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Research Article
Assessment of Sesame and Sweet Almond Oils Efficacy Against Food-Borne and Human Illness Microorganisms with Molecular Docking Study

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Abstract

Background and Objective: Human and food-born pathogenic microorganism's resistance to antibiotics has been a significant problem in the last decades. The main objective of this study was to assess the antimicrobial activities of sesame and sweet almond essential oils (EOs) alone and in dual combinations. **Materials and Methods:** The sesame oil was extracted from the heated sesame seeds at 35°C utilizing the cold pressing procedure, while almond oil was extracted at temperatures ranging from 50 to 70°C. Chemical constituents of the used EOs were determined via Gas Chromatography-Mass Spectrometry (GC-MS), antimicrobial activity was detected using well-diffusion method, while antioxidant potential was assessed using 1,1-Diphenyl-2-Picrylhydrazyl (DPPH) method. **Results:** The GC-MS analysis indicated that sesamin, sesamolin, β-sitosterol and campesterol represent the main components of sesame essential oil (EO), while β-sitosterol, glycidol oleate and vitamin E represent the main components of sweet almond EO. Some compounds such as 3-methylpentane, dodecane, (Z)-2-decenal; undec-2-enal, tetradecane, hexadecane, docosane, dihydrodehydrocostus lactone, α-tocopherol and squalene were detected in both sesame and sweet almond EOs. Almond EO was effective against *Enterococcus faecalis*, *Staphylococcus aureus*, *Escherichia coli* and *Klebsiella pneumoniae* compared to sesame EO. Less IC_{50} value (28.19 µg/mL) of sweet almond EO than the IC_{50} value (60.5 µg/mL) of sesame EO for DPPH scavenging activity was recorded. Molecular docking interaction indicated sesamin and β-sitosterol have enough potential to inhibit the proteins of *K. pneumoniae* (PDB: 8FFK) and *E. faecalis* (PDB: 2OMK). **Conclusion:** The EOs of sesame and sweet almonds have the potential to inhibit the tested microorganism *in vitro* and *in silico*.

Key words: Antimicrobial activity, sesame oil, sweet almond oil, antioxidant activity, microorganism, molecular docking

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INTRODUCTION

Finding new natural compounds that are effective against pathogenic microorganisms is necessary. Numerous plant-based natural extracts have been studied for their potential as medicines for a range of illnesses. Scientists from a variety of fields are studying plants to find molecules that can combat microbial infections. The problem of drug resistance in microorganisms today is significant. Consequently, plant-based medicines are seen as secure alternatives to synthetic drugs. Particularly, the ability of plant extracts and essential oils (EOs) to act as antimicrobial agents has served as the foundation for a wide range of applications, such as food preservation, pharmaceuticals, alternative medicine and therapies[1-6]. Various EOs, a recently identified non-antibiotic substance, as well as the chemicals that make up these substances, have demonstrated strong combative potential against drug-resistant pathogens[7,8].

The EOs are a diverse group of phytochemicals generated by medicinal and fragrant plants for a variety of protective purposes. Since the beginning of time, they have been utilised as both home cures and in conventional medicine[9]. The EOs are recognized to have several biological activities such as antibacterial, antifungal and anti-inflammatory effects. Okoh *et al.*[10] has demonstrated the potential of EOs ability to scavenge free radicals as well as their function in the prevention and treatment of infectious disorders. The fact that EOs break down fast, leaves no hazardous residues and are relatively non-toxic to humans also makes them environmentally beneficial[11].

Sesame EO is one of the most significant natural EOs which has been extensively utilized for cooking fish and as a brilliant salad EO in Japan. According to Namiki[12], sesame EO is a vital component in Ayurvedic remedies in India and is utilized to raise energy and avoid aging in Chinese medicine. Sesame EO includes sesaminollignan, sesamolin and sesamin fractions, which are important in preventing diseases including cancer, hypertension, hypercholesterolemia and ageing. Sesame EO may also be useful in the treatment of illnesses linked to oxidative stress, such as Alzheimer's disease, chronic renal failure, atherosclerosis, rheumatoid arthritis and neurological disorders[13]. Sesamol, which possesses stronger antioxidant and antibacterial capabilities than its parent molecule, is also present in greater concentrations in sesame EO[14]. Sallam *et al.*[15] reported that sesame EO decline in the counts of some food-borne microorganisms including *E. coli*, *Staphylococcus aureus*, *Listeria monocytogenes* and *Salmonella enterica* were meatballs, therefore, they Sallam *et al.*[15] suggest that this EO may use as a food additive for limiting microbial proliferation and prolonging its shelf life throughout storage.

Bitter almond EO and sweet almond EO are the two varieties of almond EO. Every variety differs in its characteristics and applications. The *Prunus amygdalus dulcis* (almond) tree's fruit is used as a source of sweet almond EO, while *P. amygdalus amara* represents the source of bitter almonds. In the present investigation, sweet almond EO was applied as an antimicrobial and antioxidant agent. The *P. amygdalus dulcis* (almond trees) are a native species of Western Asia. Almond trees are currently grown extensively abroad in other regions. The almond tree replaces other nut trees in the Mediterranean regions as a result of its rustic nature and ability to survive in dry climates and droughts[16]. The utilization of sweet almond EO has a variety of applications including the food and cosmetic industry as well as alternative medicine to cover numerous health benefits such as anti-inflammatory, immunity-boosting, antihepatotoxicity and modulatory effects on inflammation[17]. Moreover, the almond EO displays a rich lipid profile, 63.42-78.03% of monounsaturated and 14.41-27.01% of polyunsaturated fatty acids[18]. It also presents a good dietary supply of antioxidants, like flavonoids, tocopherols and polyphenols[19]. Almond EO is applied to minimize the level of lipase in blood serum[20], it is also utilized as a soothing treatment of skin allergies and to treat minor cuts and wounds. Other biological utilization such as anticancer[21], antibacterial against *Bacillus subtilis*, *Staphylococcus aureus* and fungi[22] and anti-inflammatory[23] activities were associated with almond EO.

One of the most popular techniques used in the computer-aided drug design process to find potential inhibitors against different infections is molecular docking. With this ground-breaking approach, the expensive, time-consuming and energy-intensive drug discovery process may be greatly reduced when promising therapeutic compounds are found in huge drug libraries[24,25]. The advantages of these oils in antimicrobial activity, avoid the use of chemical antibiotics that have side effects on body organs, these oils have markedly different aromas and are used in other therapies and are incorporated in dermo-cosmetics, these oils increase peroxisomal fatty acid oxidation and hepatic mitochondrial rate. Moreover, sesame oil raises plasma γ-tocopherol and improves the activity of vitamin E, which is supposed to inhibit cancer and minimize heart disease. Therefore, the current study aimed to evaluate the antimicrobial potential of sesame and sweet almond EOs and their mixture against some food-born and human pathogenic microorganisms, as well as their antioxidant activity.

MATERIALS AND METHODS

Study area: Some experiments were carried out in the Microbiology Laboratory, Science College of Jazan University, Saudi Arabia, while other experiments were carried out in the Microbiology Laboratory, Science College of Al-Azhar University, Egypt, from March, 2023 to October, 2023.

Chemicals and essential oils: The used chemicals in the recent scientific paper were in analytical grade level and were obtained from Sigma-Aldrich (St. Louis, Missouri) including Dimethyl Sulfoxide (DMSO), 2,2-Diphenyl-1-Picrylhydrazyl (DPPH), ascorbic acid, Mueller-Hinton Agar, Sabouraud Dextrose Agar and solvents. Two EOs including sesame and sweet almond were obtained from Albadawia Company for extraction of natural Oils, Mansoura, Dakahlia, Egypt. The description of the oil indicated that the sesame oil was extracted from the heated sesame seeds at 35°C utilizing the cold pressing procedure, with a moisture content of 4.7%, crude fiber of 2.87% and ash content of 3.21%. While almond oil was extracted at temperatures ranging from 50 to 70°C, with a moisture content of 4.5%, crude fiber of 3.2% and ash content of 5.11%. Standard two compounds including sesamin and β-sitosterol were obtained from Sigma-Aldrich, (St. Louis, Missouri, USA).

Essential oils analysis by Gas Chromatography-Mass Spectrometry (GC-MS): Thermo Scientific's Trace GC1310-ISQ mass spectrometer and the TG-5MS direct capillary column (30 m×0.25 mm×0.25 µm film thickness) (THERMO Scientific Corp., Dani, Rome, Italy) were used to analyze the constituents of tested EOs. The temperature of the column oven was first maintained at 50°C, then raised to 230°C by 5°C/min and held for 2 min and then increased to 290°C by 30°C/min (as a final temperature) and kept for 2 min. Helium was employed as the carrier gas, with a constant flow rate of 1 mL/min and temperatures of the injector were maintained at 260°C and the MS transfer line was maintained at 250°C. The solvent delay was 3 min and 1 µL of diluted EOs were automatically injected utilizing Autosampler AS1300 combined with GC in the split approach. Full mass spectra covering the m/z range of 40-1000 were collected at 70 eV ionization voltages. The temperature of the ion source was fixed at 200°C. The EOs constituents were recognized via comparison of their mass spectra and retention times with those of NIST 11 and WILEY 09 mass spectral databases. The main constituents (only two compounds including sesamin and β-sitosterol) were identified by comparing their mass spectra (ranging from 50-600 m/z) with those of authentic constituents which were injected in GC-MS to confirm their identification.

Antimicrobial activities of essential oils samples: *Bacillus subtilis* (ATCC 6633), *Enterococcus faecalis* (ATCC 10541), *Staphylococcus aureus* (ATTC25923), *Escherichia coli* (ATCC 25955), *Klebsiella pneumoniae* (ATCC13883), *Salmonella typhi* (ATCC 6539) *Candida albicans* (ATCC 10231) and *Aspergillus niger* were the tested microorganisms. The well-diffusion manner was used to assess the antibacterial activity of EOs. The susceptibility of tested microorganisms to different EOs was tested using Mueller-Hinton Agar plates for bacteria and Sabouraud Dextrose Agar (SDA) for *A. niger* and *C. albicans*. A sterile inoculated needle was used to uniformly disperse the 24 hrs old microbial suspension across each plate. After the solidification of media, via a 6 mm sterile cork-borer, agar plugs were cut agar medium and each plug was filled with 10 µL of used EOs. The bacterial inoculated plates were incubated at 37°C for 1 day, while fungal inoculated plates were incubated at 30°C for 4 days. At the end of the incubation period, the inhibitory zones' diameter (mm) was measured. Considering the microorganisms' susceptibility to antibiotics, the following was employed as a positive control: Ketoconazole (100 µg/mL) as antifungal and gentamicin (4 µg/mL) as antibiotic[26].

