

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-morpholinylmethyl]-1,2-dihydro-3H-1,2,4-triazol-3-one

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

MF: $C_{23}H_{21}F_7N_4O_3$

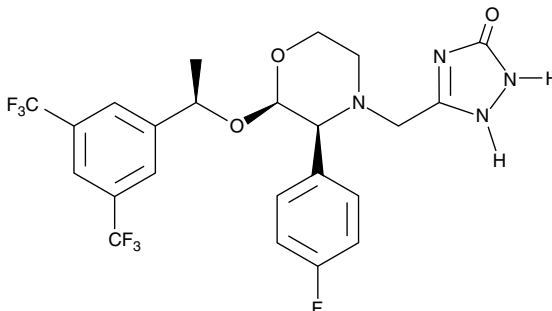
FW: 534.4

Purity: $\geq 98\%$

Stability: ≥ 2 years at -20°C

Supplied as: A crystalline solid

UV/Vis.: λ_{max} : 264, 271 nm



Laboratory Procedures

For long term storage, we suggest that aprepitant be stored as supplied at -20°C . It should be stable for at least two years.

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.

Substance P, a neurokinin peptide found in the brain and gastrointestinal tract, is thought to modulate stress responses, including the emetic reflex. Its actions are mediated through the neurokinin-1 (NK_1) receptor, one of three GPCRs that couple neurokinin binding to the inositol phosphate signal transduction pathway.¹⁻² Aprepitant is an anti-emetic compound that selectively antagonizes the human NK_1 receptor ($K_s = 3$ and 454.1 nM for h NK_1 and h NK_3 , respectively; $\text{IC}_{50} = 0.09$ nM for h NK_1).¹⁻² In *in vivo* assays to measure peripheral (guinea pig SYVAL assay) and central (gerbil foot-tapping stress response assay) inhibition of NK_1 receptors, aprepitant demonstrates ED_{50} values of 0.008 and 0.36 mg/kg, respectively.³ Through antagonism of NK_1 receptor activity, aprepitant has found clinical use to prevent chemotherapy-induced nausea and vomiting.⁴

References

1. Bissantz, C., Bohnert, C., Hoffmann, T., *et al.* *J. Med. Chem.* **55**(11), 5061-5076 (2012).
2. Finke, P.E., Meurer, L.C., Levorse, D.A., *et al.* *Bioorg. Med. Chem. Lett.* **16**(17), 4497-4503 (2006).
3. Meurer, L.C., Finke, P.E., Owens, K.A., *et al.* *Bioorg. Med. Chem. Lett.* **16**(17), 4504-4511 (2006).
4. Hesketh, P.J., Grunberg, S.M., Gralla, R.J., *et al.* *J. Clin. Oncol.* **21**(22), 4112-4119 (2003).

Related Products

For a list of related products please visit: www.caymanchem.com/catalog/14867

WARNING: THIS PRODUCT IS FOR LABORATORY RESEARCH ONLY: NOT FOR ADMINISTRATION TO HUMANS. NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until information to the contrary becomes available. Do not ingest, swallow, or inhale. Do not get in eyes, on skin, or on clothing. Wash thoroughly after handling. This information contains some, but not all, of the information required for the safe and proper use of this material. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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