

Product Name: Calhex 231 hydrochloride

Catalog No.: 4387

Batch No.: 1

CAS Number: 2387505-78-2

IUPAC Name: 4-Chloro-N-[(1S,2S)-2-[[[(1R)-1-(1-naphthalenyl)ethyl]amino]cyclohexyl]-benzamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₇ClN₂O.HCl

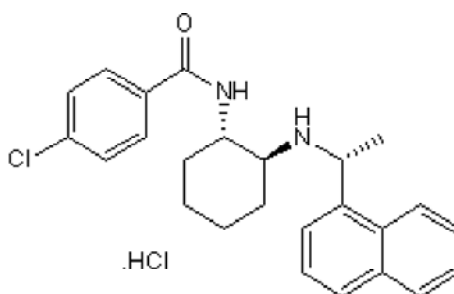
Batch Molecular Weight: 443.41

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.1 (Ethyl acetate:Petroleum ether [1:4])

HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -23.2 (Concentration = 0.28, Solvent = Chloroform)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.72	6.36	6.32
Found	67.72	6.35	6.43

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Description:

Negative allosteric modulator of the calcium sensing receptor (CaSR). Blocks increases in [³H]inositol phosphate levels elicited by wild-type hCasR activation (IC₅₀= 0.39 μM in transiently transfected HEK293 cells).

Physical and Chemical Properties:

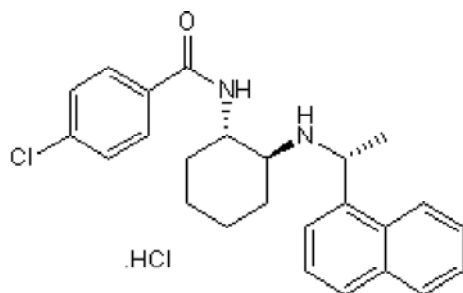
Batch Molecular Formula: C₂₅H₂₇ClN₂O.HCl

Batch Molecular Weight: 443.41

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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:

Weston et al (2008) The expression and function of Ca²⁺-sensing receptors in rat mesenteric artery; comparative studies using a model of type II diabetes. *Br.J.Pharmacol.* **154** 652. PMID: 18414396.

Kessler et al (2006) *N*¹-Benzoyl-*N*²-[1-(1-naphthyl)ethyl]-*trans*-1,2-diaminocyclohexanes: Development of 4-chlorophenylcarboxamide (Calhex 231) as a new calcium sensing receptor ligand demonstrating potent calcilytic activity. *J.Med.Chem.* **49** 5119. PMID: 16913701.

Petrel et al (2003) Modeling and mutagenesis of the binding site of Calhex 231, a novel negative allosteric modulator of the extracellular Ca²⁺-sensing receptor. *J.Biol.Chem.* **278** 49487. PMID: 14506236.

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