Minimum inhibitory concentration and minimum bactericidal concentration tests: With a little modification, the broth micro-dilution technique was used to establish the minimum inhibitory concentration (MIC) of used EOs for *C. albicans* and bacteria. Using Muller Hinton broth, a two-fold dilution series of EO was created in the range of 1.95-1000 µL/mL. According to the instructions, microbial suspension was injected into each tube holding the dilution. For 24 hrs, tubes were incubated at 37°C for bacteria and at 28±2°C for *C. albicans* for 24 and 48 hrs, respectively. Media without the EOs served as the positive controls. The minimal inhibitory concentration was defined as the lowest concentration at which there was no discernible growth (turbidity). The 96-well microtiter plate was serially diluted with the tested EOs for detection of their minimum bactericidal concentration (MBC) via micro dilution assay, which was then inoculated with tested microorganisms (1×10^6 CFU/mL) and then subsequently incubated at 37°C for 24 hrs and at 28°C for 48 hrs for bacteria and *C. albicans*, respectively. By measuring the absorbance at 660 nm using a microtiter plate reader (SciTech Global Co. Ltd., Jinan City,

Shandong Province, China), bacterial growth was measured. Transferring 5 mL of the contents onto Muller-Hinton Agar (MHA) plates and incubating under identical circumstances allowed the wells with >90% inhibition to be taken into consideration. In the current investigation, the MBC was defined as the lowest concentration of the EOs required to kill the tested bacteria. As a check, well-known antibiotics were used. To further evaluate the bactericidal efficacy of tested EOs, MBC/MIC index was computed[27].

Antioxidant activity: According to the approach employed by Al-Rajhi and Abdel Ghany[7] with slight modification, the capacity of sesame, sweet almond EOs and its mixture to scavenge free radicals were assessed using 2,2-Diphenyl-1-Picrylhydrazyl (DPPH) as a synthetic free radical agent. The reaction mixture contained 500 µL of each tested sample, 50 mL of ethyl alcohol and DPPH dissolved in 99.5% ethanol as 0.02%, w/v. The mixture was forcefully agitated and allowed to incubate in the dark. A spectrophotometer (Canfort Laboratory and Education Supplies Co. Ltd., Jinan, China) was used to measure the absorbance at 517 nm after 30 min of incubation. The activity of DPPH radical scavenging was determined as follows:

$$\text{Radical scavenging activity (\%)} = \frac{\text{Absorbance at control} - \text{Absorbance at EO treatment}}{\text{Absorbance at blank}} \times 100$$

The value of IC_{50} of EO is defined as the quantity of EO required to inhibit DPPH radical formation by 50%. Ascorbic acid as a synthetic antioxidant was applied as a positive control[5].

Experiment of molecular docking: The goal of the molecular docking experiments was to completely comprehend the molecular interactions between the drugs under study and the active sites of the targets. Molecular operating environment (MOE) software was used to conduct the docking research on Dell Core i7, a 1.99 GHz, machine with a Microsoft Windows 10 operating system. The targets' crystal structures were obtained using the Protein Data Bank (PDB)[24] which is a database of proteins: *Enterococcus faecalis* protein (PDB: 2OMK) and *K. pneumoniae* protein (PDB: 8FFK). After eliminating the proteins' binding ligand, cofactors and bound water molecules, hydrogen atoms were added. The binding affinity was assessed using the binding free energy and hydrogen bonds that had formed between proteins and molecules. Using RMSD (Root Mean Square Deviation) values, the ideal binding pose was found. Via the study of the structure of 2OMK protein, a rich electron density was recorded at pyrithiamine pyrophosphate that bound to the enzyme active site. Moreover, this structure also offers a complete perception of the binding pocket for the nucleoside triphosphate and therefore permits a detailed understanding of the catalytic requirements for catalysis of this protein. On the other hand, the structure of 8FFK allows us to understand the action mechanism for drug recognition. Residues actively participated in this structure molecule at the entrance drug-binding site. Therefore, the exact composition of these entrance residues may play a critical role in substrate specificity and selectivity.

Statistical analysis: The achieved results were studied through SPSS version 15.0 (SPSS Inc. Chicago, Illinois, USA). The values were presented as the means of three replicates analysis for standard deviation (±SD) calculation.

RESULTS AND DISCUSSION

Essential oils constituent analysis: Although, for numerous years, pluck EOs have been exploited in traditional medicinal applications, during the last decade, EO constituents began to be explored and applied in pharmaceutics as weapons for the control and management of various infections. In the present study, sesame and sweet almond EOs were investigated by Gas Chromatography/Mass Spectrometry (GC/MS) as well as their antimicrobial and antioxidant activities besides molecular docking interaction of the EO's main constituents with target ligands of some tested microorganisms. The GC/MS analysis of sesame and sweet almond EOs (Fig. 1-2) reflected the presence of several constituents associated with phenolic steroids, fatty acids, terpenoids, flavonoids and different kinds of ester compounds. Sesame EO was rich in 76 different compounds with different molecular weights and molecular formula (Table 1). According to area (%), (+)-sesamin was the main prevailed detected compound in sesame EO with area 36.59%, followed by sesamolin (20.04%), β-sitosterol (11.66%), campesterol (4.01%), butyl 9,12-octadecadienoate (2.52%), α-tocopherol (2.77%), stigmasterol (2.02%), octadecanoic acid (1.85%), elaidic acid, methyl ester (1.70%) and glycidyl palmitate (1.58%). The area (%) of the rest detected compounds in sesame EO was less than 1%. Tocotrienol was detected in sesame EO according to Weijian *et al.*[28]. Sesamin and sesamolin as sesame lignin's in the current finding was the major content of sesame EO, this result matches with other investigations[29,30]. Numerous biological utilities like anticancer, antihypertensive and minimization of cholesterol, antioxidant and antibacterial[31].

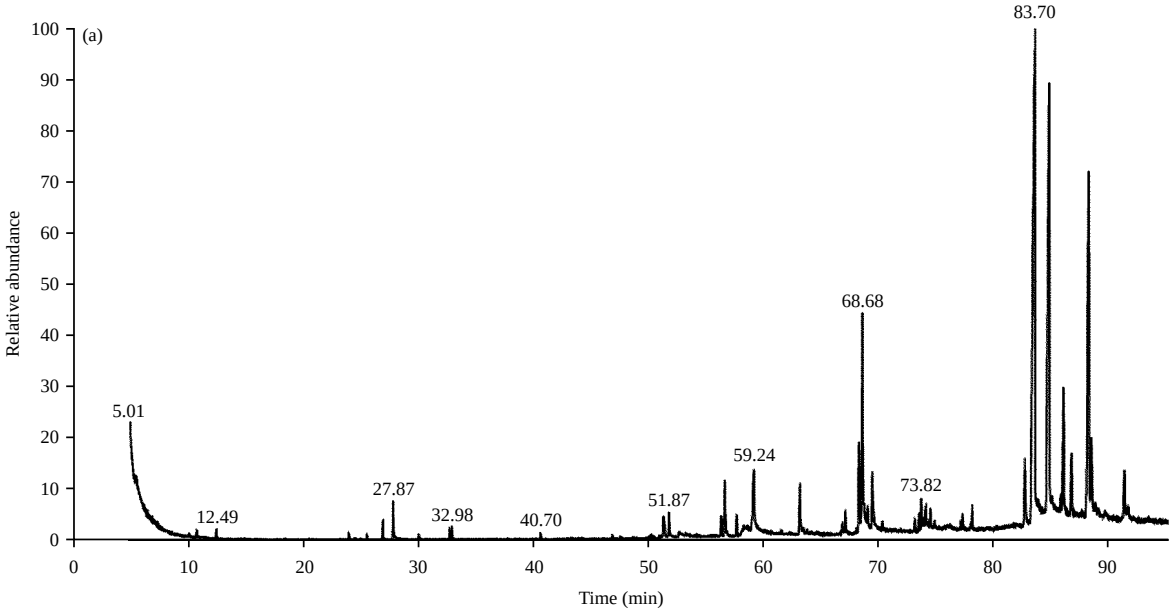

Fig. 1: GC/MS analysis chromatogram of sesame EO

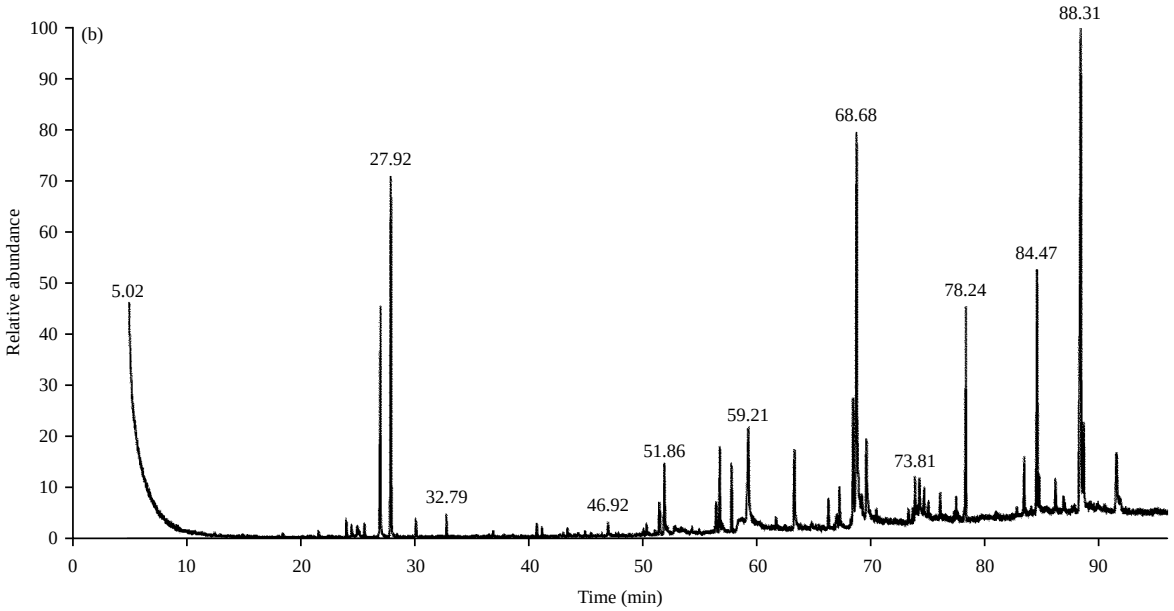

Fig. 2: GC/MS analysis chromatogram of sweet almond EO

Table 1: Detected volatile compounds in sesame EO by GC/MS analysis

Compound	Retention time	Area (%)	MF	MW
3-Methylpentane	5.02	0.07	C_6H_{14}	86
Isoleucine	5.38	0.04	$C_6H_{13}NO_2$	131
5,5-Dimethyl-1,3-diox-2-one	5.52	0.27	$C_6H_{10}O_3$	130
4-Methyl-2-propyl-1-pentanol	7.13	0.06	$C_9H_{20}O$	144
1-Propanol, 2,2-bis(methoxymethyl)-	10.12	0.13	$C_7H_{16}O_3$	148
(5E)-2,5-Dimethyl-1,5-heptadiene-3,4-diol	10.79	0.21	$C_9H_{16}O_2$	156
Pinkdpnbfyuwms-Uhfffaoysa-N	12.50	0.27	$C_{13}H_{22}O_4$	242
Dodecane	24.02	0.16	$C_{12}H_{26}$	170
Thymoquinone	24.54	0.06	$C_{10}H_{12}O_2$	164

