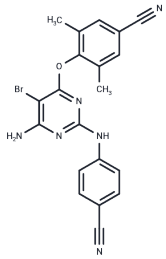
Data Sheet (Cat.No.T2551)

TargetMol

Etravirine

Chemical Properties



CAS No. : 269055-15-4

Formula: C20H15BrN6O

Molecular Weight: 435.28

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

Description	Etravirine (R165335) is a diarylpyrimidine non-nucleoside reverse transcriptase inhibitor. Etravirine is designed to be active against HIV isolates with mutations that confer resistance to the two most commonly prescribed first-generation NNRTIs. It can bind the enzyme reverse transcriptase (RT) in multiple conformations, both for native and mutant RT, thereby blocking the enzymatic activity of RT.
Targets(IC50)	HIV Protease,Reverse Transcriptase
In vitro	Etravirine (TMC125), is highly active against wild-type HIV-1 with EC50 of 1.4 nM to 4.8 nM and shows some activity against HIV-2 with EC50 of 3.5 μM. TMC125 also inhibits a series of HIV-1 group M subtypes and circulating recombinant forms and a group O virus. [1] [2]
In vivo	Etravirine (TMC125) demonstrates a high genetic barrier against resistance development and remains effective against HIV strains resistant to existing non-nucleoside reverse transcriptase inhibitors (NNRTIs), including those also resistant to protease inhibitors (PIs). Its tolerability profile, assessed in phase IIb trials with treatment-experienced patients, is comparable to the control group[3].

Solubility Information

Solubility	Ethanol: < 1 mg/mL (insoluble or slightly soluble), DMSO: 250 mg/mL (574.34 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (4.59 mM),Sonication is recommended. *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	2.2974 mL	11.4869 mL	22.9737 mL
5 mM	0.4595 mL	2.2974 mL	4.5947 mL
10 mM	0.2297 mL	1.1487 mL	2.2974 mL
50 mM	0.0459 mL	0.2297 mL	0.4595 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

Das K, et al. J Med Chem, 2004, 47(10), 2550-2560.
Ly T T G, Yun J, Ha J S, et al. Inhibitory Effect of Etravirine, a Non-Nucleoside Reverse Transcriptase Inhibitor, via Anterior Gradient Protein 2 Homolog Degradation against Ovarian Cancer Metastasis. International Journal of Molecular Sciences. 2022, 23(2): 944.
Islam S, Rahaman M H, Yu M, et al.Anti-Leukaemic Activity of Rilpivirine Is Mediated by Aurora A Kinase Inhibition. Cancers.2023, 15(4): 1044.
Andries K, et al. Antimicrob Agents Chemother, 2004, 48(12), 4680-4686.
Lazzarin A, et al. Lancet, 2007, 370(9581), 39-48.
Ekiciler A, Chen W L K, Bo Y, et al.Quantitative Cytochrome P450 3A4 Induction Risk Assessment Using Human Hepatocytes Complemented with Pregnane X Receptor-Activating Profiles.Drug Metabolism and Disposition.2023, 51(3): 276-284.
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