

Certificate of Analysis

Product Name: L-733,060 hydrochloride

Catalog No.: 1145

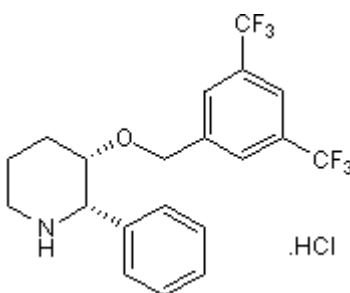
Batch No.: 5

CAS Number: 148687-76-7

IUPAC Name: (2S,3S)-3-[[3,5-bis(Trifluoromethyl)phenyl]methoxy]-2-phenylpiperidine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₁₉F₆NO.HCl
Batch Molecular Weight: 439.83
Physical Appearance: White solid
Solubility: water to 50 mM with gentle warming
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.44 (Chloroform:Methanol [9:1])
HPLC: Shows 100% purity
Chiral HPLC: Shows >99.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = +83 (Concentration = 1, Solvent = Methanol)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.62	4.58	3.18
Found	54.74	4.7	3.1

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

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Description:

Potent NK₁ antagonist (K_i values are 0.08, 0.2 and 93.13 nM for gerbil, human and rat receptors, respectively). Produces anxiolytic-like effects in the gerbil elevated plus-maze. Exhibits antitumor activity in vitro. Also decreases HER2 activity and tumor growth in mice bearing HER2⁺ or EGFR⁺ breast tumors. Orally bioavailable and brain penetrant.

Physical and Chemical Properties:

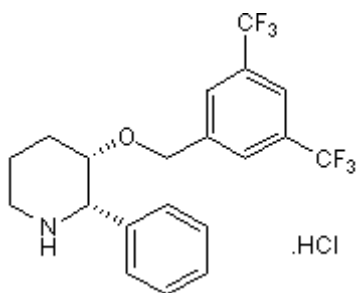
Batch Molecular Formula: C₂₀H₁₉F₆NO.HCl

Batch Molecular Weight: 439.83

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

water to 50 mM with gentle warming

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:

Seabrook et al (1996) L-733,060, a novel tachykinin NK₁ receptor antagonist; effects in [Ca²⁺]_i mobilisation, cardiovascular and dural extravasation assays. *Eur.J.Pharmacol.* **317** 129. PMID: 8982729.

Kramer et al (1998) Distinct mechanism for antidepressant blockade of central substance P receptors. *Science* **281** 1640. PMID: 9733503.

Varty et al (2002) The gerbil elevated plus-maze II: anxiolytic-like effects of selective neurokinin NK1 receptor antagonists. *Neuropsychopharmacology* **27** 371. PMID: 12225694.

Garcia-Recio et al (2013) Substance P autocrine signaling contributes to persistent HER2 activation that drives malignant progression and drug resistance in breast cancer. *Cancer Res.* **73** 6424. PMID: 24030979.

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