Table 1: Continue

Compound	Retention time	Area (%)	MF	MW
(Z)-2-Decenal	25.59	0.11	$C_{10}H_{18}O$	154
2,4-Decadienal, (E,E)-	26.97	0.49	$C_{10}H_{16}O$	152
Undec-2-enal	30.11	0.14	$C_{11}H_{20}O$	168
Tetradecane	32.79	0.21	$C_{14}H_{30}$	198
1,2-Benzenedicarboxylic acid, dimethyl ester	32.98	0.33	$C_{10}H_{10}O_4$	194
Hexadecane	40.70	0.14	$C_{16}H_{34}$	226
2-Methylhexadecan-1-ol	43.38	0.05	$C_{17}H_{36}O$	256
Docosane	44.35	0.05	$C_{22}H_{46}$	310
Costunolide	46.93	0.10	$C_{15}H_{20}O_2$	232
2-cis-9-octadecenyloxyethanol	47.65	0.05	$C_{20}H_{40}O_2$	312
1-Chloro-7-heptadecyne	48.74	0.05	$C_{17}H_{31}Cl$	270
1-Acetyl-16-methoxyaspidospermidin-17-ol	50.10	0.06	$C_{22}H_{30}N_2O_3$	370
Dihydrodehydrocostus lactone	50.30	0.11	$C_{15}H_{20}O_2$	232
9-Hexadecenoic acid	50.52	0.05	$C_{16}H_{30}O_2$	254
2,2-Dideutero octadecanal	51.03	0.07	$C_{18}H_{34}D_2O$	270
Methyl 14-methylpentadecanoate	51.41	1.04	$C_{17}H_{34}O_2$	270
Dehydrocostus lactone	51.87	0.68	$C_{15}H_{18}O_2$	230
2,3-Dihydroxypropyl palmitate	52.72	0.15	$C_{19}H_{38}O_4$	330
9-Octadecenoic acid (Z)-	53.34	0.08	$C_{18}H_{34}O_2$	282
Ethyl octadecanoate	53.16	0.03	$C_{20}H_{40}O_2$	312
Tetraneurin-A-diol	54.27	0.07	$C_{15}H_{20}O_5$	280
7-Methyl-Z-tetradecen-1-ol acetate	55.92	0.07	$C_{17}H_{32}O_2$	268
Linoleic acid, methyl ester	56.40	0.15	$C_{19}H_{34}O_2$	294
Elaidic acid, methyl ester	56.72	1.70	$C_{19}H_{36}O_2$	296
10-Octadecenoic acid, methyl ester	56.40	0.02	$C_{19}H_{36}O_2$	296
Methyl stearate	57.75	0.60	$C_{19}H_{38}O_2$	298
Cis-Vaccenic acid	58.71	0.11	$C_{18}H_{34}O_2$	282
Octadecanoic acid	59.24	1.85	$C_{18}H_{36}O_2$	284
2-Hydroxy-1-[(palmitoyloxy) methyl]ethyl palmitate	61.64	0.13	$C_{35}H_{68}O_5$	568
Glycidol oleate	62.37	0.08	$C_{21}H_{38}O_3$	338
2,3-Dihydroxypropyl stearate	63.56	0.11	$C_{21}H_{42}O_4$	358
Dasycarpidan-1-methanol, acetate (ester)	63.88	0.09	$C_{20}H_{26}N_2O_2$	326
1-Heptatriacotanol	66.74	0.07	$C_{37}H_{76}O$	536
Linolein, 2-mono-	66.92	0.26	$C_{21}H_{38}O_4$	354
Glyceryl monooleate	67.20	0.60	$C_{21}H_{40}O_4$	356
Octadecanoic acid, 2-hydroxy-1,3-propanediyl di-ester	68.01	0.03	$C_{39}H_{76}O_5$	624
Octadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	68.17	0.15	$C_{21}H_{42}O_4$	358
Butyl 9,12-octadecadienoate	68.39	2.52	$C_{22}H_{40}O_2$	336
Glycidyl palmitate	69.54	1.58	$C_{19}H_{36}O_3$	312
1,2-Benzenedicarboxylic acid	70.43	0.24	$C_{24}H_{38}O_4$	390
Hydrocinnamic acid, o-[(1,2,3,4-tetrahydro-2-naphthyl)methyl]-	73.81	0.80	$C_{20}H_{22}O_2$	294
(Z,Z)-1,3-dioctadecenoyl glycerol	74.19	0.59	$C_{39}H_{72}O_5$	620
Tetrakis(1,1-dimethylethyl)-28-methoxyp entacyclo[19.3.1.1(3,7).1(9,13).1(15,19)] Octacosa-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecene-25,26,27-triol	76.00	0.06	$C_{45}H_{58}O_4$	662
2-Hydroxy-3-[(9E)-9-octadecenoyloxy]propyl(9E)-9-octadecenoate	76.29	0.09	$C_{39}H_{72}O_5$	620
Olean-12-ene-3,28-diol, (3 β)-	77.40	0.39	$C_{30}H_{50}O_2$	442
(22S,23S,25R)-3-ü-methoxy-16á,23:22,26-diepoxy-5 β-cholestane	78.12	0.16	$C_{28}H_{46}O_3$	430
Squalene	78.22	0.66	$C_{30}H_{50}$	410
6,8-Di-C-β-glucosylluteolin	79.64	0.05	$C_{27}H_{30}O_{16}$	610
3',4',7-trimethylquercetin	80.40	0.08	$C_{18}H_{16}O_7$	344
Ethyl iso-allocholate	80.70	0.04	$C_{26}H_{44}O_5$	436
α-tocopherol	82.81	2.27	$C_{28}H_{48}O_2$	416
(+)-Sesamin	83.69	36.59	$C_{20}H_{18}O_6$	354
Sesamolin	84.93	20.04	$C_{20}H_{18}O_7$	370
Ergosta-5,24(28)-dien-3 β-ol	85.92	0.40	$C_{28}H_{46}O$	398
Campesterol	86.17	4.01	$C_{28}H_{48}O$	400
Stigmasterol	86.86	2.02	$C_{29}H_{48}O$	412
β-sitosterol	88.37	11.66	$C_{29}H_{50}O$	414
(E)-24-propylidenecholesterol	88.61	2.14	$C_{30}H_{50}O$	426
9,10-secoergosta-5,7,10(19),22-tetraene-1,3,25-trio, (3 β,5Z,7E,22E)-	89.17	0.22	$C_{28}H_{44}O_3$	428
Testosterone cypionate	91.47	1.65	$C_{27}H_{40}O_3$	412
Flavone 4'-OH,5-OH,7-di-O-glucoside	91.78	0.38	$C_{27}H_{30}O_{15}$	594
Isochiapin B	93.50	0.08	$C_{19}H_{22}O_6$	346

Table 2 shows the 71 compounds that recognized in sweet almond EO at different retention times. The detected compounds were recognized at different area%, for instance, the main area was associated to β-sitosterol (17.83%), followed by glycidol oleate (12.48%), 2,4-decadienal, (E,E)-(11.63%), vitamin E (7.86%), squalene (6.24%), linolein, 2-mono-(4.18%), octadecanoic acid (3.29%), stigmasta-5,24(28)-dien-3á-ol, (Z)- (2.80%), 9-octadecenoic acid, methyl ester, (E)-(2.58%), dehydrocostuslactone (2.30%), cis-sitostenone (2.12%), methyl stearate (1.78%), (+)-sesamin (1.97%), glyceryl monooleate (1.27%), campesterol (1.26%) and 3-(methoxymethoxy)-2,3-dimethyl-1-undecene (1.30%). The rest of the other compounds were found at an area (%) of less than 1%. According to the obtained findings Zhao *et al.*[32], 44 compounds sweet identified in almond EO but methyl stearate, methyl oleate and methyl palmitate represent the main components in this EO. Via GC/MS analysis, methyl stearate; 9-octadecenoic acid (Z)-, methyl ester; hexadecanoic acid and methyl ester was recognized in sweet almond EO[33]. Banjanin *et al.*[34] indicated that sweet almond EO is mainly composed of unsaturated fatty acids as well as other phytoconstituents. In the present study, β-sitosterol represents the major constituent in almond-sweet EO, in another study Matthäus and Özcan[35] found that β-sitosterol followed by 5-avenasterol, campesterol, 5,24-stigmastadienol, stigmasterol, sitostanol and cholesterol represent main sterols in different samples almond EO. From GC/MS analysis, it is clear that certain compounds were detected in sesame and sweet almond EOs but at different retention times and with different levels of area (%). For example, 3-methylpentane, dodecane, (Z)-2-decenal, 2,4-decadienal (E,E)-, undec-2-enal, tetradecane, hexadecane, docosane, dihydrodehydrocostus lactone, 2-dideutero octadecanal, dehydrocostuslactone, 2,3-dihydroxypropyl palmitate, 9-octadecenoic acid (Z)-, glycidol oleate, isochiapin B, β-sitosterol, α-tocopherol and squalene were detected in both sesame and sweet almond EOs. Tir *et al.*[36] noticed the occurrence of a peak in the GC-MS chromatogram, which was identified as sesamin. This compound is among the constituents of sesame oil that give notable stability to the oil, besides it is responsible for numerous unique oil health properties. According to Czaplicki *et al.*[37], β-sitosterol and sesamin were recognized in sesame oil. Recently, GC-MS was used to identify the four tocopherols, eight phytosterols and 16 fatty acids in different samples of sesame oils[38]. According to Xue *et al.*[39], β-sitosterol was detected in sweet almond EO via GC-MS.

