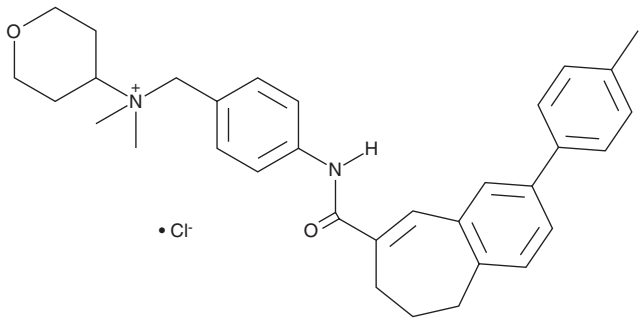
PRODUCT INFORMATION

TAK-779

Item No. 26744

CAS Registry No.: 229005-80-5
Formal Name: N-[[4-[[[6,7-dihydro-2-(4-methylphenyl)-5H-benzocyclohepten-8-yl]carbonyl]amino]phenyl]methyl]tetrahydro-N,N-dimethyl-2H-pyran-4-aminium, monochloride
MF: $C_{33}H_{39}N_2O_2 \bullet Cl$
FW: 531.1
Purity: ≥98%
UV/Vis.: λ_{max}: 261 nm
Supplied as: A crystalline 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

TAK-779 is supplied as a crystalline solid. A stock solution may be made by dissolving the TAK-779 in the solvent of choice, which should be purged with an inert gas. TAK-779 is soluble in the organic solvent DMSO. It is also soluble in water. The solubility of TAK-779 in DMSO and water is approximately 20 and 10 mg/ml, respectively. We do not recommend storing the aqueous solution for more than one day.

Description

TAK-779 is an antagonist of chemokine receptor 5 (CCR5), CCR2b, and CXC chemokine receptor 3 (CXCR3).[1,2] It inhibits CCR5 and CXCR3 (IC_{50}s = 236 and 369 nM, respectively, for mouse recombinant receptors expressed in 2B4 T cells) and CCR5 and CCR2b (IC_{50}s = 1.4 and 27 nM, respectively, for human recombinant receptors expressed in CHO cells). TAK-779 inhibits the replication of clinical isolates of R5, but not X4, HIV-1 in human peripheral blood mononuclear cells (PBMCs; EC_{50}s = 1.6-3.5 and >20,000 nM, respectively).[1] TAK-779 (250 mg/animal per day) inhibits ovalbumin-induced increases in CCR5, CXCR3, IFN-γ, and TNF-α expression in mouse lung, as well as the number of total cells, lymphocytes, and eosinophils in bronchoalveolar lavage fluid (BALF), in a mouse model of asthma.[3] It also increases intestinal allograft survival in a rat model of small intestine transplantation when administered at a dose of 10 mg/kg per day.[4]

References

1. Baba, M., Nishimura, O., Kanzaki, N., *et al.* A small-molecule, nonpeptide CCR5 antagonist with highly potent and selective anti-HIV-1 activity. *Proc. Natl. Acad. Sci. U.S.A.* **96(10)**, 5698-5703 (1999).
2. Gao, P., Zhou, X.-Y., Yashiro-Ohtani, Y., *et al.* The unique target specificity of a nonpeptide chemokine receptor antagonist: Selective blockade of two Th1 chemokine receptors CCR5 and CXCR3. *J. Leukoc. Biol.* **73(2)**, 273-280 (2003).
3. Suzaki, Y., Hamada, K., Nomi, T., *et al.* A small-molecule compound targeting CCR5 and CXCR3 prevents airway hyperresponsiveness and inflammation. *Eur. J. Respir. J.* **31(4)**, 783-789 (2008).
4. Takama, Y., Miyagawa, S., Yamamoto, A., *et al.* Effects of a calcineurin inhibitor, FK506, and a CCR5/CXCR3 antagonist, TAK-779, in a rat small intestinal transplantation model. *Transpl. Immunol.* **25(1)**, 49-55 (2011).

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