

Product Data Sheet

Product Name: Aprepitant

Cat. No.: GC15200

Chemical Properties

Cas. No. 170729-80-3

Chemical Name 5-[[[(2R,3S)-2-[1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]-3-(4-fluorophenyl)morpholin-4-yl]methyl]-1,2-dihydro-1,2,4-triazol-3-one

SMILES CC(C1=CC(=CC(=C1)C(F)(F)F)C(F)(F)F)OC2C(N(CCO2)CC3=NC(=O)NN3)C4=CC=C(C=C4)F

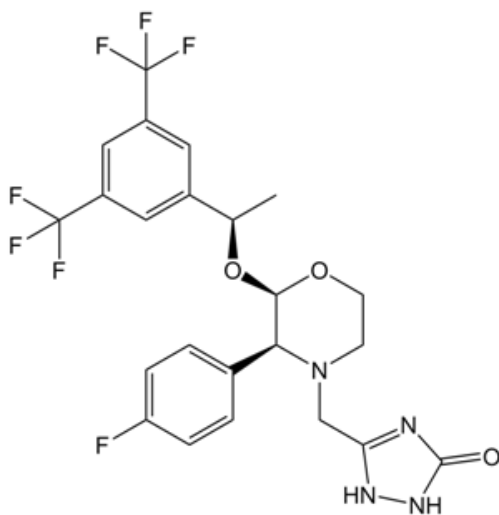
Formula $C_{23}H_{21}F_7N_4O_3$ M.Wt 534.43

Solubility $\geq 26.7\text{mg/mL}$ in DMSO Storage 4°C , protect from light

General tips For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



Protocol

Cell experiment [1]:

Caution: Product has not been fully validated for medical applications. For research use only.

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Cell lines	Nalm-6
Preparation Method	A stock solution of Aprepitant at the concentration of 10mM was prepared by dissolving the compound in 0.1% DMSO. Cells were treated with relevant amounts of the Aprepitant stock solution to attain concentration of 5, 10, 15, 20 and 30μM. In addition to the 4 negative controls (no inhibitor), cells were treated with the corresponding concentration of DMSO as an alternative negative control.
Reaction Conditions	5, 10, 15, 20 and 30μM; 24-36h
Applications	Aprepitant decreased the viability and cell counts, induced rate of DNA synthesis, induced accumulation of the cells in G1 phase, and decreased the cells population in S phase in a dose- and time-dependent manner.
Animal experiment [2]:	
Animal models	Male C57BL/6J mice
Preparation Method	Aprepitant was dissolved in DMSO and diluted with saline, resulting in a final DMSO concentration of 0.002%.
Dosage form	10mg/kg/d; 3d; i.p.
Applications	When compared to vehicle, Aprepitant significantly reduced the CPP expression and locomotor activation.

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References:

- [1] Bayati S, Bashash D, Ahmadian S, et al. Inhibition of tachykinin NK μ receptor using aprepitant induces apoptotic cell death and G1 arrest through Akt/p53 axis in pre-B acute lymphoblastic leukemia cells. *Eur J Pharmacol*. 2016;791:274-283.
- [2] Mannangatti P, Sundaramurthy S, Ramamoorthy S, Jayanthi LD. Differential effects of aprepitant, a clinically used neurokinin-1 receptor antagonist on the expression of conditioned psychostimulant versus opioid reward. *Psychopharmacology (Berl)*. 2017;234(4):695-705.

Background

Aprepitant is a novel and highly selective Neurokinin-1 (NK-1) receptor antagonist^[1]. Aprepitant has a K_d value of 86pM for the human NK-1 receptor, and IC₅₀ values of 0.1nM, 4nM, and 0.7nM for human, rat, and ferret NK-1 receptors, respectively^[2].

In vitro, treatment with Aprepitant (5-30μM) for 24-48h exerted cytotoxic and anti-proliferative effects on Nalm-6 cells in a dose- and time-dependent manner^[3]. IC₅₀ for Aprepitant against HEK 293 cells was >90μM^[2]. Aprepitant, at 10-60mM concentrations for 72h, elicits cell growth inhibition in a concentration-dependent manner in all melanoma cell lines^[4].

In vivo, Intraperitoneal administration of aprepitant (10mg/kg/d) for 3 days attenuated the expression of Conditioned place preference (CPP) induced by psychostimulants, AMPH and cocaine while enhancing morphine induced CPP^[5].

References:

- [1] Tattersall FD1, Rycroft W, Cumberbatch M, Mason G, Tye S, Williamson DJ, Hale JJ, Mills SG, Finke PE, MacCoss M, Sadowski S, Ber E, Cascieri M, Hill RG, MacIntyre DE, Hargreaves RJ. The novel NK1 receptor antagonist MK-0869 (L-754,030) and its water soluble phosphoryl prodrug, L-758,298, inhibit acute and delayed cisplatin-induced emesis in ferrets. *Neuropharmacology*. 2000 Feb 14;39(4):652-63.
- [2] Muñoz M, Rosso M. The NK-1 receptor antagonist aprepitant as a broad spectrum antitumor drug. *Invest New Drugs*. 2010;28(2):187-193.
- [3] Bayati S, Bashash D, Ahmadian S, et al. Inhibition of tachykinin NK μ receptor using aprepitant

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induces apoptotic cell death and G1 arrest through Akt/p53 axis in pre-B acute lymphoblastic leukemia cells. *Eur J Pharmacol.* 2016;791:274-283.

[4] Muñoz M, Rosso M, Robles-Frias MJ, et al. The NK-1 receptor is expressed in human melanoma and is involved in the antitumor action of the NK-1 receptor antagonist aprepitant on melanoma cell lines. *Lab Invest.* 2010;90(8):1259-1269.

[5] Mannangatti P, Sundaramurthy S, Ramamoorthy S, Jayanthi LD. Differential effects of aprepitant, a clinically used neurokinin-1 receptor antagonist on the expression of conditioned psychostimulant versus opioid reward. *Psychopharmacology (Berl).* 2017;234(4):695-705.

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