Antimicrobial activity of essential oils: Sesame and sweet almond EOs exhibited antimicrobial activities but with different levels of inhibitions (Table 3 and Fig. 3). More inhibition zones were observed using sweet almond EO than the inhibition zones using sesame EO against all tested bacteria and *C. albicans*. For example, inhibition zones of *E. faecalis*, *E. coli* and *S. typhi* were 24±0.2, 25±0.3 and 29±0.2 mm using sweet almond EO while it was 21±0.5, 22±0.4 and 27±0.4 mm using sesame oil. A mixture of sesame and sweet almond oils showed synergistic action toward *S. aureus*, *S. typhi* and *C. albicans*, while reflecting antagonistic potential against *B. subtilis*, *E. faecalis* and *K. pneumoniae*, where the effect of EOs mixture was better than the effect of each EO alone. Moreover, both EOs reflected more inhibitory potential against the most tested bacteria and *C. albicans* compared to the positive control (Ketoconazole/Gentamicin). Stored vegetables paste fortified with sesame EOs were repelled to spoilage fungi and bacteria[40]. Different levels of inhibition zones may depend on the type of test microorganism or the efficacy of the used EO, in this context, a previous report indicated that sesame EO exhibited excellent antibacterial activity against most but not all tested microorganisms by Zaki *et al.*[41], including *Acinetobacter* spp., *Pseudomonas aeruginosa*, *Enterobacter* spp., *E. coli*, *Staphylococcus* spp., *Salmonella* spp., *Serratia* spp. and *Streptococcus* spp. Surprisingly, Mohamed *et al.*[42] reported that ciprofloxacin resistance and biofilm-producing *K. pneumoniae* become sensitive when the ciprofloxacin is loaded with EOs. Gram +ve bacteria were more sensitive than Gram -ve bacteria because of the constitution of their cell wall; however, the results show a special case for the bacterial strain *S. typhi*, which is a Gram -ve bacterium. These findings may indicate the existence of mechanisms other than cell wall composition for resistance of antibacterial agents, for instance, Alenazy[43] mentioned that multidrug resistance properties of *Salmonella* are represented by efflux pumps which extrude the antibacterial agents from the bacterial cells. Therefore, scientific investigators focused on the efflux pumps as an antibacterial agent target for novel drug discoveries. In this context, the ability of *S. typhi* to form biofilm is considered one of the mechanisms for antibacterial agent resistance.

According to an earlier study, the growth of spoilage bacteria and fungi in the stored potato paste was strongly inhibited by sesame EOs, therefore the utilization of these EOs as an antioxidant, antibacterial agent and coating of food can be applied as suggested by Fallah *et al.*[40]. Unfortunately, the two EOs don't exhibit inhibitory action against *A. niger*. However, Uniyal *et al.*[44], investigated the antifungal potential of sesame EO. They found this EO able to control the growth of *Aspergillus* spp., that causes aspergilloma. Also, *A. niger*

Table 2: Detected volatile compounds in sweet almond EO by GC/MS analysis

Compound	Retention time	Area (%)	MF	MW
3-Methylpentane	5.02	0.13	C_6H_{14}	86
2-Methylhexadecan-1-ol	12.47	0.09	$C_{17}H_{36}O$	256
p-Cymene	14.95	0.09	$C_{10}H_{14}$	134
Nonanal	18.45	0.12	$C_9H_{18}O$	142
Dodecane	24.02	0.48	$C_{12}H_{26}$	170
1-Cyclohexene-1-acetaldehyde, β,2-dimethyl-	24.47	0.38	$C_{10}H_{16}O$	152
Propanal, 3-cyclohexylidene-2-methyl-	24.99	0.33	$C_{10}H_{16}O$	152
1-Ethynylcycloheptanol	25.15	0.11	$C_9H_{14}O$	138
2-Decenal, (E)-	25.60	0.41	$C_{10}H_{18}O$	154
2,4-Decadienal, (E,E)-	27.91	11.63	$C_{10}H_{16}O$	152
Undec-2-enal	30.11	0.44	$C_{11}H_{20}O$	168
Tetradecane	32.78	0.65	$C_{14}H_{30}$	198
Docosane	36.86	0.19	$C_{22}H_{46}$	310
Hexadecane	40.69	0.37	$C_{16}H_{34}$	226
13-Heptadecyn-1-ol	43.00	0.12	$C_{17}H_{32}O$	252
8-Heptadecene	43.38	0.26	$C_{17}H_{34}$	238
3',4',7-Trimethylquercetin	44.32	0.17	$C_{18}H_{16}O_7$	344
Heptacosane	44.91	0.05	$C_{27}H_{56}$	380
1-Naphthalenol, 1,2,3,4,4a,5,6,8a-octahydro-4a,8-dimethyl-2-(2-propenyl)-	45.43	0.12	$C_{15}H_{24}O$	220
Costunolide	46.92	0.41	$C_{15}H_{20}O_2$	232
1H-Purin-6-amine, [(2-fluorophenyl)methyl]-	49.89	0.07	$C_{12}H_{10}FN_5$	243
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	50.04	0.18	$C_{17}H_{24}O_3$	276
Dihydrodehydrocostus lactone	50.29	1.09	$C_{15}H_{20}O_2$	232
2,2-Dideutero octadecanal	51.03	0.12	$C_{18}H_{34}D_2O$	270
Hexadecanoic acid, methyl ester	51.42	0.78	$C_{17}H_{34}O_2$	270
Dibutyl phthalate	51.48	0.55	$C_{16}H_{22}O_4$	278
Dehydrocostuslactone	51.86	2.30	$C_{15}H_{18}O_2$	230
Benzene, (2-decyldodecyl)-	52.12	0.11	$C_{28}H_{50}$	386
Estra-1,3,5(10)-trien-17 β -ol	52.69	0.28	$C_{18}H_{24}O$	256
9-Octadecenoic acid (z)	53.33	0.20	$C_{18}H_{34}O_2$	282
01297107001Tetraneurin-A-diol	54.26	0.18	$C_{15}H_{20}O_5$	280
1H-purin-6-amine, [(2-fluorophenyl)methyl]-	54.91	0.09	$C_{12}H_{10}FN_5$	243
8,11-Octadecadienoic acid, methyl ester	56.39	1.00	$C_{19}H_{34}O_2$	294
9-Octadecenoic acid, methyl ester, (E)-	56.70	2.58	$C_{19}H_{36}O_2$	296
10-Octadecenoic acid, methyl ester	56.90	0.28	$C_{19}H_{36}O2$	296
Methyl stearate	57.74	1.78	$C_{19}H_{38}O_2$	298
Oleic acid	58.37	2.06	$C_{18}H_{34}O_2$	282
Octadecanoic acid	59.20	3.29	$C_{18}H_{36}O_2$	284
Hexadecanoic acid, 2,3-dihydroxypropyl ester	61.64	0.39	$C_{19}H_{38}O_4$	330
Glycidyl palmitate	63.23	2.67	$C_{20}H_{36}O_3$	312
2,2,3,3,4,4 Hexadeutero octadecanal	64.71	0.19	$C_{18}H_{30}D_6O$	274
Octadecanoic acid, 2-hydroxy-1,3-propanediyl di-ester	64.81	0.11	$C_{39}H_{76}O_5$	624
p-Cresol, 2,2'-methylenebis[6-tert-butyl-	66.22	0.96	$C_{23}H_{32}O_2$	340
Glyceryl monooleate	67.19	1.27	$C_{21}H_{40}O_4$	356
Stearin, 2-mono-	68.16	0.18	$C_{21}H_{42}O_4$	358
Linolein, 2-mono-	68.37	4.18	$C_{21}H_{38}O_4$	354
Glycidol oleate	68.68	12.48	$C_{21}H_{38}O_3$	338
10-Methoxy-NB-à-methylcorynantheol	70.42	0.38	$C_{21}H_{29}N_2O_2$	341
(Z,Z)-1,3-Dioctadecenoyl glycerol	71.32	0.14	$C_{39}H_{72}O_5$	620
2,9-Bis(2',6'-dimethylphenyl)-1,10-phenanthroline	73.22	0.42	$C_{28}H_{24}N_2$	388
3-(Methoxymethoxy)-2,3-dimethyl-1-undecene	73.80	1.30	$C_{15}H_{28}D_2O_2$	244
1,3-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	75.99	0.79	$C_{24}H_{38}O_4$	390
Olean-12-ene-3,28-diol	77.39	0.72	$C_{30}H_{50}O_2$	442
Squalene	78.24	6.24	$C_{30}H_{50}$	410
6,8-DI-C- β -Glucosylluteolin	80.38	0.09	$C_{27}H_{30}O_{16}$	610
α-Tocopherol	82.71	0.27	$C_{28}H_{48}O_2$	416
(+)-Sesamin	83.35	1.97	$C_{20}H_{18}O_6$	354
Vitamin E	84.74	7.86	$C_{29}H_{50}O_2$	430
Campesterol	86.09	1.26	$C_{28}H_{48}O$	400
Ethyl iso-allocholate	86.80	0.66	$C_{26}H_{44}O_5$	436
β-sitosterol	88.31	17.83	$C_{29}H_{50}O$	414
Stigmasta-5,24(28)-dien-3 β -ol, (Z)-	88.55	2.80	$C_{29}H_{48}O$	412
3-Hydroxyspirost-8-en-11-one	89.16	0.35	$C_{27}H_{40}O_4$	428
Isochiapin B	89.44	0.18	$C_{19}H_{22}O_6$	346
1-Heptatriacotanol	89.77	0.30	$C_{37}H_{76}O$	536
cis-Sitostenone	91.43	2.12	$C_{29}H_{48}O$	412

