Doravirine

Catalog No.C11942 Batch:C1194203

Product Datasheet

Technical Data

Formula	$C_{17}H_{11}C_1F_3N_5O_3$					
Molecular Weight	425.75	**CAS No.**	1338225-97-0			
Solubility (25°C)*	In vitro	DMSO	85 mg/mL (199.64 mM)			
		Water	Insoluble			
		Ethanol	Insoluble			
	In vivo (Add solvents to the product individually and in order)	Oral Administration	Homogeneous suspension	CMC-NA	≥5mg/ml	Taking the 1 mL working solution as an example, add 5 mg of this product to 1 ml of CMC-Na solution, mix evenly to obtain a homogeneous suspension with a final concentration of 5 mg/ml.
		Injection	Clear solution	5%DMSO [1] → 40%PEG300 [2] → 5%Tween80 [3] → 50%ddH2O Validated by Capsid Bio labs. Should you need adjustments to this formulation, contact our sales team for custom testing.	2.125mg/ml (4.99mM)	Taking the 1 mL working solution as an example, add 50 μL of 42.5 mg/ml clarified DMSO stock solution to 400 μL of PEG300, mix evenly to clarify it; add 50 μL of Tween80 to the above system, mix evenly to clarify; then continue to add 500 μL of ddH2O to adjust the volume to 1 mL. The mixed solution should be used immediately for optimal results.
			Clear solution	5% DMSO [1] → 95% Corn oil Validated by Capsid Bio labs. Should you need adjustments to this formulation, contact our sales team for custom testing.	0.700mg/ml (1.64mM)	Taking the 1 mL working solution as an example, add 50 μL of 14 mg/ml clear DMSO stock solution to 950 μL of corn oil and mix evenly. The mixed solution should be used immediately for optimal results.

* <1 mg/ml means slightly soluble or insoluble.
* Please note that Capsid Bio tests the solubility of all compounds in-house, and the actual solubility may differ slightly from published values. This is normal and is due to slight batch-to-batch variations.
* Room temperature shipping (Stability testing shows this product can be shipped at 2-8°C for storage purposes.)

Preparing Stock Solutions

Concentration \ Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.3488 mL	11.7440 mL	23.4880 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	0.0470 mL	0.2349 mL	0.4698 mL

Biological Activity

Description	Doravirine is a novel **HIV-1 nonnucleoside reverse transcriptase** inhibitor with IC50 values of 12, 9.7, and 9.7 nM against the wild type (WT) and K103N and Y181C reverse transcriptase (RT) mutants, respectively, in a biochemical assay. It is highly specific with minimum off-target activities.
Targets	K103N HIV-1 RT [1] 9.7 nM; Y181C HIV-1 RT [1] 9.7 nM; WT HIV-1 RT [1] 12 nM
In vitro	MK-1439 exhibits greater than 10,000-fold selectivity with respect to the cellular DNA polymerases α, ß, and γ with IC50s of >100 μM. In the screen with more than 110 protein targets including enzymes, transporters, ion channels, and receptor, MK-1439 shows an IC50 of greater than 10 μM against all targets except 5-HT2ß, where an IC50 of 2.5 μM is noted in a ligand binding assay. However, the 5-HT2ß activity is not observed in a functional cell-based assay monitoring the accumulation of inositol-1-phosphate. Therefore, the binding activity does not appear to translate into a 5-HT2ß functional response. MK-1439 does not display cytotoxicity in activated CD4+ T cells, PBMCs, monocytes, macrophages proliferating transformed cell lines, such as MT4, SupT1, and HL60 cell lines at concentrations of up to 100 μM[1].
In vivo	In rats dosed IV at 1 mpk (60%PEG200), the clearance (CL) of MK-1439 is 5.4 mL/min/kg and the half time is 4.4 hr. Its volume of distribution (Vd) is 2.3 L/kg. The oral bioavailability of MK-1439 is 57% (doesed PO at 5 mpk). In dogs dosed IV at 0.5 mpk, the CL of MK-1439 is 0.36 mL/min/kg and half-time is 37 hr. The oral bioavailability of MK-1439 is 52% (doesed PO at 1 mpk). Overall, The pharmacokinetic profile of MK-1439 in preclinical species is favorable[2].

Protocol (from reference)

Animal Study:[2]

- **Animal Models**
  60% PEG200 (IV); Ball-milled, 0.5% methocel (PO in rats); Ball-milled, 10% Tween (PO in dogs)
- **Dosages**
  1 mpk (IV in rats); 5 mpk (PO in rats); 0.5 mpk (IV in dogs); 1 mpk (PO in dogs)
- **Administration**
  IV or PO

References

https://pubmed.ncbi.nlm.nih.gov/24379202/ https://pubmed.ncbi.nlm.nih.gov/24412110/

RETURN POLICY

Capsid Bio's Unconditional Return Policy ensures a smooth online shopping experience for our customers. If you are in any way unsatisfied with your purchase, you may return any item(s) within 7 days of receiving it. In the event of product quality issues, either protocol related or product related problems, you may return any item(s) within 365 days from the original purchase date. Please follow the instructions below when returning products.

SHIPPING & STORAGE

Capsid Bio products are transported at room temperature. If you receive the product at room temperature, please rest assured, the Capsid Bio Quality Inspection Department has conducted experiments to verify that the normal temperature placement of one month will not affect the biological activity of powder products. After collecting, please store the product according to the requirements described in the datasheet. Most Capsid Bio products are stable under the recommended conditions.

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