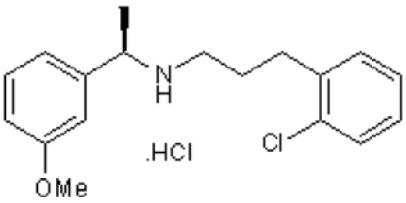
Batch Molecular Formula: $C_{18}H_{22}ClNO.HCl$

Batch Molecular Weight: 340.29

Physical Appearance: White solid

**Minimum Purity:** ≥99%

**Batch Molecular Structure:**




**Storage:** Desiccate at RT

**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.

**References:**

**Ying Lin Lu** *et al* (2009) Effect of the calcimimetic R-568 [3-(2-chlorophenyl)-*N*-((1*R*)-1-(3-methoxyphenyl)ethyl)-1-propanamine] on correcting inactivating mutations in the human calcium-sensing receptor. J.Pharmacol.Exp.Ther. ***331*** 775. PMID: 19759318.

**Fox** *et al* (1999) NPS R-568: a type II calcimimetic compound that acts on parathyroid cell calcium receptor of rats to reduce plasma levels of parathyroid hormone and calcium. J.Pharmacol.Exp.Ther. ***290*** 473. PMID: 10411552.

**Wada** *et al* (1997) The calcimimetic compound NPS R-568 suppresses parathyroid cell proliferation in rats with renal insufficiency. J.Clin.Invest. ***100*** 2977. PMID: 9399943.