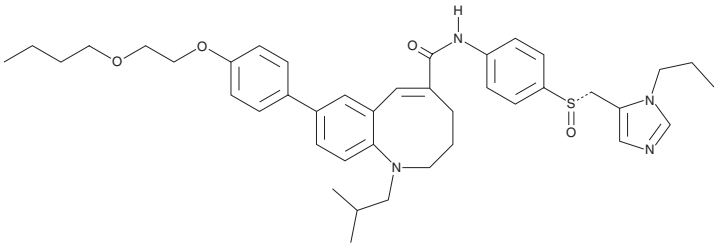
PRODUCT INFORMATION

Cenicriviroc

Item No. 23927

CAS Registry No.: 497223-25-3
Formal Name: 8-[4-(2-butoxyethoxy)phenyl]-1,2,3,4-tetrahydro-1-(2-methylpropyl)-N-[4-[(S)-[(1-propyl-1H-imidazol-5-yl)methyl]sulfinyl]phenyl]-1-benzazocine-5-carboxamide
Synonym: TAK-652
MF: $C_{41}H_{52}N_4O_4S$
FW: 696.9
Purity: ≥95%
UV/Vis.: λ_{max}: 295 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

Cenicriviroc is supplied as a crystalline solid. A stock solution may be made by dissolving the cenicriviroc in the solvent of choice. Cenicriviroc is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of cenicriviroc is approximately 5 mg/ml in ethanol and approximately 20 mg/ml in DMSO and DMF.

Cenicriviroc is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, cenicriviroc should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Cenicriviroc has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Cenicriviroc is an orally bioavailable antagonist of C-C chemokine receptor type 5 (CCR5) and CCR2 that inhibits binding of macrophage inflammatory protein 1α (MIP-1α; IC_{50} = 2.3 nM) and monocyte chemotactic protein 1 (MCP-1; IC_{50} = 5.9 nM), respectively, in CHO cells.[1] Cenicriviroc is also an antagonist of CCR3 and CCR4 (IC_{50}s = 2.4 and 1.1 µM, respectively), however, it does not inhibit agonist binding to CCR1 or CCR7 at concentrations up to 10 µM. At a concentration of 100 nM, cenicriviroc completely inhibits replication of R5 HIV-1 in U87.CD4.CCR5 cells. Cenicriviroc inhibits replication of the R5 HIV-1 strains JR-FL and KK in peripheral blood mononuclear cells (PBMCs) with EC_{50} values ranging from 21 to 210 pM and 33 to 91 pM, respectively. *In vivo*, cenicriviroc (20 mg/kg per day) reduces collagen deposition, levels of collagen type 1 protein and mRNA expression, and non-alcoholic fatty liver disease activity score in a mouse model of non-alcoholic steatohepatitis (NASH).[2] It also reduces collagen type 1 protein levels, mRNA expression, and collagen deposition in a mouse model of unilateral ureter obstruction and a rat model of thioacetamide-induced liver fibrosis.

References

1. Baba, M., Takashima, K., Miyake, H., *et al.* TAK-652 inhibits CCR5-mediated human immunodeficiency virus type 1 infection *in vitro* and has favorable pharmacokinetics in humans. *Antimicrob. Agents Chemother.* **49(11)**, 4584-4591 (2005).
2. Lefebvre, E., Moyle, G., Reshef, R., *et al.* Antifibrotic effects of the dual CCR2/CCR5 antagonist cenicriviroc in animal models of liver and kidney fibrosis. *PLoS One* **11(6):e0158156**, (2016).

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