

Product Name: Atovaquone

Catalog No.: 6358

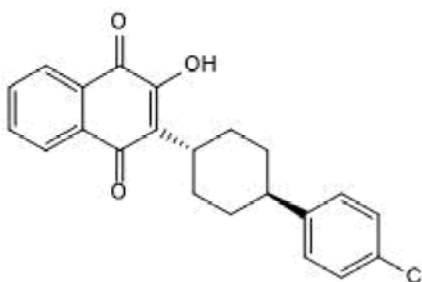
Batch No.: 1

CAS Number: 95233-18-4

IUPAC Name: 2-[*trans*-4-(4-Chlorophenyl)cyclohexyl]-3-hydroxy-1,4-naphthalenedione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₁₉ClO₃
Batch Molecular Weight: 366.84
Physical Appearance: Orange solid
Solubility: DMSO to 20 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	72.03	5.22	
Found	72.11	5.16	

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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IUPAC Name: 2-[*trans*-4-(4-Chlorophenyl)cyclohexyl]-3-hydroxy-1,4-naphthalenedione

Description:

Broad spectrum antiparasitic and antipneumocystic compound. Inhibits bc₁ complex (complex III) of mitochondrial electron transport chain (EC₅₀ = 0.26 μM), causing cell death in *Plasmodium yoelii* infected erythrocytes. Also inhibits DHODH. Also exhibits anti-MERS-CoV activity in Vero cells in vitro (IC₅₀ = 0.72 μM).

Physical and Chemical Properties:

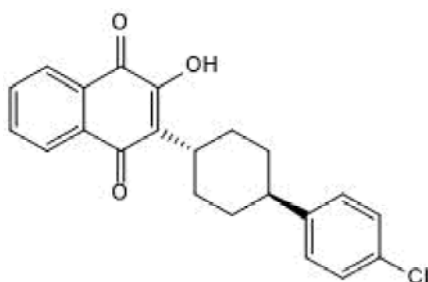
Batch Molecular Formula: C₂₂H₁₉ClO₃

Batch Molecular Weight: 366.84

Physical Appearance: Orange solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 20 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Ko et al (2020) Screening of FDA-approved drugs using a MERS-CoV clinical isolate from South Korea identifies potential therapeutic options for COVID-19. *BioRxiv* - Paper not yet peer reviewed.

Srivastava et al (1997) Atovaquone, a broad spectrum antiparasitic drug, collapses mitochondrial membrane potential in a malarial parasite. *J.Biol.Chem.* **272** 3961. PMID: 9020100.

Hughes et al (1990) Efficacy of a hydroxynaphthoquinone, 566C80, in experimental *Pneumocystis carinii* pneumonitis. *Antimicrob.Agents Chemother.* **34** 225. PMID: 2327770 .

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