

PRODUCT INFORMATION



Aprepitant

Item No. 14867

CAS Registry No.: 170729-80-3

Formal 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

Synonyms: Emend, L-754,030, MK-869, ONO-7436

MF: C₂₃H₂₁F₇N₄O₃

FW: 534.4

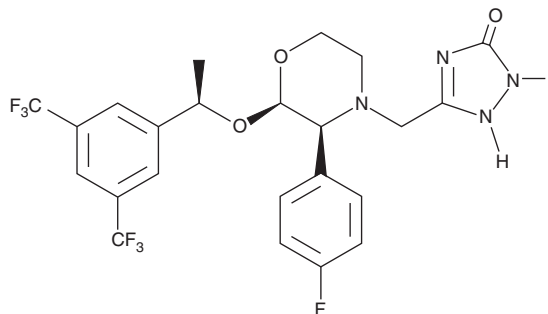
Purity: ≥98%

UV/Vis.: λ_{max}: 264, 271 nm

Supplied as: A crystalline solid

Storage: -20°C

Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Aprepitant is supplied as a crystalline solid. A stock solution may be made by dissolving the aprepitant in the solvent of choice. Aprepitant is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of aprepitant in these solvents is approximately 3, 16, and 25 mg/ml, respectively.

Aprepitant is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, aprepitant should first be dissolved in DMF and then diluted with the aqueous buffer of choice. Aprepitant has a solubility of approximately 0.33 mg/ml in a 1:2 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Aprepitant is an antiemetic and antagonist of the neurokinin-1 (NK₁) receptor (K_i = 3 nM; IC₅₀ = 0.09 nM for the human receptor).^{1,2} It is selective for NK₁ over NK₃ receptors (K_i = 454.1 nM for human NK₃).¹ *In vivo*, aprepitant (1 mg/kg) prevents plasma extravasation into the esophagus of guinea pigs induced by substance P (Item No. 24035).³ It also reduces NK₁-agonist-induced foot tapping in gerbils. Formulations containing aprepitant have been used to prevent chemotherapy-induced nausea and vomiting.

References

1. Bissantz, C., Bohnert, C., Hoffmann, T., *et al.* Identification of a crucial amino acid in the helix position 6.51 of human tachykinin neurokinin 1 and 3 receptors contributing to the insurmountable mode of antagonism by dual NK₁/NK₃ antagonists. *J. Med. Chem.* **55**(11), 5061-5076 (2012).
2. Finke, P.E., Meurer, L.C., Levorse, D.A., *et al.* Cyclopentane-based human NK₁ antagonists. Part 1: Discovery and initial SAR. *Bioorg. Med. Chem. Lett.* **16**(17), 4497-4503 (2006).
3. Meurer, L.C., Finke, P.E., Owens, K.A., *et al.* Cyclopentane-based human NK₁ antagonists. Part 2: Development of potent, orally active, water-soluble derivatives. *Bioorg. Med. Chem. Lett.* **16**(17), 4504-4511 (2006).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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