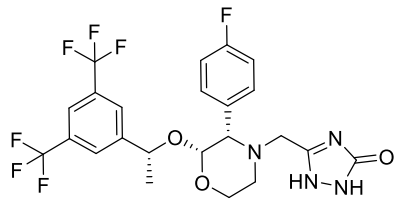
Product data sheet

MedKoo Cat#: 100065 Name: Aprepitant CAS#: 170729-80-3 Chemical Formula: $C_{23}H_{21}F_7N_4O_3$ Exact Mass: 534.1502 Molecular Weight: 534.43	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:

Aprepitant is a small molecule, high-affinity substance P antagonist (SPA) with antiemetic activity. Crossing the blood brain barrier, aprepitant binds selectively to the human substance P/neurokinin 1 receptor in the central nervous system (CNS), thereby inhibiting receptor binding of endogenous substance P and substance P-induced emesis. This agent has little or no affinity for serotonin type 3 (5-HT3), dopamine, and corticosteroid receptors.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	69.11	129.32
Ethanol	11.11	20.79
DMF	25.0	46.78
DMF:PBS (pH 7.2) (1:2)	0.33	0.62

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.87 mL	9.36 mL	18.71 mL
5 mM	0.37 mL	1.87 mL	3.74 mL
10 mM	0.19 mL	0.94 mL	1.87 mL
50 mM	0.04 mL	0.19 mL	0.37 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Zhao XN, Bai ZZ, Li CH, Sheng CL, Li HY. The NK-1R Antagonist Aprepitant Prevents LPS-Induced Oxidative Stress and Inflammation in RAW264.7 Macrophages. Drug Des Devel Ther. 2020 May 20;14:1943-1952. doi: 10.2147/DDDT.S244099. PMID: 32546961; PMCID: PMC7246327.
2. Wang X, Douglas SD, Song L, Wang YJ, Ho WZ. Neurokinin-1 receptor antagonist (aprepitant) suppresses HIV-1 infection of microglia/macrophages. J Neuroimmune Pharmacol. 2008 Dec;3(4):257-64. doi: 10.1007/s11481-008-9117-3. Epub 2008 Jul 25. PMID: 18654860; PMCID: PMC2675876.

In vivo study

1. Wu H, Cheng X, Huang F, Shao G, Meng Y, Wang L, Wang T, Jia X, Yang T, Wang X, Fu C. Aprepitant Sensitizes Acute Myeloid Leukemia Cells to the Cytotoxic Effects of Cytosine Arabinoside in vitro and in vivo. Drug Des Devel Ther. 2020 Jun 18;14:2413-2422. doi: 10.2147/DDDT.S244648. PMID: 32606608; PMCID: PMC7308242.

2. Martinez AN, Burmeister AR, Ramesh G, Doyle-Meyers L, Marriott I, Philipp MT. Aprepitant limits in vivo neuroinflammatory responses in a rhesus model of Lyme neuroborreliosis. J Neuroinflammation. 2017 Feb 15;14(1):37. doi: 10.1186/s12974-017-0813-x. PMID: 28202084; PMCID: PMC5312540.

7. Bioactivity

Biological target:

Aprepitant (MK-0869) is a selective and high-affinity neurokinin 1 receptor antagonist with a Kd of 86 pM.

In vitro activity

Aprepitant treatment decreased the levels of ROS and MDA obviously. These findings suggested that aprepitant could protect macrophages by inhibiting oxidative stress. Furthermore, activated macrophages induced by LPS released various pro-inflammatory cytokines and chemokines such as MCP-1 and TNF-α. Excessive production of these factors takes an important part in affecting the development of inflammation. TNF-α is described as a primary inflammatory regulator in the pathogenesis of inflammation. For example, TNF-α is consumedly increased in synovial tissue in rheumatoid arthritis (RA). Interestingly, overexpression of NOX-4 has also been associated with the upregulation of TNF-α. In this study, the expression of these pro-inflammatory factors was decreased significantly by aprepitant. In addition, LPS stimulation activates COX-2 and iNOS transcription which lead to the overexpression of PGE2 and NO in macrophages, respectively. These inflammatory mediators are highly increased in inflammation. The results in this study show that aprepitant reduced PGE2 and NO production induced by LPS, due to its inhibition on the production of COX-2 and iNOS.

Reference: Drug Des Devel Ther. 2020; 14: 1943–1952. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7246327/

In vivo activity

Analysis of mRNA expression in the dura mater and spinal cord within the cervical region revealed that expression of mRNA encoding CXCL13, CCL2, and IL-17A was significantly elevated at 2 weeks following B. burgdorferi administration (Fig. 4a–c), while levels of mRNA encoding IL-6 were higher at 4 weeks following infection (Fig. 4d). Similarly, levels of mRNA encoding IL-17A were higher in thoracic region dura mater and spinal cord at 2 weeks following B. burgdorferi challenge (Fig. 4e). Importantly, daily treatment with aprepitant significantly attenuated these infection-associated increases in inflammatory mediator mRNA expression (Fig. 4).

Reference: J Neuroinflammation. 2017; 14: 37. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5312540/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.