

Product Name: L 760735

Catalog No.: 4013

Batch No.: 1

CAS Number: 188923-01-5

IUPAC Name: 5-[[[(2*R*,3*S*)-2-[(1*R*)-1-[3,5-Bis(trifluoromethyl)phenyl]ethoxy]-3-(4-fluorophenyl)-4-morpholinyl]methyl-*N,N*-dimethyl-1*H*-1,2,3-triazole-4-methanamine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₂₈F₇N₅O₂.HCl.½H₂O

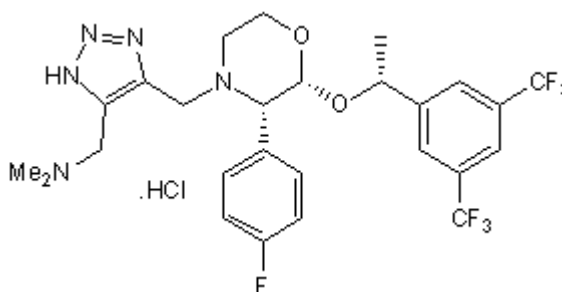
Batch Molecular Weight: 620.99

Physical Appearance: Off-white solid

Solubility: water to 30 mM
DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Dichloromethane:Methanol:Acetic acid [9:1:0.1])

HPLC: Shows 100% purity

¹H NMR: consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +67.5 (Concentration = 0.5, Solvent = Water)

Microanalysis:

Carbon Hydrogen Nitrogen

	Carbon	Hydrogen	Nitrogen
Theoretical	50.29	4.87	11.28
Found	50.33	4.86	11.12

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Description:

High affinity NK₁ receptor antagonist (IC₅₀ = 0.19 nM at human NK₁ receptors). Selective (>300-fold) over h-NK₂ and h-NK₃ receptors. Exhibits anxiolytic and antidepressant-like effects. Orally active.

Physical and Chemical Properties:

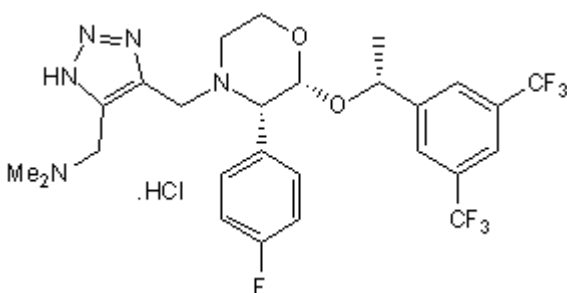
Batch Molecular Formula: C₂₆H₂₈F₇N₅O₂.HCl.½H₂O

Batch Molecular Weight: 620.99

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 30 mM
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:

Harrison *et al* (2001) An orally active, water-soluble neurokinin-1 receptor antagonist suitable for both intravenous and oral clinical administration. *J.Med.Chem.* **44** 4296. PMID: 11708932.

Duffy *et al* (2002) Correlation of neurokinin (NK) 1 receptor occupancy in gerbil striatum with behavioral effects of NK1 antagonists. *J.Pharmacol.Exp.Ther* **301** 536. PMID: 11961054.

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