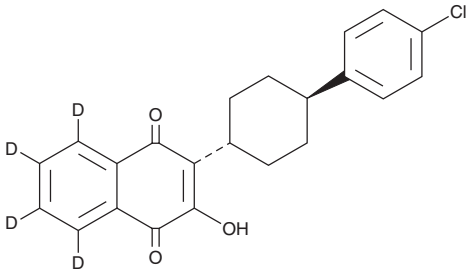
PRODUCT INFORMATION

Atovaquone-d_4

Item No. 28491

CAS Registry No.:	2070015-14-2
Formal Name:	2-[*trans*-4-(4-chlorophenyl)cyclohexyl]-3-hydroxy-1,4-naphthalenedione-5,6,7,8-d_4
MF:	$C_{22}H_{15}ClD_4O_3$
FW:	370.9
Chemical Purity:	≥98% (Atovaquone)
Deuterium Incorporation:	≥99% deuterated forms (d_1-d_4); ≤1% d_0
Supplied as:	A solid
Storage:	-20°C
Stability:	≥4 years



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

Laboratory Procedures

Atovaquone-d_4 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_4 is supplied as a solid. A stock solution may be made by dissolving the atovaquone-d_4 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 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.

References

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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).

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