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## Original Article

# An investigation of the olive phenols activity as a natural medicine

Q6 Faik Gökalp

Kırkkale University, Faculty of Education, Science Education, Yahşihan, Kırkkale, Turkey

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## ABSTRACT

The natural antioxidants of olive oil have phenolic structure and their activities are related to the formation of stable derivatives. In this study, the single components of the phenolic fraction of olive oil (1,4-hydroquinone, Semiquinone and 1,4-benzoquinone) have been studied as theoretical by using DFT (Density functional Theory). The behaviors of phenolic compounds of olive against to the alkyl peroxy radicals were investigated. Our data show that 1,4-benzoquinone is the best electron transfer agent in primary metabolic processes to human life. The frontier orbital gap, namely HOMO (highest occupied molecular orbital) –LUMO (lowest unoccupied molecular orbital) gap is the smallest for 1,4-benzoquinone. Hence, it is more stable than the others in blood. The natural phenolic compound's mechanism of many plants can be explained by using DFT method without consuming time and money. In this study, we have indicated the behaviors of natural antioxidants of olive oil's single components phenolic structure in blood phase.

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## 1. Introduction

Olive phenols have been studied to indicate healthy effects recently [1–4]. The chemical composition of EVOO and the phenolic compounds of it were effective to decrease the risk of cardiovascular disease [4]. Furthermore, some studies related to the Olive phenols showed that the daily consumption of it was too beneficial to be healthy for human because of the reduction in the peroxidation of blood lipids due to having phenolic functional groups. The most important antioxidants in olive were lipophilic and hydrophilic phenols [7], and the other effective structures such as carotenoids.

Phenolic acids, phenolic alcohols, hydroxy-isochromans, flavonoids, lignans and secoiridoids were effective phenolic

compounds in these olive oils [1,4]. Phenolic acids, vanillic, syringic, p-coumaric, o-coumaric, protocatechuic, sinapic, p-Q1 hydroxybenzoic and gallic acid were the initially discovered phenolic compounds in olive oil [7,8].

Antioxidants, were the mainly part of olive oil because of their biological activity effecting oxidation processes. The phenolic compounds of olive acted as chain breakers by donating radical hydrogen to alkylperoxyl radicals, which were produced by lipid oxidation. The formation of stable derivatives of olive phenols were given in Fig. 1 [4].

The reaction mechanism of 1,4-hydroquinone against the free radical as antioxidant could be explained in Fig. 2 [5].

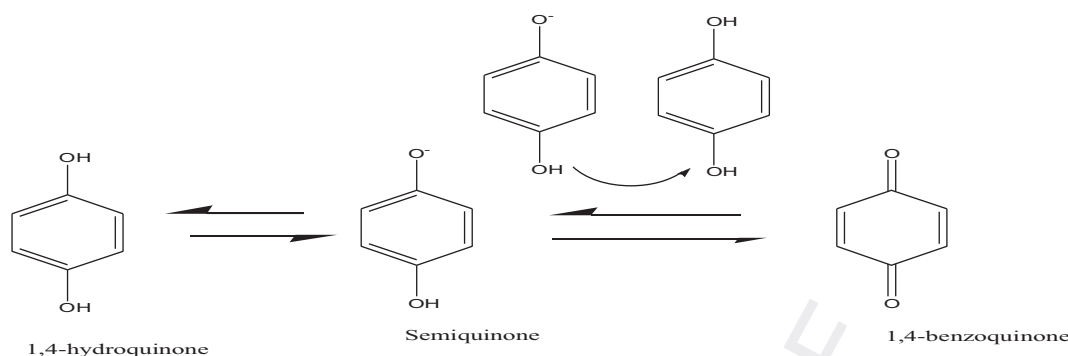
1,4-hydroquinone, Semiquinone and 1,4-benzoquinone's electron transfer mechanism that allows the formation of the stable free radicals is given in Fig. 3 [6].

E-mail address: [akgokalp@gmail.com](mailto:akgokalp@gmail.com).

