Product Data Sheet

Product Name: Aplaviroc (AK 602)
Cat. No.: GC32336

Chemical Properties

Cas. No.	461443-59-4		
SMILES	O=C(O)C1=CC=C(OC2=CC=C(CN(CC3)CCC3(N(CCCC)C([C@@H]([C@@H](C4CCCCC4)O)N5)=O)C5=O)C=C2)C=C1		
Formula	$C_{33}H_{43}N_3O_6$	M.Wt	577.71
Solubility	Soluble in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	Aplaviroc (AK 602)		

Background

Aplaviroc, a SDP derivative, is a CCR5 antagonist, with IC50s of 0.1-0.4 nM for HIV-1Ba-L, HIV-1JRFL and HIV-1MOKW.

Aplaviroc (AK602) is identified as the most potent agent among newly designed and synthesized SDP derivatives. Aplaviroc exerts potent activity against three wild-type R5 HIV-1 strains (HIV-1Ba-L, HIV-1JRFL and HIV-1MOKW) with IC50 values of 0.1 to 0.4 nM. It is of note that Aplaviroc is substantially more potent than two previously published CCR5 inhibitors, E921/TAK-779 and AK671/SCH-C. The activity of Aplaviroc's anti-HIV-1 is limited and similar to that seen for zidovudine. Moreover, Aplaviroc suppresses the infectivity and replication of two HIV-1MDR variants, HIV-1MM and HIV-1JSL, at extremely low concentrations (IC50 values of 0.4 to 0.6 nM), while these two R5 HIV-1 variants are less susceptible to zidovudine, nelfinavir, and saquinavir. Aplaviroc binds to CCR5 with high affinity. The Kd values thus determined for Aplaviroc, E913, E921/TAK-779, and AK671/SCH-C are 2.9±1.0, 111.7±3.5, 32.2±9.6, and 16.0±1.5 nM, respectively. Aplaviroc potently blocks rgp120/sCD4 binding to CCR5 with an IC50 value of 2.7 nM. These results suggest that the potent activity of Aplaviroc against R5 HIV-1 stems from

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com
Address: 10292 Central Ave. #205, Montclair, CA, USA

its binding to ECL2B and/or its vicinity with high affinity, resulting in inhibition of gp120/CD4 binding to CCR5[1].

[1]. Maeda K, et al. Spirodiketopiperazine-based CCR5 inhibitor which preserves CC-chemokine/CCR5 interactions and exerts potent activity against R5 human immunodeficiency virus type 1 in vitro. J Virol. 2004 Aug;78(16):8654-62.

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