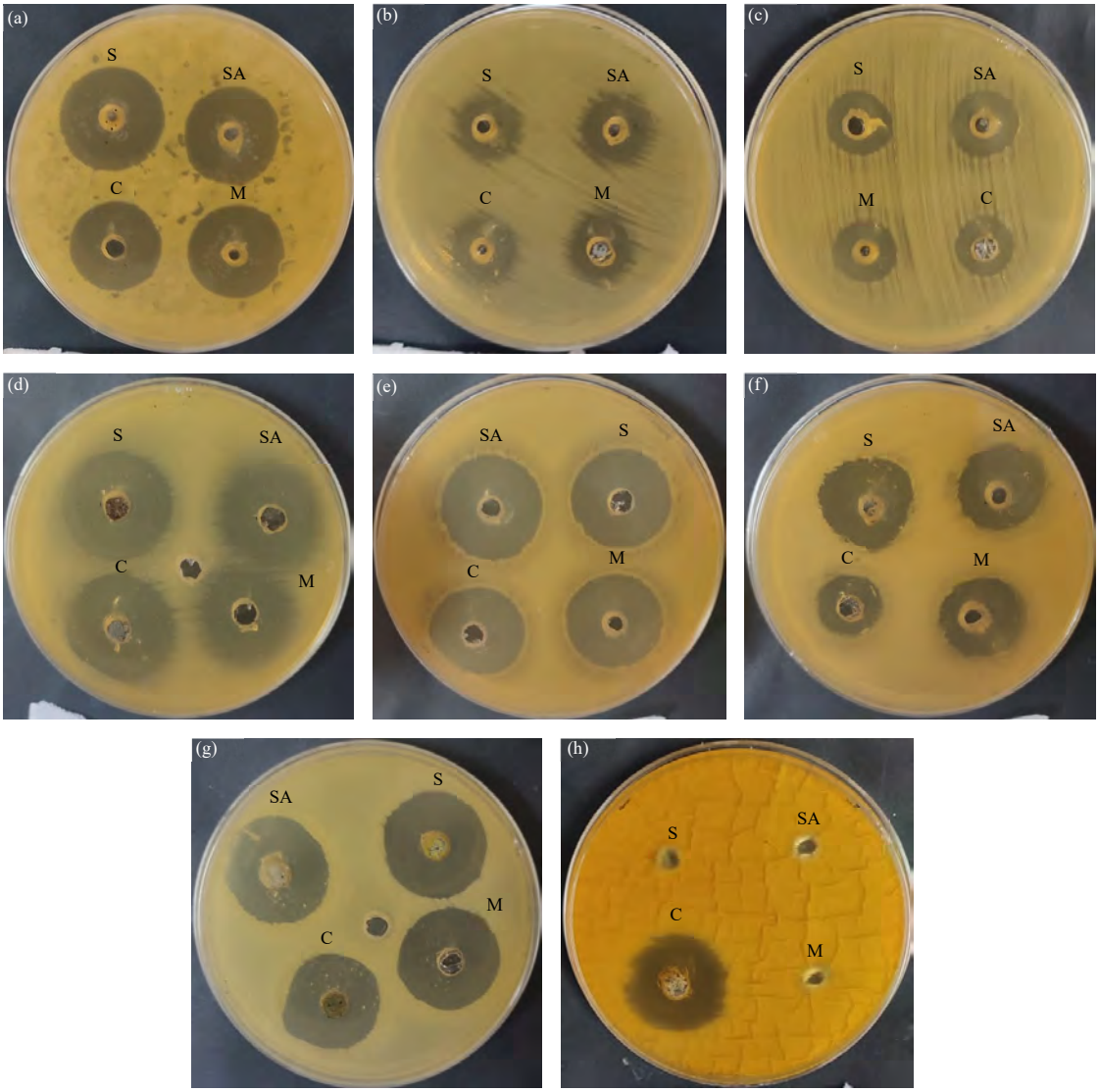

Fig. 3(a-h): Antimicrobial activity of sesame (S), sweet almond (SA) EOs, their mixture (M) and standard control (C) against different microorganisms, (a) *Staphylococcus aureus*, (b) *Escherichia coli*, (c) *Klebsiella pneumoniae*, (d) *Salmonella typhi*, (e) *Bacillus subtilis*, (f) *Enterococcus faecalis*, (g) *Candida albicans* and (h) *Aspergillus niger*

Table 3: Antimicrobial activity of sesame, sweet almond EOs and their mixture

	Inhibition zone (mm)			
Test organisms	Sesame EO	Sweet almond EO	Mixture of EOs	*Control
Bacillus subtilis (ATCC 6633)	25±0.3	26±0.4	26±0.1	23±0.2
Enterococcus faecalis (ATCC 10541)	21±0.5	24±0.2	23±0.2	15±0.2
Staphylococcus aureus (ATCC 6538)	22±0.1	25±0.1	26±0.2	23±0.3
Escherichia coli (ATCC 8739)	22±0.4	25±0.3	25±0.4	21±0.4
Klebsiella pneumoniae (ATCC 13883)	24±0.3	27±0.2	26±0.4	20±0.2
Salmonella typhi (ATCC 6539)	27±0.4	29±0.2	31±0.2	24±0.2
Candida albicans (ATCC 10221)	26±0.1	27±0.1	28±0.2	25±0.2
Aspergillus niger	NA	NA	NA	22±0.3

*Control: Ketoconazole/Gentamicin for fungi/bacteria

Table 4: MIC and MBC of sesame essential oil (SEO) and sweet almond oil (SAEO) against tested microorganisms

	MIC (µg/mL)			MBC (µg/mL)			MBC/MIC index		
Test microbes	SEO	SAEO	Mixture	SEO	SAEO	Mixture	SEO	SAEO	Mixture of Eos
Bacillus subtilis	7.83±0.06	7.67±0.23	7.93±0.12	31.33±0.14	7.87±0.15	15.60±0.17	4.00	1.03	1.97
Enterococcus faecalis	31.20±0.09	15.46±0.19	15.61±0.01	62.47±0.06	15.61±0.01	31.25±0.25	2.00	1.01	2.00
Staphylococcus aureus	15.58±0.07	3.93±0.25	3.90±0.17	62.40±0.17	3.90±0.10	7.83±0.15	4.00	0.99	2.00
Escherichia coli	31.17±0.14	3.97±0.21	7.87±0.12	62.57±0.40	7.80±0.17	15.67±0.06	2.00	1.96	1.99
Klebsiella pneumoniae	62.33±0.29	7.93±0.12	15.64±0.05	250.00±5.0	31.25±0.25	62.33±1.26	4.01	3.94	3.99
Salmonella typhi	7.73±0.12	1.97±0.03	1.92±0.20	31.33±0.38	1.96±0.02	3.93±0.25	4.05	0.99	2.04
Candida albicans	15.54±0.07	7.87±0.12	7.83±0.21	31.33±0.14	15.62±0.02	15.61±0.10	2.01	1.98	1.99

Table 5: DPPH scavenging (%) of sesame EO, sweet almond EO and ascorbic acid

	DPPH scavenging (%)			
Concentration (µg/mL)	Sesame EO	Sweet almond EO	Mixture of EOs	Ascorbic acid
1000	74.9	82.6	77.1	97.1
500	68.9	76.4	71.5	94.6
250	63.2	70.3	65.2	92.6
125	57.2	64.0	58.8	87.9
62.50	50.6	57.6	52.4	80.9
31.25	44.1	51.3	46.5	74.2
15.63	37.7	44.8	39.5	65.9
7.81	31.4	38.1	33.7	59.4
3.90	24.8	31.5	27.3	52.2
1.95	18.6	25.1	21.5	46.3
0	0.0	0.0	0.0	0.0
IC_{50} (µg/mL)	60.5	28.19	47.51	2.45

and *A. fumigatus* were inhibited using sesame EO[22]. Sweet almond EO was used as a food preservative; therefore, the counts of *S. aureus* were decreased, while *E. coli* was completely inhibited in the labneh fortified with this EO[45]. Also, the antibacterial effects were associated with sweet almond EOs as mentioned[46].

MIC and MBC of essential oils: The MIC value of sweet almond EO was very lower (15.46±0.19, 3.93±0.25, 3.97±0.21, 7.93±0.12, 1.97±0.03 and 7.87±0.12 µg/mL) than the MIC value of sesame EO (31.20±0.09, 15.58±0.07, 31.17±0.14, 62.33±0.29, 7.73±0.12 and 15.54±0.07 µg/mL) against all tested microorganisms including *E. faecalis*, *S. aureus*, *E. coli*, *K. pneumoniae*, *S. typhi* and *C. albicans*, respectively except *B. subtilis* where negligible change in the values of MIC of sesame EO (7.83±0.06 µg/mL) and sweet almond EO (7.67±0.23 µg/mL) (Table 4). Slight minimization of the MIC was observed using a mixture of the two EOs against *S. aureus* and *S. typhi*, but unfortunately, the value of MIC increased against the rest of the tested microorganisms. The same observation was recorded in the case MBC, where sweet almond EO exhibited a promising value of MBC particularly *S. aureus* and *S. typhi* compared to sesame EO and its mixture (Table 4). In an earlier study, food-borne pathogens were inhibited using sesame EO[14]. According to French[27], the drug possesses bactericidal properties, if its MBC/MIC value is fewer than 4 times its MIC. Therefore, sesame EO alone has bactericidal activity for *E. faecalis*, *E. coli* and *C. albicans* only, while sweet almond EO alone and the mixture of EOs possess bactericidal activity against all tested microorganisms (Table 4).

Antioxidant activity of essential oils: The antioxidant potential of both sesame and sweet almond EOs was evaluated (Table 5). The DPPH scavenging (%) increased with increasing the concentration of EOs and their mixture. It's clear that sweet almond EO possesses high antioxidant capacity compared to sesame EO at all applied concentrations, for instance, DPPH scavenging (%) was 64.0 and 57.2%, respectively at 125 µg/mL and 76.4 and 68.9%, respectively at 500 µg/mL. The IC_{50} value of sesame EO (60.5 µg/mL) was more twofold than the IC_{50} value of sweet almond EO (28.19 µg/mL). Antioxidant activity of EOs mixture exhibited a higher IC_{50} value (47.51 µg/mL) than the IC_{50} value of sweet almond EO, indicating the antagonistic action of both EOs. The antioxidant potential of both EOs was compared to the antioxidant potential of ascorbic acid reflecting IC_{50} value of 2.45 µg/mL. As mentioned in a Lange *et al.*[47], the unsaturated fatty acids in plant EO are strongly related to antioxidant properties. Current findings were in agreement with Zhao *et al.*[32], where who mentioned that sweet almond EO has antioxidant abilities and it is suggested to develop nutritive

Table 6: Docking scores and energies of (+)- sesamin and β-sitosterol with structure of *E. faecalis* 2OMK

Mol	S	rmsd_refine	E_conf	E_place	E_score1	E_refine	E_score2
(+)- Sesamin	-5.12225	2.102249	52.46055	-48.3424	-9.77703	-24.2093	-5.12225
(+)- Sesamin	-5.09339	1.992562	54.31136	-78.5494	-10.0509	-25.7701	-5.09339
(+)- Sesamin	-5.07636	1.745321	54.56289	-58.7166	-9.97134	-25.3386	-5.07636
(+)- Sesamin	-5.07363	2.750735	53.99917	-77.7847	-10.1562	-23.7046	-5.07363
(+)- Sesamin	-5.07318	1.607661	53.98363	-76.0768	-10.3108	-25.1755	-5.07318
β-Sitosterol	-5.53883	3.964647	48.76462	-36.6845	-8.16154	-26.4915	-5.53883
β-Sitosterol	-5.24251	2.635749	47.6861	-36.8963	-8.25049	-25.0757	-5.24251
β-Sitosterol	-5.2063	2.8653	41.29132	-17.3072	-8.23689	-25.2824	-5.2063
β-Sitosterol	-5.19076	2.352433	44.24205	-26.4321	-7.96337	-23.7446	-5.19076
β-Sitosterol	-5.18719	2.220733	39.21606	-22.869	-8.09841	-23.8644	-5.18719

