PRODUCT INFORMATION



Atovaquone-d_₄

Item No. 28491

CAS Registry No.:	2070015-14-2	
Formal Name:	2-[trans-4-(4-chlorophenyl)cyclohexyl]-3-	CI
	hydroxy-1,4-naphthalenedione-5,6,7,8-d ₄	
MF:	$C_{22}H_{15}CID_4O_3$	
FW:	370.9	₽ o ĺ ľ
Chemical Purity:	≥98% (Atovaquone)	
Deuterium		
Incorporation:	≥99% deuterated forms (d_1-d_4) ; ≤1% d_0	
Supplied as:	A solid	D
Storage:	-20°C	D O
Stability:	≥4 years	

Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Atovaquone-d4 is intended for use as an internal standard for the quantification of atovaquone (Item No. 23802) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated versus unlabeled).

Atovaquone- d_1 is supplied as a solid. A stock solution may be made by dissolving the atovaquone- d_1 in the solvent of choice, which should be purged with an inert gas. Atovaquone- d_4 is soluble in chloroform.

Description

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 $(IC_{50}s = 0.23 \text{ and } 6.8 \mu\text{M}, \text{ respectively}).^4$ It inhibits the growth of T. gondii in MRC-5 human lung fibroblasts in vitro (IC₅₀ = ~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.

References

- 1. Kessl, J.J., Lange, B.B., Merbitz-Zahradnik, T., et al. J. Biol. Chem. 278(33), 31312-31318 (2003).
- 2. Fry, M. and Pudney, M. Biochem. Pharmacol. 43(7), 1545-1553 (1992).
- 3. Srivastava, I.K., Rottenberg, H., and Vaidya, A.B. J. Biol. Chem. 272(7), 3961-3966 (1997).
- 4. Rijpma, S.R., van den Heuvel, J.J., van der Velden, M., et al. Malar. J. 13, 359 (2014).
- 5. Romand, S., Pudney, M., and Derouin, F. Antimicrob. Agents Chemother. 37(11), 2371-2378 (1993).

WARNING THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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