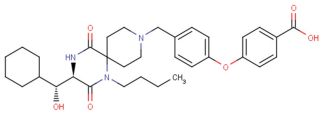
Data Sheet (Cat.No.T14307)

TargetMol
A DRUG SCREENING EXPERT

Aplaviroc

Chemical Properties



CAS No.:	461443-59-4
Formula:	C33H43N3O6
Molecular Weight:	577.71
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	Aplaviroc (AK 602), a SDP derivative, is a CCR5 antagonist. With IC50s of 0.1-0.4 nM for HIV-1Ba-L, HIV-1JRFL and HIV-1MOKW.
Targets(IC_{50})	HIV-1Ba-L: 0.4 nM HIV-1JRFL: 0.1 nM HIV-1MOKW: 0.2 nM CCR5: None
In vitro	Aplaviroc (AK602) is identified as the most potent agent among newly designed and synthesized SDP derivatives and it also is substantially more potent than two previously published CCR5 inhibitors, E921/TAK-779 and AK671/SCH-C. 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 and it potently blocks rgp120/sCD4 binding to CCR5 with an IC50 value of 2.7 nM. The activity of Aplaviroc's anti-HIV-1 is limited and similar to that seen for zidovudine. 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 and it also 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. These results suggest that the potent activity of Aplaviroc against R5 HIV-1 stems from its binding to ECL2B and/or its vicinity with high affinity, resulting in inhibition of gp120/CD4 binding to CCR5[1].

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.731 mL	8.655 mL	17.31 mL
5 mM	0.346 mL	1.731 mL	3.462 mL
10 mM	0.173 mL	0.865 mL	1.731 mL
50 mM	0.035 mL	0.173 mL	0.346 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

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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