Product Data Sheet

Product Name: Atovaquone D4
Cat. No.: GC38889

Chemical Properties

Cas. No.	2070015-14-2		
SMILES	O=C1C2=C(C(C(O)=C1[C@@H]3CC[C@@H](C4=CC=C(Cl)C=C4)CC3)=O)C([2H])=C([2H])C([2H])=C2[2H]		
Formula	$C_{22}H_{15}D_4ClO_3$	M.Wt	370.86
Solubility	Chloroform: soluble	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	Atovaquone D4		

Background

Atovaquone-d_4 is intended for use as an internal standard for the quantification of atovaquone by GC- or LC-MS. Atovaquone is a broad-spectrum antiprotozoal agent that is active against *Plasmodium*, *Toxoplasma*, and *Babesia*, among other protozoa.[1] It inhibits complex III activity on dihydroorotate in isolated *P. falciparum* and *P. yoelii* mitochondria more potently than in rat liver mitochondria (EC_{50}s = 0.95, 0.94, and 510 nM, respectively) and depolarizes the mitochondrial membrane in *P. yoelii*-infected mouse erythrocytes (EC_{50} = 260 nM).[2,3] Atovaquone also inhibits transport mediated by human breast cancer resistance protein (BCRP) and P-glycoprotein in membrane vesicles (IC_{50}s = 0.23 and 6.8 µM, respectively).[4] It inhibits the growth of *T. gondii* in MRC-5 human lung fibroblasts *in vitro* (IC_{50} = ~64 nM) and increases mean survival of *T. gondii*-infected mice from 5.5 to 21.2 days when administered at a dose of 100 mg/kg per day.[5] Formulations containing atovaquone have been used in the treatment of *Pneumocystis* pneumonia and toxoplasmosis as well as in combination with proguanil in the treatment of malaria and babesiosis.

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1.Kessl, J.J., Lange, B.B., Merbitz-Zahradnik, T., et al.Molecular basis for atovaquone binding to the cytochrome bc1 complexJ. Biol. Chem.278(33)31312-31318(2003) 2.Fry, M., and Pudney, M.Site of action of the antimalarial hydroxynaphthoquinone, 2-[trans-4-(4'-chlorophenyl) cyclohexyl]-3-hydroxy-1,4-naphthoquinone (566C80)Biochem. Pharmacol.43(7)1545-1553(1992) 3.Srivastava, I.K., Rottenberg, H., and Vaidya, A.B.Atovaquone, a broad spectrum antiparasitic drug, collapses mitochondrial membrane potential in a malarial parasiteJ. Biol. Chem.272(7)3961-3966(1997) 4.Rijpma, S.R., van den Heuvel, J.J., van der Velden, M., et al.Atovaquone and quinine anti-malarials inhibit ATP binding cassette transporter activityMalar. J.13359(2014) 5.Romand, S., Pudney, M., and Derouin, F.In vitro and in vivo activities of the hydroxynaphthoquinone atovaquone alone or combined with pyrimethamine, sulfadiazine, clarithromycin, or minocycline against Toxoplasma gondiiAntimicrob. Agents Chemother.37(11)2371-2378(1993)

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