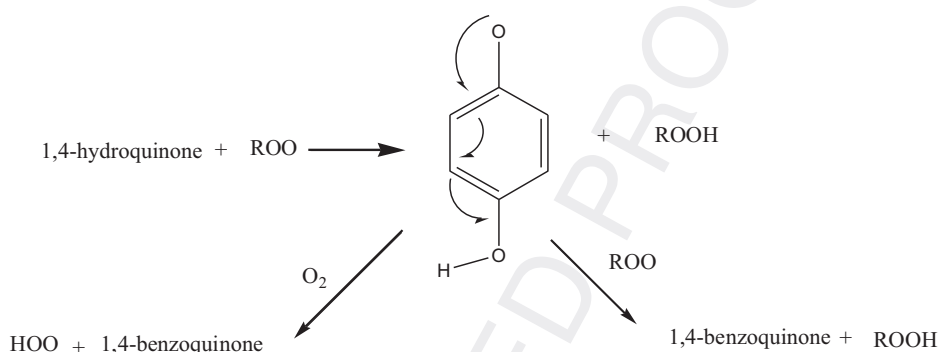
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**Fig. 1 – The mechanism of the antioxidant activity of Olive phenols.**



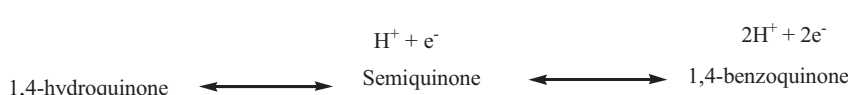
**Fig. 2 – The reaction mechanism of 1,4-hydroquinone against the free radical as antioxidant.**

The cananga tree alkaloid sampangine had been investigated for having antimicrobial and antitumor potential effects. The biological activities formed as the reduction of cellular oxygen, the induction of reactive oxygen species (ROS) in vivo [9]. “Ubiquinone was possible that this compound was reduced to more reactive Semiquinone form by mitochondria then readily reduces oxygen to superoxide. In support of this idea, ascorbate, an electron donor for a variety of compounds. For the heme biosynthesis can be coupled to the mitochondrial electron transport chain for energy production, oxidative stress disregulates heme production, ROS induced by the herbicide paraquat disrupts heme biosynthesis, and ROS suppresses uroporphyrinogen III synthase gene expression. Redox cycling appears responsible for the observed immediate increase of cellular oxygen consumption, but defects in heme biosynthesis may disrupt an array of biochemical processes. ROS-mediated side effects and toxicity may significantly limit the clinical potential of sampangine and its analogs as antifungal and antitumor agents” [9].

There were two major groups as determining antioxidant capacity. One of them is single electron transfer and the other is hydrogen atom transfer reaction. The main important method for single electron transfer is the Trolox equivalent

antioxidant capacity [10]. The oxygen radical absorbance capacity is the most applied method for hydrogen atom transfer reaction. Phenolic compounds are acted as effective radical chain-breaking antioxidants by the hydrogen atom transfer reaction [11,12]. With this mechanism, it is effected to the alkylperoxyl radicals, formed during the initiation step of lipid oxidation. In this step phenolics groups play important role as strong antioxidant [13] correlated to the total phenolics of it [10].

The risk of atherosclerosis may be decreased by the consumption of olive oil having a lot of phenolic compounds by decreasing inflammation and improving the antioxidant profile in the vascular endothelium [15]. Moreover, the high concentration of phenolic compounds have postprandial anti-inflammatory effects and decreases the gene expression of genes related to inflammation and oxidative stress [15,16]. “It may reduce the risk of developing atherosclerosis in metabolic syndrome patients by decreasing inflammation and improving the antioxidant profile in the vascular endothelium. These results provide further evidence of the reduction in the risk factors for developing cardiovascular disease observed in Mediterranean regions, where the main source of dietary fat is virgin olive oil” [14].



**Fig. 3 – Electron transfer mechanism of 4-hydroquinone, Semiquinone and 1,4-benzoquinone.**

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