Table 7: Docking scores and energies of (+)- sesamin and β-sitosterol with *K. pneumoniae* 8FFK

Mol	S	rmsd_refine	E_conf	E_place	E_score1	E_refine	E_score2
(+)- Sesamin	-7.48578	2.282297	56.78818	-66.2752	-10.3004	-40.3707	-7.48578
(+)- Sesamin	-7.17779	1.682334	54.64922	-75.4525	-10.2934	-37.9065	-7.17779
(+)- Sesamin	-7.07175	2.061245	64.16233	-48.8616	-9.96928	-36.8002	-7.07175
(+)- Sesamin	-6.96311	1.407056	57.97913	-83.9847	-10.2426	-38.3116	-6.96311
(+)- Sesamin	-6.91184	3.223817	55.02187	-48.6821	-10.6997	-35.8151	-6.91184
β-Sitosterol	-7.66918	2.597712	57.51109	-45.054	-8.4473	-37.6114	-7.66918
β-Sitosterol	-7.58909	3.061845	86.97365	-82.406	-9.15214	-28.5992	-7.58909
β-Sitosterol	-7.5857	3.641331	58.65593	-58.5693	-9.04714	-40.2255	-7.5857
β-Sitosterol	-7.54364	1.947424	70.5992	-54.9462	-9.35724	-32.893	-7.54364
β-Sitosterol	-7.53889	2.350388	74.87484	-98.6482	-9.51165	-23.8191	-7.53889

antioxidants based on this EO. According to Kumar and Singh[14], the constituents of sesame EO such as sesamin and sesamolin, are acknowledged for their antioxidant potential. Due to the presence of natural antioxidants in both EOs, the utilisation of these EOs as food additives can minimize the side effects resulting from oxidative stress. Tit and Bungau[48] mentioned that fatty acid content EOs rise in antioxidant potential but a more significant role was associated with the lignan content of EO. The differences between the antioxidant capacities of the two EOs may be due to the quantitative and qualitative differences in EOs' chemical composition. For example, as documented by Gharehcheshmeh *et al.*[49], sweet almond EO includes 95% of oleic acid and linoleic acid as unsaturated fatty acids but sesame EO includes 41% of linoleic acid besides tocopherols and phenolic constituents that play a vital role in the balance of oxidative stress. The antioxidant of yogurt samples supplemented with sweet almond and sesame EOs was estimated via DPPH reflecting IC_{50} values 45.35±1.44 and 31.05±2.16 µg/mL, respectively[49].

Molecular docking interaction of sesamin and β-sitosterol: One of the most popular techniques used in the process of computer-aided drug generation to find possible inhibitors against different infections is molecular docking. With this ground-breaking technique, the expensive, time-consuming and energy-intensive drug discovery process can be greatly reduced when promising drug molecules are found in enormous drug libraries. Throughout the current investigation, molecular docking was done using *E. faecalis* protein (PDB: 2OMK) and *K. pneumoniae* protein (PDB: 8FFK) as inhibitors that interact with (+)- sesamin and β-sitosterol as ligands.

The results of the experiments have been further supported by investigations on molecular docking. The two-dimensional and three-dimensional models were displayed with docking scores with higher negative values. Using the top-ranked intermolecular, electrostatic and binding free energies, Table 6 and 7 display the docking results. Figure 4-27 depict the active sites used to discover the interaction of proteins and ligands.

Based on the docking results shown below were attained:

- Docking of (+)- sesamin and β-sitosterol with *K. pneumoniae* protein (PDB: 8FFK) having negative free binding energy of (-7.48578 and -7.66918 kcal/mol, respectively) ratings that are higher than docking with *E. faecalis* protein (PDB: 2OMK) which determined to be (-5.12225 and -5.53883 kcal/mol, respectively)
- β-Sitosterol binds to 8FFK and 2OMK proteins through hydrogen bonds, demonstrating that it has the highest affinity for binding compared to (+)- sesamin. The experimental research produced the same outcome
- It was found that the presence of a wide attractive region close to the ASP 760 and GLU 171 residues corroborates the inhibitor H-donor interactions in 8FFK and 2OMK docking respectively with β-Sitosterol, the results suggested that the O 76 atom may be necessary for the inhibitor complexation step

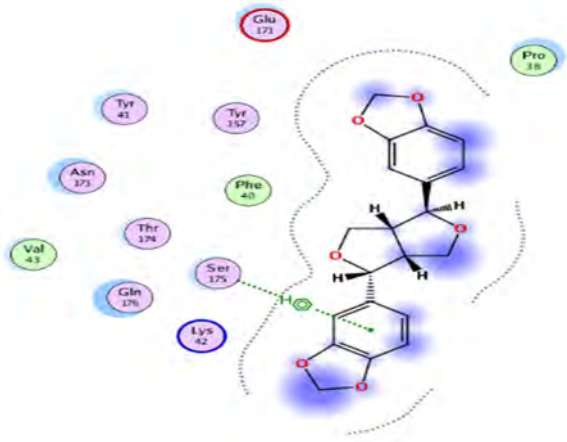

Fig. 4: Molecular docking of (+)- sesamin with 2OMK (interaction between (+)- sesamin and active sites of 2OMK protein)

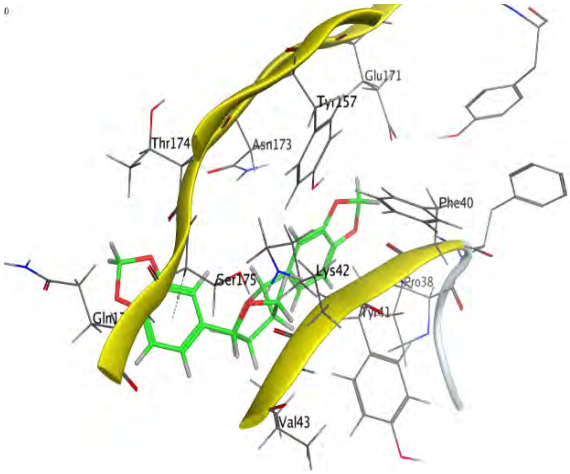

Fig. 5: Molecular docking of (+)- sesamin with 2OMK (identified binding conformation of (+)- sesamin and the corresponding intermolecular interactions)

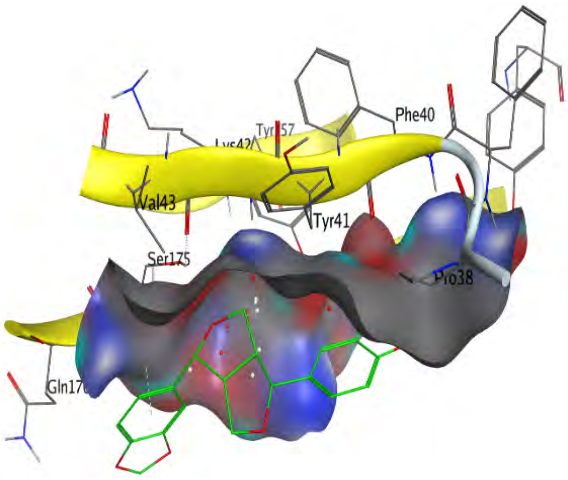

Fig. 6: Molecular docking process of (+)- sesamin with 2OMK (molecular surface of (+)- sesamin with 2OMK)

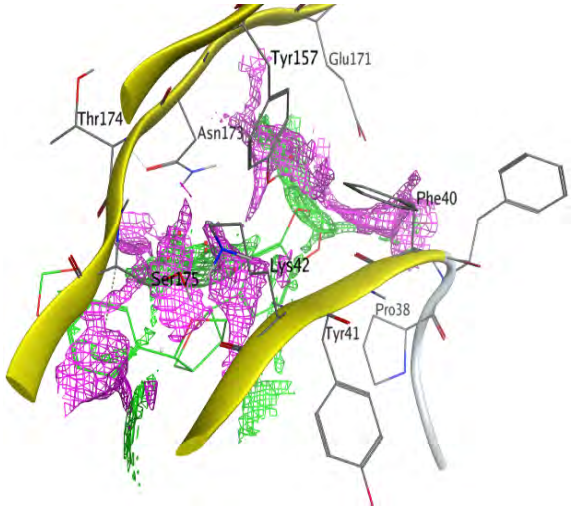

Fig. 7: Molecular docking of (+)- sesamin with 2OMK (contact preference of (+)- sesamin with 2OMK)

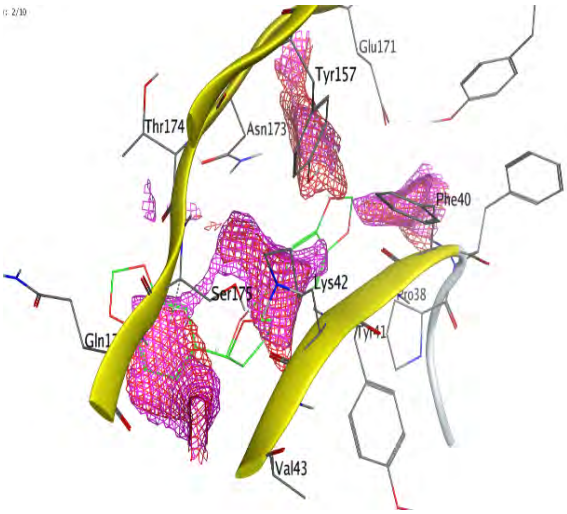

Fig. 8: Molecular docking of (+)- sesamin with 2OMK (interaction potential of (+)- sesamin with 2OMK)

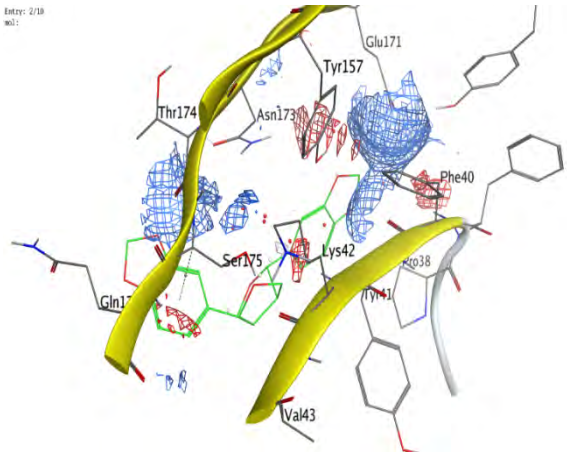

Fig. 9: Molecular docking of (+)- sesamin with 2OMK (electrostatic map of (+)- sesamin with 2OMK)

