

Product Name: Aprepitant

Catalog No.: 6486

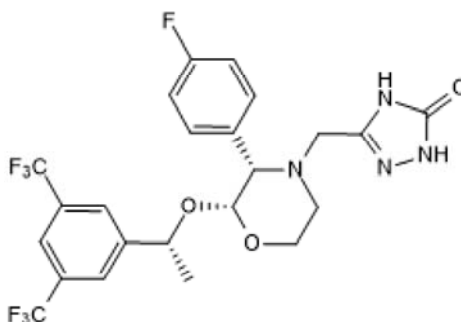
Batch No.: 1

CAS Number: 170729-80-3

IUPAC Name: 5-[[[(2R,3S)-2-[(1R)-1-[3,5-Bis(trifluoromethyl)phenyl]ethoxy]-3-(4-fluorophenyl)-4-morpholinyl]methyl]-1,2-dihydro-3H-1,2,4-triazol-3-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₁F₇N₄O₃
Batch Molecular Weight: 534.43
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 10 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = +65.2 (Concentration = 1, Solvent = Methanol)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.69	3.96	10.48
Found	51.67	3.82	10.42

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

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Description:

Potent long-acting hNK-1 antagonist, (IC₅₀ = 0.09 nM and K_d = 19 pM). Inhibits induced foot-tapping in gerbils. CNS penetrant and orally bioavailable. Antiemetic.

Physical and Chemical Properties:

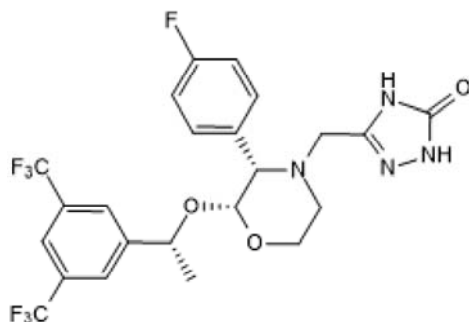
Batch Molecular Formula: C₂₃H₂₁F₇N₄O₃

Batch Molecular Weight: 534.43

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 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:

Hale *et al* (1998) Structural optimization affording 2-(*R*)-(1-(*R*)-3, 5-bis(trifluoromethyl)phenylethoxy)-3-(*S*)-(4-fluoro)phenyl-4-(3-oxo-1,2,4-triazol-5-yl)methylmorpholine, a potent, orally active, long-acting morpholine acetal human NK-1 receptor antagonist. *J.Med.Chem.* **41** 4607. PMID: 9804700.

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