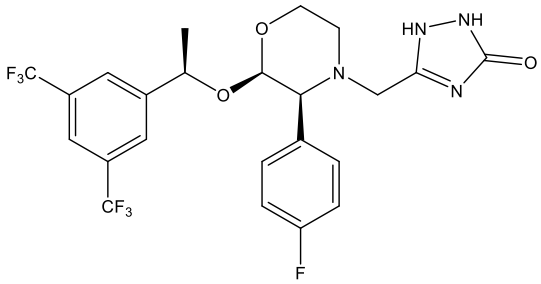
Catalog # 10-4366
Aprepitant

CAS# 170729-80-3

3-[[(2R,3S)-2-[(1R)-1-bis(Trifluoromethyl)phenyl]ethoxy]-3-(4-fluorophenyl)morpholin-4-yl]methyl]-1,4dihydro-1,2,4-triazol-5-one; MK-0869

Lot # FBS21



Aprepitant is a potent human neurokinin-1 (NK-1) antagonist.[1] It is an FDA approved medication for the treatment of chemotherapy-induced and postoperative nausea and vomiting.[2] Aprepitant is also a selective activator of the K2P channel TRAAK.[3] It also has been shown to have multiple anticancer effects.[4]

1) Hale *et al*. (1998), *Structural optimization affording 2-(R)-(1-(R)-3,5-bis(trifluoromethyl)phenylethoxy)-3-(S)-(4-fluoro)phenyl-4-(3-oxo-1,2,4-triazol-5-yl)methylmorpholine, a potent, orally active, long-acting morpholine acetal human NK-1receptor antagonist*; J. Med. Chem. **41** 4607
2) Rapoport and Smit (2017); *Clinical pharmacology of neurokinin-1 receptor antagonists for the treatment of nausea and vomiting associated with chemotherapy*, Expert Opin. Drug Saf., **16** 697
3) McCoull *et al*. (2022); *Aprepitant is a novel, selective activator of the K2P channel TRAAK*, Biochem. Biophys. Res. Commun., **588** 41
4) Muñoz and Coveñas (2020); *The Neurokinin-1 Receptor Antagonist Aprepitant: An Intelligent Bullet against Cancer?*, Cancer (Basel), **12** 2682

PHYSICAL DATA

Molecular Weight:	534.43
Molecular Formula:	$C_{23}H_{21}F_7N_4O_3$
Purity:	>98% by HPLC
	NMR: (Conforms)
Solubility:	DMSO (>25 mg/ml)
Physical Description:	White solid
Storage and Stability:	Store as supplied at -20°C for up to 2 years from the date of purchase. Solutions in DMSO may be stored at -20°C for up to 3 months.

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