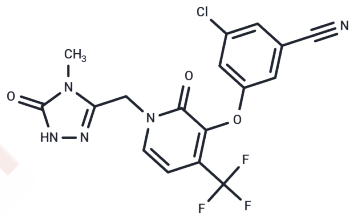
Data Sheet (Cat.No.T3632)

TargetMol

Doravirine

Chemical Properties



CAS No. : 1338225-97-0

Formula: C17H11ClF3N5O3

Molecular Weight: 425.75

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	Doravirine (MK-1439) is a non-nucleoside reverse transcriptase inhibitor used for the treatment of HIV/AIDS.
Targets(IC50)	HIV Protease,Reverse Transcriptase
In vitro	Doravirine exhibits potent antiviral activity against wild-type virus and K103N, Y181C, and K103N/Y181C mutant viruses, with IC50 value of 12, 21, 31, and 33 nM, respectively. [1]? MK-1439 exhibited similar antiviral activities against 10 different HIV-1 subtype viruses (a total of 93 viruses).[2]
In vivo	Administration of 50 mg doravirine with a high-fat meal is associated with slight elevations in AUC time zero to infinity (AUC0-∞) and C24 h with no change in Cmax. Midazolam AUC0-∞ is slightly reduced by coadministration of doravirine (geometric mean ratio 0.82, 90% CI 0.70, 0.97). [3]
Kinase Assay	FS-3 substrate is solubilized in assay buffer at 500 μM and frozen at -20°C in single-use aliquots for up to 4 weeks. Recombinant autotaxin is diluted in Tris-buffered saline (140 mM NaCl, 5 mM KCl, 1 mM CaCl2, 1 mM MgCl2, 50 mM Tris, pH 8.0) and incubated with compound in DMSO or DMSO alone (final 1% DMSO) for 15 min at 37°C, and the reaction is started with the addition of FS-3 at a final concentration of 1 μM. The reaction is allowed to proceed at 37°C for 30 min and monitored at 520 nm until the uninhibited control compared with a no-enzyme control gave a Z′≥0.5. IC50s are determined in triplicate by using a four-parameter fit[1].

Solubility Information

Solubility	DMSO: 100 mg/mL (234.88 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: < 10 mg/mL (23.49 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 10 mg/mL (23.49 mM),Solution. 10% DMSO+90% Corn Oil: 2 mg/mL (4.7 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	2.3488 mL	11.744 mL	23.488 mL
5 mM	0.4698 mL	2.3488 mL	4.6976 mL
10 mM	0.2349 mL	1.1744 mL	2.3488 mL
50 mM	0.047 mL	0.2349 mL	0.4698 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

Lai MT, et al. Antimicrob Agents Chemother. 2014;58(3):1652-63.
Fical L, Khalikova M, Kočová Vlčková H, et al. Determination of Antiviral Drugs and Their Metabolites Using Micro-Solid Phase Extraction and UHPLC-MS/MS in Reversed-Phase and Hydrophilic Interaction Chromatography Modes. Molecules. 2021, 26(8): 2123.
Anderson MS, et al. Antivir Ther. 2015;20(4):397-405.
Fical L. Vývoj UHPLC-MS/MS metody pro analýzu vybraných antivirotik v HILIC a RP módu[J]. 2020
Fical L, Khalikova M, Kočová Vlčková H, et al. Determination of Antiviral Drugs and Their Metabolites Using Micro-Solid Phase Extraction and UHPLC-MS/MS in Reversed-Phase and Hydrophilic Interaction Chromatography Modes [J]. Molecules. 2021, 26(8): 2123.