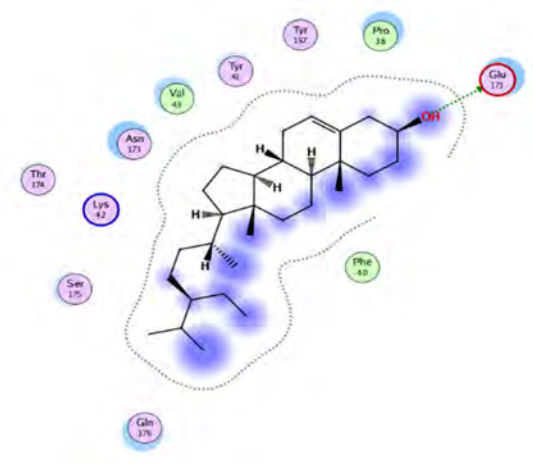

Fig. 10: Molecular docking of β-sitosterol with 2OMK (interaction between β-sitosterol and active sites of 2OMK protein)

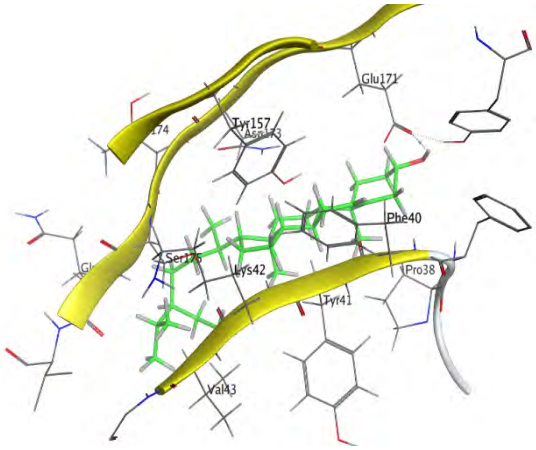

Fig. 11: Molecular docking process of β-sitosterol with 2OMK (identified binding conformation of β-sitosterol and the corresponding intermolecular interactions)

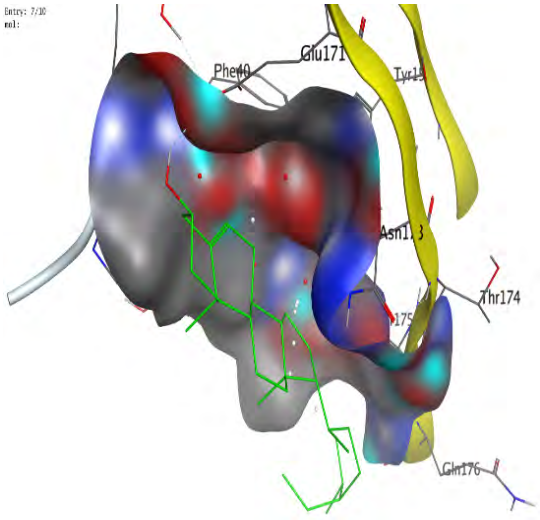

Fig. 12: Molecular docking of β-sitosterol with 2OMK (molecular surface of β-sitosterol with 2OMK)

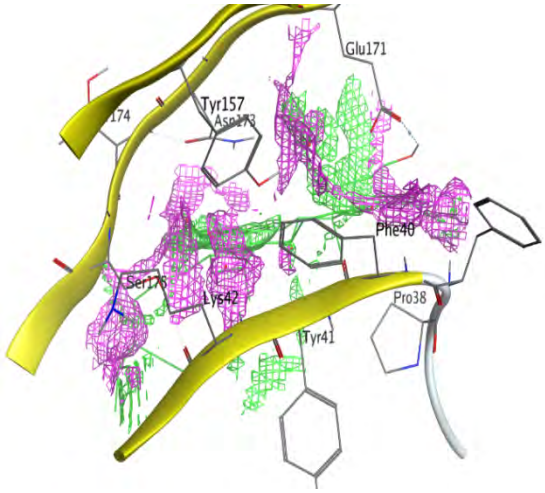

Fig. 13: Molecular docking of β-sitosterol with 2OMK (contact preference of β-sitosterol with 2OMK)

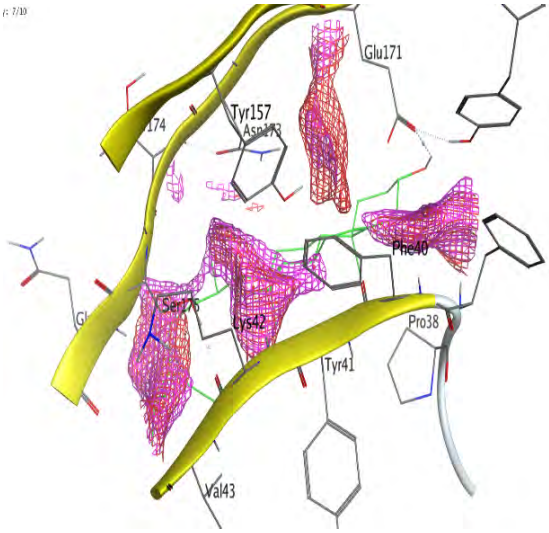

Fig. 14: Molecular docking of β-sitosterol with 2OMK (interaction potential of β-sitosterol with 2OMK)

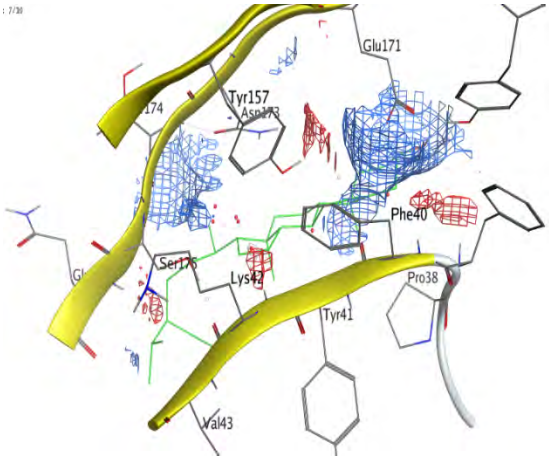

Fig. 15: Molecular docking of β-sitosterol with 2OMK (electrostatic map of β-sitosterol with 2OMK)

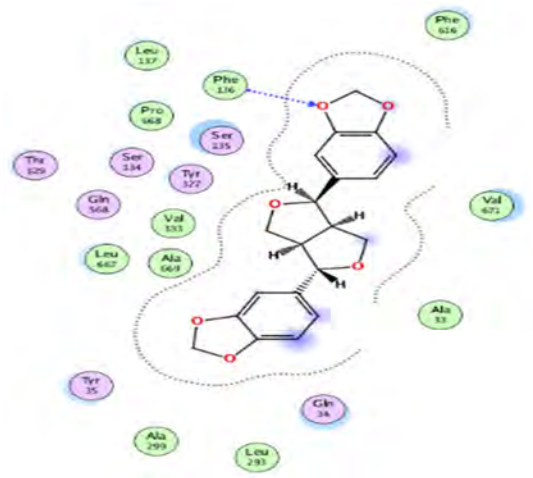

Fig. 16: Molecular docking of (+)- sesamin with 8FFK (interaction between (+)- sesamin and active sites of 8FFK protein)

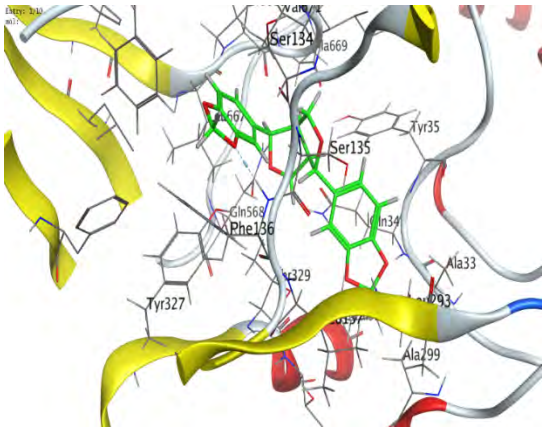

Fig. 17: Molecular docking of (+)- sesamin with 8FFK (identified binding conformation of (+)- sesamin and the corresponding intermolecular interactions)

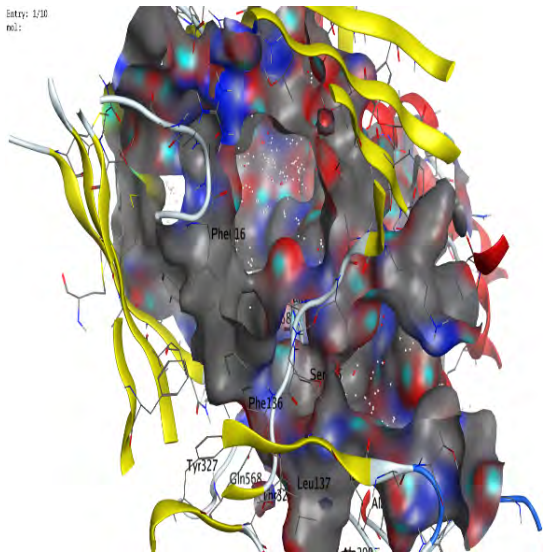

Fig. 18: Molecular docking of (+)- sesamin with 8FFK (molecular surface of (+)- sesamin with 8FFK)

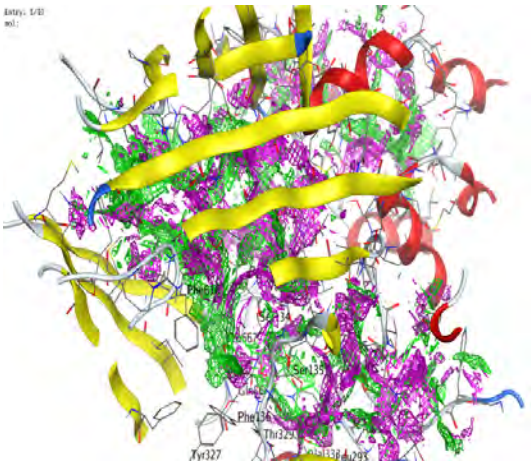

Fig. 19: Molecular docking (+)- sesamin with 8FFK (contact preference of (+)- sesamin with 8FFK)

