Product Name: Aprepitant

Revision Date: 6/30/2018

Product Data Sheet

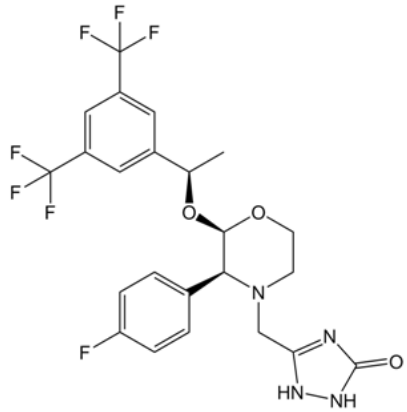
Chemical Properties

Product Name: Aprepitant

Cas No.: 170729-80-3

M.Wt: 534.43

Formula: C23H21F7N4O3



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

Canonical 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

Solubility: ≥26.7mg/mL in DMSO

Storage: Store at -20°C

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.

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

Biological Activity

Targets : Neuroscience

Pathways: Substance P/NK1 Receptor

Description:

Aprepitant (also known as MK-0869) is a novel and highly selective Neurokinin-1 (NK-1) receptor antagonist that inhibits the activity of substance P (SP), an undecapeptide belonging to the tachykinin family of peptides, on the NK-1 receptor with the dissociation constant Kd of 86 pM for human NK-1 receptor and the half maximal inhibition concentration IC50 of 0.1 nM, 4 nM and

0.7 nM for human, rat and ferret NK-1 receptors respectively [1,2].
Since SP has been demonstrated to induce cell proliferation in several human cancer cell lines with overexpressed NK-1 receptors, aprepitant has also been found to concentration-dependently induce growth inhibition in a variety of tumor cell lines, including glioma (GAMG), neuroblastoma (SKN-BE2, IMR-32 and KELLY), retinoblastoma (Y-79 and WERI-Rb-1), pancreas carcinoma (PA-TU-8902 and CAPAN-1), larynx carcinoma (HEp-2), gastric carcinoma (23132-87) and colon carcinoma (SW-403), with IC50 of 33.1 μM, 24.6 μM, 19.6 μM, 27.7 μM, 30.4 μM, 23 μM, 31.2 μM, 27.4 μM, 22.7 μM, 24.2 μM and 30.5 μM respectively [2].

***Reference**:*

[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 M1, Rosso M. The NK-1 receptor antagonist aprepitant as a broad spectrum antitumor drug. Invest New Drugs. 2010 Apr;28(2):187-93. doi: 10.1007/s10637-009-9218-8. Epub 2009 Jan 17.

Protocol

Cell experiment:

Cell lines	Nalm-6 cells
Preparation method	The solubility of this compound in DMSO is >26.7mg/mL. General tips for obtaining a higher concentration: Please warm the tube at 37 ℃ for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below -20℃ for several months.
Reacting conditions	
Applications	Aprepitant decreased the metabolic activity with an estimated IC50 value of 20 μM. Aprepitant induced cell-growth inhibition and G1 cell-cycle arrest. Aprepitant significantly induced apoptosis in Nalm-6 cells. Aprepitant (20 μM) induced p53 accumulation and expression of pro-apoptotic p53 target genes.

Animal experiment [3]:

Animal models	Male C57BL/6J mice
Dosage form	Intraperitoneal injection, 10 mg/kg
Applications	Aprepitant (10 mg/kg, i.p.) significantly attenuated AMPH-induced

	CPP expression and locomotor activation produced by AMPH and cocaine in mice. Aprepitant significantly enhanced the expression of CPP produced by morphine while significantly suppressing the locomotor activity of the mice conditioned with morphine.
Other notes	Please test the solubility of all compounds indoor, and the actual solubility may slightly differ with the theoretical value. This is caused by an experimental system error and it is normal.

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

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.

ApexBio Technology

www.apexbt.com

7505 Fannin street, Suite 410, Houston, TX 77054.

Tel: +1-832-696-8203 | Fax: +1-832-641-3177 | Email: info@apexbt.com