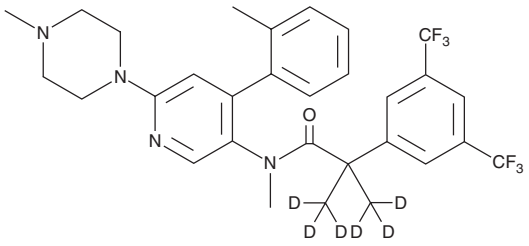
PRODUCT INFORMATION

Netupitant-d_6

Item No. 28901

CAS Registry No.:	2070015-31-3
Formal Name:	N-methyl-α,α-dimethyl-d3-N-[4-(2-methylphenyl)-6-(4-methyl-1-piperazinyl)-3-pyridinyl]-3,5-*bis*(trifluoromethyl)-benzeneacetamide
MF:	$C_{30}H_{26}D_6F_6N_4O$
FW:	584.6
Chemical Purity:	≥98% (Netupitant)
Deuterium Incorporation:	≥99% deuterated forms (d_1-d_6); ≤1% d_0
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

Netupitant-d_6 is intended for use as an internal standard for the quantification of netupitant (Item No. 23809) 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).

Netupitant-d_6 is supplied as a solid. A stock solution may be made by dissolving the netupitant-d_6 in the solvent of choice, which should be purged with an inert gas. Netupitant-d_6 is soluble in methanol and DMSO.

Description

Netupitant is an insurmountable antagonist of the neurokinin-1 (NK_1) receptor (K_i = 0.95 nM in CHO cells expressing the human recombinant receptor).[1] It is selective for human NK_1 over human NK_2 and NK_3 and rat NK_1 (K_is = >1,500 nM) and over 50 G protein-coupled receptors, monoamine transporters, and ion channels when used in the nanomolar range.[2] Netupitant decreases the maximal response to substance P-induced contractions in isolated guinea pig ileum with long-lasting effects. It also dose-dependently inhibits the substance P-induced scratching, biting, and licking response in mice when used at doses ranging from 1 to 10 mg/kg and decreases NK agonist-induced foot tapping in gerbils (ID_{50}s = 1.5 mg/kg, i.p., or 0.5 mg/kg, oral).

References

1. Hoffmann, T., Bös, M., Stadler, H., *et al.* Design and synthesis of a novel, achiral class of highly potent and selective, orally active neurokinin-1 receptor antagonists. *Bioorg. Med. Chem. Lett.* **16(5),** 1362-1365 (2006).
2. Rizzi, A., Campi, B., Camarda, V., *et al.* In vitro and in vivo pharmacological characterization of the novel NK_1 receptor selective antagonist Netupitant. *Peptides* **37(1),** 86-97 (2012).

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