

PRODUCT INFORMATION



rac-Aprepitant-d₄ Item No. 25232

CAS Registry No.: 2748471-42-1
Formal Name: 5-((2-(1-(3,5-bis(trifluoromethyl)phenyl)ethoxy)-3-(4-fluorophenyl-2,3,5,6-d₄)morpholino)methyl)-2,4-dihydro-3H-1,2,4-triazol-3-one

MF: C₂₃H₁₇D₄F₇N₄O₃
FW: 538.5

Chemical Purity: ≥98% (Aprepitant)

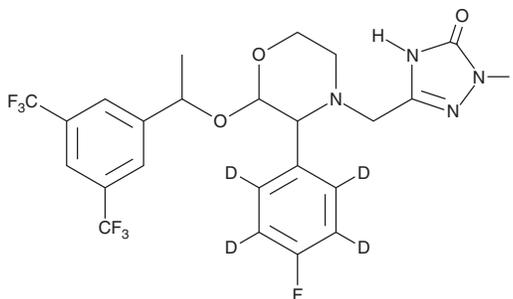
Deuterium

Incorporation: ≥99% deuterated forms (d₁-d₄); ≤1% d₀

Supplied as: A solid

Storage: -20°C

Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

rac-Aprepitant-d₄ is intended for use as an internal standard for the quantification of aprepitant (Item No. 14867) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated *versus* unlabeled).

rac-Aprepitant-d₄ is supplied as a solid. A stock solution may be made by dissolving the *rac*-aprepitant-d₄ in the solvent of choice. *rac*-Aprepitant-d₄ is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide, which should be purged with an inert gas. The solubility of *rac*-aprepitant-d₄ in these solvents is approximately 3, 16, and 25 mg/ml, respectively.

Description

Aprepitant an antiemetic compound and antagonist of the neurokinin-1 (NK₁) receptor (K_i = 3 nM; IC₅₀ = 0.09 nM for the human receptor).^{1,2} It is selective for NK₁ over NK₃ receptors (K_i = 454.1 nM for human NK₃).¹ *In vivo*, aprepitant (1 mg/kg) prevents plasma extravasation into the esophagus of guinea pigs induced by substance P (Item No. 24035).³ It also reduces NK₁-agonist-induced foot tapping in gerbils. Formulations containing aprepitant have been used to prevent chemotherapy-induced nausea and vomiting.

References

1. Bissantz, C., Bohnert, C., Hoffmann, T., *et al.* Identification of a crucial amino acid in the helix position 6.51 of human tachykinin neurokinin 1 and 3 receptors contributing to the insurmountable mode of antagonism by dual NK₁/NK₃ antagonists. *J. Med. Chem.* **55(11)**, 5061-5076 (2012).
2. Finke, P.E., Meurer, L.C., Levorse, D.A., *et al.* Cyclopentane-based human NK₁ antagonists. Part 1: Discovery and initial SAR. *Bioorg. Med. Chem. Lett.* **16(17)**, 4497-4503 (2006).
3. Meurer, L.C., Finke, P.E., Owens, K.A., *et al.* Cyclopentane-based human NK₁ antagonists. Part 2: Development of potent, orally active, water-soluble derivatives. *Bioorg. Med. Chem. Lett.* **16(17)**, 4504-4511 (2006).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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