

Antibacterial Efficacy and Molecular Docking of Leaf Extract of *Laurus nobilis* L Against some Isolated Pathogenic UTI Bacteria

Amani Abd Al-Ridha Al-Abdullah¹, Ekhlal Qanber Jasim² and Munther Abduljaleel Muhammad-Ali³

^{1,2}Department of Pathological Analyses, College of Science, Basrah University, Basrah, Iraq.

³Department of Ecology, College of Science, University of Basrah, Basrah, Iraq.

³E-mail: munther.ali@uobasrah.edu.iq

Abstract. The objective of the current study was to analyze the chemical compositions and antibacterial properties of *Laurus nobilis*. The bacterial strain was isolated from urine sample of female patients have urinary tract infection in Al-Basrah Teaching Hospital. Two solvents (hot and cold aqueous and ethanol) were used to extract the dried leaves of *L. nobilis*. While there were differences in the inhibition zones that solvent extracts demonstrated against bacterial pathogens, all of them significantly inhibited pathogens. The diameters of the inhibition zones on *Staphylococcus aureus* where the alcoholic extract was in the range of 17-29 mm, 22-28 mm for hot water and 12-14 mm for cold aqueous extract. The diameters of the inhibition zones on *Klebsiella pneumoniae* for alcoholic extract were 18-20 mm, 19-21.5 mm for hot aqueous extract and 12-17 mm for cold water extract. The GC-MS analysis demonstrated the presence of different phytochemical compounds in the extract of *Laurus nobilis*. A total of 60 compounds were identified, for ethanolic extract, tris (2-methylenecyclopropyl)methanol, (3aS,6aR,9aR,9bS)-3,6,9-trimethylenedecahydroazuleno[4,5-b]furan-2(3H)-one and (3aS,6aR,9aR,9bS)-6-methyl-3,9-dimethylene-3a,4,6a,7,8,9,9a,9b-octahydroazuleno[4,5-b]furan-2(3H)-one were the major compounds with percentage values 9.64%, 8.86% and 7.43%, respectively. For hot water extract, the major three compounds were 5-(hydroxymethyl)furan-2-carbaldehyde 11.64%, 2-methyl-5-nitro-2H-1,2,3-triazol-4-amine 8.39% and tris(2-methylenecyclopropyl)methanol 6.81%. Whereas, for cold water extract, the major compounds were n-Hexadecanoic acid 26.05%, Bis(2-ethylhexyl) phthalate 22.94% and Octadecanoic acid 8.25%. Molecular docking showed that these nine major compounds had an excellent binding affinity -4.25 to -8.56 kcal/mol against *S. aureus* using protein 1JJJ. The binding affinity of these compounds against *K. pneumoniae* (protein 6PIB) were in the range -4.03 to -8.22 kcal/mol.

Keywords. Plant extract, Antibacterial activity, Molecular docking, GC-MS instrument, Phytochemical analysis.

1. Introduction

A variety of biological activity, including antibacterial, anti-inflammatory, and antioxidant ones, have been identified for extracts extracted from medicinal plants [1]. The antimicrobial compounds from

