

LEMON ESSENTIAL OIL: MOLECULAR DOCKING ANALYSIS AND INVESTIGATION OF THE ANTIBACTERIAL AND ANTIOXIDANT ACTIVITIES

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Abstract

Lemon essential oil is widely used in both commercial and domestic products. It consists of a mixture of volatile liposoluble compounds responsible for its characteristic fragrance and bioactive properties such as antimicrobial, anti-inflammatory and antioxidant activity. The importance of lemon essential oil is even more significant when considering the increasing interest in natural products that offer positive effects on human health. In this study, lemon grown domestically in the area of Mostar, in the south of Bosnia and Herzegovina, was used. The essential oil was extracted from the peel using the hydrodistillation method in a Clevenger apparatus, which is completely environmentally safe. The composition of the resulting essential oil was analyzed by gas chromatography coupled with mass spectrometry (GC-MS). GC-MS identified the presence of 18 constituents, of which the most abundant components in lemon essential oil were monoterpene olefins with a content of 95,97%. D-limonene was the main component, with a content of 63,48%, followed by β -pinene and γ -terpinene with content of 13,3% and 10,42% respectively. The antimicrobial activity of the essential oil was tested, demonstrating effectiveness against *Staphylococcus aureus* with a clear inhibitory zone in a diameter of 21 mm, which is considered as bacterial sensitivity to the testing substance. Molecular docking analysis revealed that all three principal compounds were able to bind to the DNA gyrase enzyme. Among them, d-limonene exhibited the lowest binding energy (-5.9 kcal/mol), which was comparable to that of ciprofloxacin (-5.9 kcal/mol), a well-known DNA gyrase inhibitor. The lemon essential oil also exhibited significant DPPH radical scavenging activity, highlighting its potential as an antioxidant. The results indicate that both the concentration and incubation time affect the antioxidant capacity of the essential oil. Our study results indicate that the antioxidant activity of lemon essential oil increases as the concentration rises, both after 20 minutes and 60 minutes of incubation. At the highest concentration of 150 mg/mL, LEO had a good DPPH free radical scavenging rate (76.0% for 20 min incubation time; 82.1% for 60 min incubation time).

Keywords: Essential oil, Limonene, Molecular docking, *S. aureus*, Antioxidant