

**Product Name:** Aprepitant

**Catalog No.:** 6486

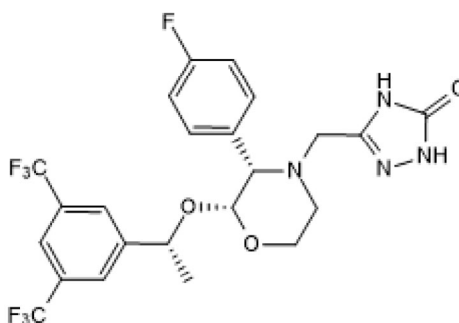
**Batch No.:** 2

CAS Number: 170729-80-3

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

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>23</sub>H<sub>21</sub>F<sub>7</sub>N<sub>4</sub>O<sub>3</sub>.  
**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 100% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = +63.7 (Concentration = 1.00, Solvent = Methanol)  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	51.69	3.96	10.48
Found	51.6	3.93	10.28

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

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**Description:**

Aprepitant is a potent long-acting hNK-1 antagonist ( $IC_{50} = 0.09$  nM and  $K_d = 19$  pM) that inhibits the effect of substance P on NK-1 receptors. Inhibits metastasis and impairs tumor growth in patient derived xenografts and breast cancer cells. In an animal model of intracerebral hemorrhage, Aprepitant reduces neurological impairment, neuronal damage and neuronal death. Suppresses pain and inflammation induced by formalin. Inhibits induced foot-tapping in gerbils. CNS penetrant and orally bioavailable. Antiemetic.

**Physical and Chemical Properties:**

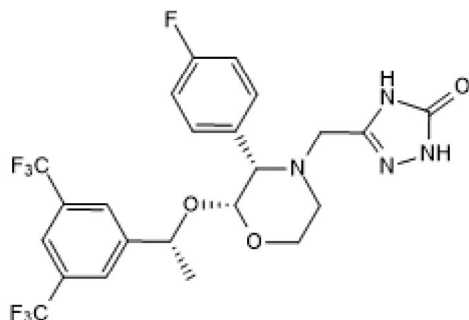
Batch Molecular Formula:  $C_{23}H_{21}F_7N_4O_3$ .

Batch Molecular Weight: 534.43

Physical Appearance: White solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**Storage:** Store at  $-20^{\circ}C$

**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  $45-60^{\circ}C$  water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

**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  $-20^{\circ}C$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

**Padmanaban et al (2024)** Neuronal substance P drives metastasis through an extracellular RNA-TLR7 axis. *Nature* **633** 207. PMID: 39112700.

**Jin et al (2022)** Aprepitant attenuates NLRC4-dependent neuronal pyroptosis via NK1R/PKC $\delta$  pathway in a mouse model of intracerebral hemorrhage. *J.Neuroinflammation* **19** 198. PMID: 35922848.

**Yang et al (2022)** Aprepitant inhibits JNK and p38/MAPK to attenuate inflammation and suppresses inflammatory pain. *Front.Pharmacol.* **12** 811584. PMID: 35087409.

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