Atovaquone

Cat. No.: HY-13832

CAS No.: 95233-18-4

Molecular Formula: $C_{22}H_{19}ClO_3$

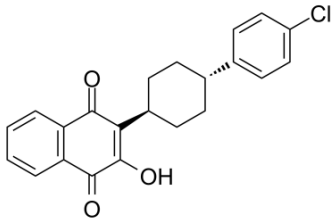
Molecular Weight: 366.84

Target: Parasite; Cytochrome P450; Antibiotic

Pathway: Anti-infection; Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 8.33 mg/mL (22.71 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.7260 mL	13.6299 mL	27.2598 mL
	5 mM	0.5452 mL	2.7260 mL	5.4520 mL
	10 mM	0.2726 mL	1.3630 mL	2.7260 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: 0.83 mg/mL (2.26 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 0.83 mg/mL (2.26 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Atovaquone (Atavaquone) is a potent, selective and orally active inhibitor of the parasite's mitochondrial cytochrome ***bc1*** complex. Atovaquone is against human and P. falciparum cytochrome bc1 activity with IC_{50} values of 460 nM and 2.0 nM, respectively. Atovaquone is an antimalarial agent and has the potential for the investigation of neumocystis pneumonia, toxoplasmosis, malaria, and babesia[1][2].

IC_{50} & Target

IC50: 460 nM (human cytochrome bc1); 2.0 nM (P. falciparum cytochrome bc1)[1]

In Vitro

Atovaquone targets to the Q_o site of the Plasmodium cytochrome bc1 complex of the mitochondrial electron transport chain[1].

Atovaquone is against the development in the mosquito from gamete production, through fertilization, zygote formation

	and finally, to the development of the mature ookinete, and demonstrates an IC_{50} of 67 nM providing further evidence of the transmission blocking potential of this molecule[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Atovaquone (oral administration; 100 mg/kg; once daily) is against survival rates of mice, mice treated orally died within 22 days after discontinuation of sulfadiazine,while the control group died at day 14[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	ICSBP$^{-/-}$ mice infected with 10 cysts of the ME49 strain of T. gondii[2]
Dosage:	100 mg/kg
Administration:	Oral administration
Result:	Improved mice survival rate to 22 days compared to vehicle.

CUSTOMER VALIDATION

- Biomed J. 2020 Aug;43(4):368-374.

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REFERENCES

[1]. Nilsen A, et al. Quinolone-3-diarylethers: a new class of antimalarial drug.Sci Transl Med. 2013 Mar 20;5(177):177ra37.

[2]. Schöler N, et al. Atovaquone nanosuspensions show excellent therapeutic effect in a new murine model of reactivated toxoplasmosis.Antimicrob Agents Chemother. 2001 Jun;45(6):1771-9.

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