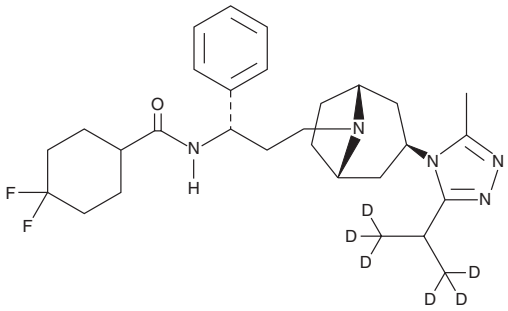
PRODUCT INFORMATION

Maraviroc-d_6

Item No. 28767

CAS Registry No.: 1033699-22-7
Formal Name: 4,4-difluoro-N-[(1S)-3-[(3-*exo*)-3-[3-methyl-5-(1-(methyl-d_3)ethyl-2,2,2-d_3)-4H-1,2,4-triazol-4-yl]-8-azabicyclo[3.2.1]oct-8-yl]-1-phenylpropyl]-cyclohexanecarboxamide
MF: $C_{29}H_{35}D_6F_2N_5O$
FW: 519.7
Chemical Purity: ≥98% (Maraviroc)
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

Maraviroc-d_6 is intended for use as an internal standard for the quantification of maraviroc (Item No. 14641) 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).

Maraviroc-d_6 is supplied as a solid. A stock solution may be made by dissolving the maraviroc-d_6 in the solvent of choice, which should be purged with an inert gas. Maraviroc-d_6 is slightly soluble in chloroform.

Description

Maraviroc is an antagonist of the chemokine (C-C motif) receptor 5 (CCR5; K_i = 0.24 nM for the rhesus monkey recombinant receptor).[1] It inhibits binding of chemokine (C-C motif) ligand 3 (CCL3), CCL4, and CCL5 to HEK293 cell membranes expressing CCR5 (IC_{50}s = 3.3, 7.2, and 5.2 nM, respectively) and inhibits HIV-1 binding to CCR5 *via* glycoprotein 120 (gp120) and gp160 (IC_{50}s = 11 and 0.22 nM, respectively).[2] Maraviroc is selective for CCR5 over CCR1, -2, -3, -4, -7, and -8, and chemokine (C-X-C motif) receptor 1 (CXCR1) and CXCR2 in a panel of immunological assays for ligand-induced cell chemotaxis and ligand-receptor binding (IC_{50}s = >10 µM for all). It has antiviral activity against laboratory and clinical isolates of CCR5-tropic (IC_{50}s = 0.1-1.1 nM), but not CXCR4-tropic or dual tropic (IC_{50}s = >10 µM for all), HIV-1 in isolated human peripheral blood mononuclear cells (PBMCs). Maraviroc prevents infection upon exposure to HIV-1 in humanized RAG-hum mice when administered at a dose of 62 mg/kg.[3]

References

1. Yuan, Y., Arnatt, C.K., El-Hage, N., *et al.* A bivalent ligand targeting the putative mu opioid receptor and chemokine receptor CCR5 heterodimers: Binding affinity versus functional activities. *Medchemcomm.* **4(5),** 847-851 (2013).
2. Dorr, P., Westby, M., Dobbs, S., *et al.* Maraviroc (UK-427,857), a potent, orally bioavailable, and selective small-molecule inhibitor of chemokine receptor CCR5 with broad-spectrum anti-human immunodeficiency virus type 1 activity. *Antimicrob. Agents Chemother.* **49(11),** 4721-4732 (2005).
3. Neff, C.P., Ndolo, T., Tandon, A., *et al.* Oral pre-exposure prophylaxis by anti-retrovirals raltegravir and maraviroc protects against HIV-1 vaginal transmission in a humanized mouse model *PLoS One* **5(12),** e15257 (2010).

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