

Thymohydroquinone

Chemical Properties

CAS No. :	2217-60-9
Formula:	C10H14O2
Molecular Weight:	166.217
Storage:	Powder: -20°C for 3 years In solvent: -80°C for 1 year Actual storage temperature shall be subject to the COA.

Biological Description

Description	Thymohydroquinone (Thymoquinol) is a monoterpenoid phenolic compound found in thyme, oregano, and other plants in the labiaceae family. Thymohydroquinone inhibits cancer cell growth, reduces oxidative stress and modulates inflammatory responses, scoured 2, 2-diphenyl-1-PicrylHydrazyl radicals in a cell-free assay (IC50 = 2.4 µg/ml), In the oxygen radical absorption capacity (ORAC) test at concentrations of 1.6 to 6.4 µg/ml, Its Trolox value was 2.6. Thymus hydroquinone inhibited the growth of A2780, OVCAR-8 and CIS-A2780 ovarian cancer cells (IC50 were 3.1, 8.9 and 9.8 µM, respectively) and human ovarian immortalized epithelial cells (IC50 = 14 µM). It also inhibited Plasmodium falciparum in vitro (IC50 = 15.9 µM).
Targets(IC50)	Antioxidant, Reactive Oxygen Species, ROS
In vitro	Thymohydroquinone, a quinone compound derived from Nigella sativa seeds, exhibits a wide range of biological activities. It demonstrates potent scavenging activity against DPPH free radicals in a cell-free assay (IC50 = 2.4 µg/ml). In addition, thymohydroquinone exhibits a Trolox equivalent value of 2.6 in an oxygen radical absorbance capacity (ORAC) assay, when tested at concentrations ranging from 1.6 to 6.4 µg/ml. [1] Thymohydroquinone inhibits the growth of A2780, OVCAR-8, and CIS-A2780 ovarian cancer cells (IC50s = 3.1, 8.9, and 9.8 µM, respectively), as well as immortalized human ovarian epithelial cells (IC50 = 14 µM). ² It is also active against P. falciparum in vitro (IC50 = 15.9 µM).[2]
In vivo	In vivo evaluation of the antitumor efficacy of Thymohydroquinone (THQ) was conducted using two murine tumor models, namely fibrosarcoma (FsaR) and squamous cell carcinoma (SCC VII). The antitumor effect of THQ was assessed by comparing the tumor growth kinetics between animals treated with four intratumoral injections of THQ at a dose of 5 mg/kg and control animals. In the in vitro study, THQ exhibited statistically significant cytotoxic activity (p < 0.01), which was dose-dependent. Moreover, the cytotoxic activity was more pronounced against tumor cells compared to L929 fibroblasts. The in vivo evaluation of THQ's antitumor activities resulted in a tumor growth inhibition (TGI) of 52%, and this effect was statistically significant (p < 0.05).[3]

Solubility Information

A DRUG SCREENING EXPERT

Solubility	Ethanol:PBS (pH 7.2) (1:9): 0.10 mg/mL (0.60 mM),Sonication is recommended. DMSO: 0.90 mg/mL (5.41 mM),Sonication is recommended. Ethanol: 1.80 mg/mL (10.83 mM),Sonication is recommended. DMF: 1.00 mg/mL (6.02 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	6.0161 mL	30.0806 mL	60.1612 mL
5 mM	1.2032 mL	6.0161 mL	12.0322 mL
10 mM	0.6016 mL	3.0081 mL	6.0161 mL
50 mM	0.1203 mL	0.6016 mL	1.2032 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Tesarova H, et al. Determination of oxygen radical absorbance capacity of black cummin (*Nigella sativa*) seed quinone compounds. *Nat Prod Commun.* 2011;6(2):213-216.

Johnson-Ajinwo OR, et al. The synthesis and evaluation of thymoquinone analogues as anti-ovarian cancer and antimalarial agents. *Bioorg Med Chem Lett.* 2018;28(7):1219-1222.

Ivankovic S, et al. The antitumor activity of thymoquinone and thymohydroquinone in vitro and in vivo. *Exp Oncol.* 2006;28(3):220-224.

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