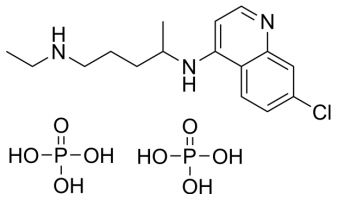
Desethyl chloroquine diphosphate

Cat. No.:	HY-135811A
CAS No.:	247912-76-1
Molecular Formula:	$C_{16}H_{28}ClN_3O_8P_2$
Molecular Weight:	487.81
Target:	Parasite; Toll-like Receptor (TLR); Autophagy
Pathway:	Anti-infection; Immunology/Inflammation; Autophagy
Storage:	4°C, protect from light, stored under nitrogen * In solvent : -80°C, 6 months; -20°C, 1 month (protect from light, stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

H_2O : 20 mg/mL (41.00 mM; ultrasonic and warming and heat to 80°C)
DMSO : 2.63 mg/mL (5.39 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0500 mL	10.2499 mL	20.4998 mL
	5 mM	0.4100 mL	2.0500 mL	4.1000 mL
	10 mM	0.2050 mL	1.0250 mL	2.0500 mL

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

In Vivo

1. Add each solvent one by one: PBS
   Solubility: 50 mg/mL (102.50 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (5.12 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.12 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Desethyl chloroquine diphosphate is a major desethyl metabolite of Chloroquine. Chloroquine diphosphate is an inhibitor of autophagy and toll-like receptors (TLRs). Desethyl chloroquine diphosphate possesses antiplasmodic activity[1][2].

IC_{50} & Target		
	Plasmodium	TLRs

In Vivo

Intraperitoneal injections of Chloroquine are administered to wild-type and Huntington's disease (Q175/Q175) mice. LC-MS/MS is used to compare the levels Chloroquine and its metabolites in blood, brain and muscle tissue. Concentrations of

Chloroquine are lower (5-15M), but more stable in brain tissue compared to blood or muscle between 4 and 24 hours after the last dose. Levels of the active Chloroquine metabolite Desethyl chloroquine decreased in muscle and blood over the 24 hour post-injection period, while brain Desethyl chloroquine levels are lower and rose slightly over the same time frame[3].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Cell Death Dis. 2021 Jan 7;12(1):42.

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REFERENCES

[1]. Ajayi FO, et al. Comparison of the partitioning in vitro of chloroquine and its desethyl metabolites between the erythrocytes and plasma of healthy subjects and those with falciparum malaria. Afr J Med Med Sci. 1989 Jun;18(2):95-100.

[2]. Vodicka P, et al. Assessment of chloroquine treatment for modulating autophagy flux in brain of WT and HD mice. J Huntingtons Dis. 2014;3(2):159-74.

[3]. Said A, et al. Chloroquine promotes IL-17 production by CD4+ T cells via p38-dependent IL-23 release by monocyte-derived Langerhans-like cells. J Immunol. 2014 Dec 15;193(12):6135-43.

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