# Data Sheet (Cat.No.T16973)

TAK-220

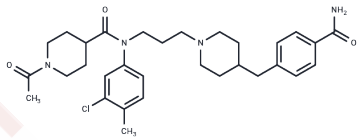
## Chemical Properties

CAS No. : 333994-00-6

Formula: C31H41ClN4O3

Molecular Weight: 553.14

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.



## Biological Description

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|---|---|
| Description | TAK-220 is a selective and orally bioavailable CCR5 antagonist with IC50 values of 3.5 nM for RANTES binding inhibition and 1.4 nM for MIP-1α binding inhibition to CCR5. |
| Targets(IC50) | HIV Protease,CCR |
| In vitro | TAK-220 inhibits R5 HIV-1 (JR-FL) envelope-mediated membrane fusion (IC50: 0.42 nM). TAK-220 shows potent inhibitory activity against the R5 isolates, with IC50s of 3.12 nM against HIV-1 R5-08, 13.47 nM against HIV-1 R5-06, and 2.26 nM against HIV-1 R5-18. TAK-220 (>100 nM) has no toxicity in uninfected PBMCs. TAK-220 (0-1000 nM) interacts with CCR5 but not with RANTES and inhibits the CCR5-mediated Casup>2+ signaling. TAK-220 also selectively inhibits HIV-1, with EC50s of 1.2 nM (HIV-1 KK), 0.72 nM (HIV-1 CTV), 1.7 nM (HIV-1 HKW), 1.7 nM (HIV-1 HNK), 0.93 nM (HIV-1 HTN), and 0.55 nM (HIV-1 HHA), and EC90s of 12 nM (HIV-1 KK), 5 nM (HIV-1 CTV), 12 nM (HIV-1 HKW), 28 nM (HIV-1 HNK), 15 nM (HIV-1 HTN), and 4 nM (HIV-1 HHA) in PBMCs [1][2]. |

## Solubility Information

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|---|---|
| Solubility | DMSO: 50 mg/mL (90.39 mM),Sonication is recommended.<br>(< 1 mg/ml refers to the product slightly soluble or insoluble) |
| In vivo Formulation | 10% DMSO+40% PEG300+5% Tween-80+45% Saline: 2.5 mg/mL (4.52 mM),Sonication is recommended.<br>*Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.* |

Preparing Stock Solutions

| | 1mg | 5mg | 10mg |
|---|---|---|---|
| 1 mM | 1.8079 mL | 9.0393 mL | 18.0786 mL |
| 5 mM | 0.3616 mL | 1.8079 mL | 3.6157 mL |
| 10 mM | 0.1808 mL | 0.9039 mL | 1.8079 mL |
| 50 mM | 0.0362 mL | 0.1808 mL | 0.3616 mL |

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Takashima K, et al. Highly potent inhibition of human immunodeficiency virus type 1 replication by TAK-220, an orally bioavailable small-molecule CCR5 antagonist. Antimicrob Agents Chemother. 2005 Aug;49(8):3474-82.
Tremblay CL, et al. TAK-220, a novel small-molecule CCR5 antagonist, has favorable anti-human immunodeficiency virus interactions with other antiretrovirals in vitro. Antimicrob Agents Chemother. 2005 Aug;49 (8):3483-5.