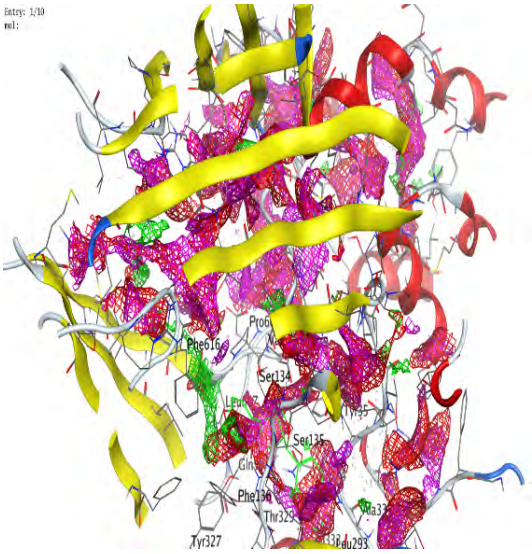

Fig. 20: Molecular docking of (+)- sesamin with 8FFK (interaction potential of (+)- sesamin with 8FFK)

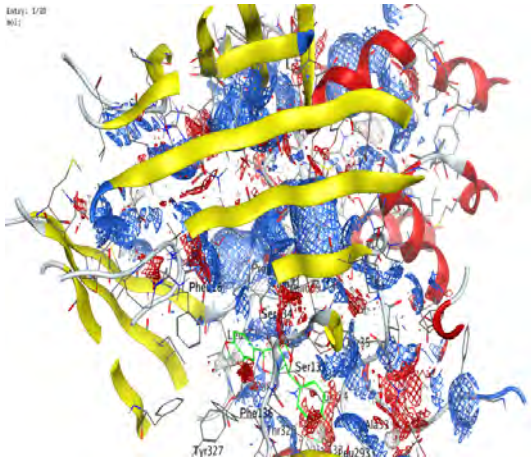

Fig. 21: Molecular docking of (+)- sesamin with 8FFK (electrostatic map of (+)- sesamin with 8FFK)

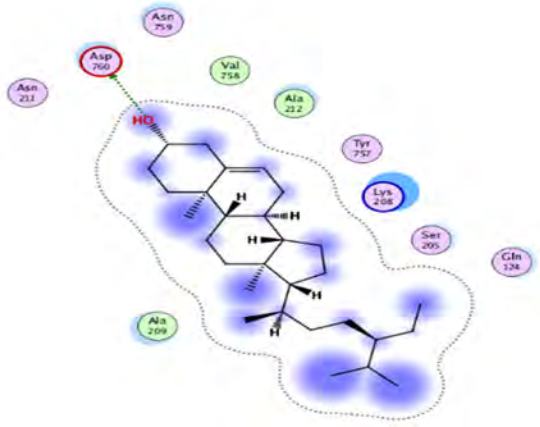

Fig. 22: Molecular docking of β-sitosterol with 8FFK (interaction between β-sitosterol and active sites of 8FFK protein)

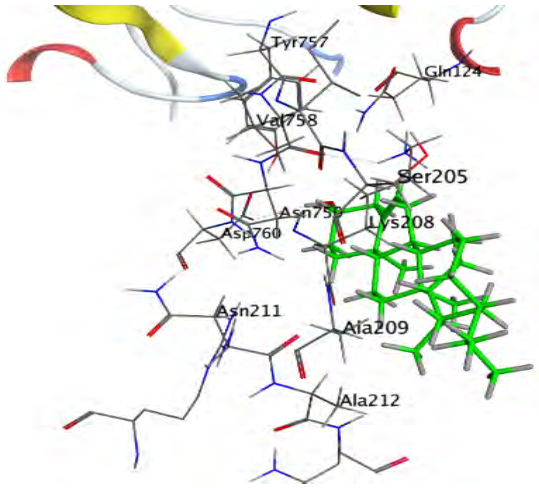

Fig. 23: Molecular docking of β-sitosterol with 8FFK (identified binding conformation of β-sitosterol and the corresponding intermolecular interactions)

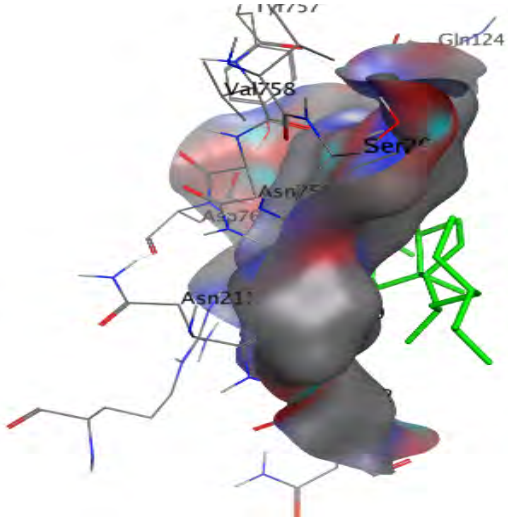

Fig. 24: Molecular docking of β-sitosterol with 8FFK (molecular surface of β-sitosterol with 8FFKK)

Fig. 25: Molecular docking of β-sitosterol with 8FFK (contact preference of β-sitosterol with 8FFK)

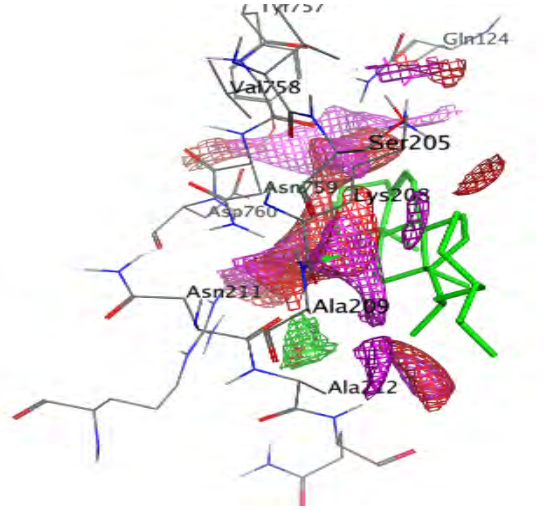

Fig. 26: Molecular docking of β-sitosterol with 8FFK (interaction potential of β-sitosterol with 2OMK)

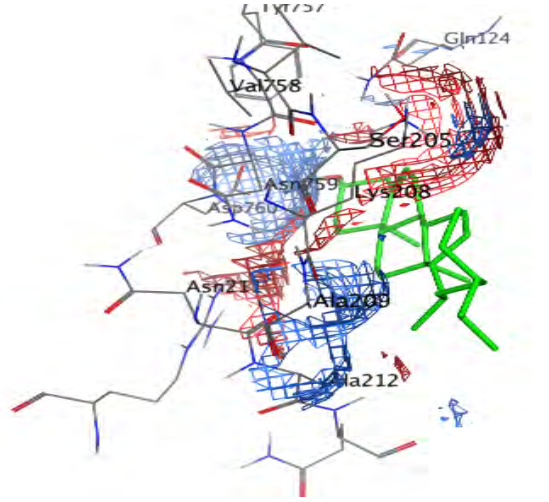

Fig. 27: Molecular docking of β-sitosterol with 8FFK (electrostatic map of β-sitosterol with 2OMK)

Table 8: Interaction of (+)- sesamin and β-sitosterol with structure of *E. faecalis* 2OMK

Mol	Ligand	Receptor	Interaction	Distance	E (kcal/mol)
(+)- Sesamin	6-ring	CA SER 175 (A)	pi-H	3.97	-0.6
β-Sitosterol	O 76	OE1 GLU 171 (A)	H-donor	3.15	-1.1

Table 9: Interaction of (+)- sesamin and β-sitosterol with *K. pneumoniae* 8FFK

Mol	Ligand	Receptor	Interaction	Distance	E (kcal/mol)
(+)- Sesamin	O 10	N PHE 136 (A)	H-acceptor	2.94	-2.0
β-Sitosterol	O 76	OD2 ASP 760 (A)	H-donor	3.08	-1.4

The details of interactions that occur between screened compounds and target proteins intermolecularly, including hydrogen bond and hydrophobic interaction are displayed in Table 8 and 9.

Some natural active constituents of sesame EO namely sesamolinol, sesamin, sesamolin and sesaminol were docked with $3CL^{pro}$ (protease enzyme) which plays a vital role in viral replication in COVID-19. These constituents possess higher binding energy ranging from -6.7 to -6.1[50].

The antibacterial activity of sesamin and β-sitosterol via interaction with the structure of *E. faecalis* 2OMK and *K. pneumoniae* 8FFK was verified by the detected negative score with the greatest value of the free binding energy in the current inquiry, which was noted in scientific investigations that were comparable but utilized other natural ingredients[3,6,51,52]. Numerous investigations supported the practical experiments findings about the effectiveness of some natural molecules via molecular docking interaction against *E. coli* and *Proteus vulgaris*[51], *S. typhi*[7], *S. aureus* and *C. albicans*[8]. The β-Sitosterol as a natural constituent of *Ocimum basilicum* L. showed antibacterial activity against *Enterococcus faecalis*, *Streptococcus mutans* and *Streptococcus sanguinis*[53]. Docking result showed this constituent reflected low binding affinity of -7.8, -7.6, -6.7 and -6.0 kcal/mol for the potential targets PBP, MurB, MurA and SrtA, respectively[54].

CONCLUSION

Several constituents were detected in sesame and sweet almond EOs via GC/MS analysis. These EOs were effective against tested bacteria and *C. albicans*, but the sweet almond EO was more effective than sesame EO. Moreover, slight synergistic action of the combined two EOs was recorded against certain microorganisms including *S. aureus*, *S. typhi* and *C. albicans* while antagonistic action was observed against the rest tested microorganisms. The ability of sweet almond EO to DPPH scavenging activity was more than sesame EO. Because of the presence of several phenolic and flavonoids, the antimicrobial and antioxidant activities of oils were performed. Also, the human body was protected from their destructive effects as well as decelerating the development of numerous diseases such as microbial infection via the removal of free radicals and reactive oxygen species by antioxidants. The current study suggested that the screened chemicals [(+)- sesamin and β-sitosterol] have enough potential to inhibit the proteins of *K. pneumoniae* (PDB: 8FFK) and *E. faecalis* (PDB: 2OMK) and may be used as efficient drug candidates for the development of new treatments. However, the tested EOs are very effective against tested microorganisms.

SIGNIFICANCE STATEMENT

Several plant-based essential oils have been investigated for their potential as pharmaceutical agent. Therefore, search for natural compounds that are effective against pathogenic microorganisms and their mechanisms is essential. Findings of the current investigation reveal that EOs of sesame and sweet almond were effective on some food-born and human pathogenic microorganisms, besides their antioxidant activity which play a vital role in the human balance during stress conditions. Molecular docking in this study will help the investigators to predict for the activity and mechanism of EOs against pathogenic bacteria, thus a critical theory on the management of food and microbial infection may be arrived at.

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