Product Data Sheet

Atovaquone-d₅

 Cat. No.:
 HY-13832S2

 CAS No.:
 1329792-63-3

 Molecular Formula:
 $C_{22}H_{14}D_5ClO_3$

Molecular Weight: 371.87

Target: Cytochrome P450; Parasite; Antibiotic; Isotope-Labeled Compounds

Pathway: Metabolic Enzyme/Protease; Anti-infection; Others

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.

BIOLOGICAL ACTIVITY

Description	Atovaquone-d ₅ is the deuterium labeled Atovaquone. 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 IC50 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	Plasmodium
In Vitro	Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

 $[1]. \ Russak\ EM, et\ al.\ Impact\ of\ Deuterium\ Substitution\ on\ the\ Pharmacokinetics\ of\ Pharmaceuticals.\ Ann\ Pharmacother.\ 2019; 53(2): 211-216.$

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

[3]. 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.

Caution: Product has not been fully validated for medical applications. For research use only.

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