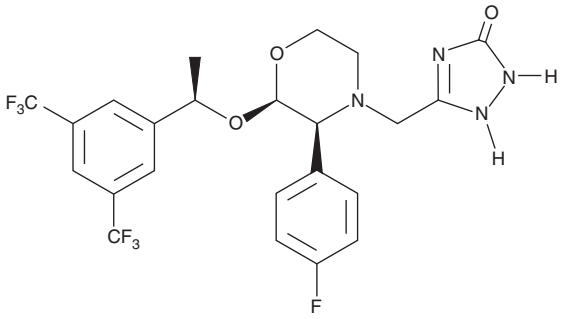
PRODUCT INFORMATION

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:	$C_{23}H_{21}F_7N_4O_3$
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 an antiemetic and antagonist of the neurokinin-1 (NK_1) receptor (K_i = 3 nM; IC_{50} = 0.09 nM for the human receptor).[1,2] It is selective for NK_1 over NK_3 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 NK_1-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 NK_1/NK_3 antagonists. *J. Med. Chem.* **55(11)**, 5061-5076 (2012).
2. Finke, P.E., Meurer, L.C., Levorse, D.A., *et al.* Cyclopentane-based human NK_1 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 NK_1 antagonists. Part 2: Development of potent, orally active, water-soluble derivatives. *Bioorg. Med. Chem. Lett.* **16(17)**, 4504-4511 (2006).

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