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Research article

Spectroscopic analysis of wild medicinal desert plants from wadi sanor (beni-suef), Egypt, and their antimicrobial and antioxidant activities

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ABSTRACT

Desert plants possess untapped potential for medicinal applications due to their rich phytochemical profiles. However, they need to be more explored. Thus, this study integrates advanced analytical, biochemical, and molecular techniques to investigate the phytochemical composition and biological activities (antimicrobial and antioxidant) of four desert plants (*Pergularia tomentosa, Zygophyllum coccineum, Pulicaria undulata*, and *Ochradenus baccatus)*, collected from Wadi Sannor, Beni-Suef Governorate, Egypt, in March 2021. The volatile chemicals in the 70 % ethanol extracts of the selected plants were also analyzed using GC-MS. The extract exhibited strong antioxidant properties, as demonstrated by its FRAP (Ferric reducing ability of plasma) values, anti-lipid peroxidation, superoxide anion scavenging activity, and DPPH scavenging activity. Additionally, plants extracts showed high antimicrobial activities against seven pathogens, including three Gram-negative bacteria (*Pseudomonas aeruginosa*, *Salmonella typhimurium*, *Escherichia coli*) and four Gram-positive bacteria (Staphylococcus saprophyticus, Staphylococcus epidermidis, *Enterococcus faecalis*, Streptococcus salivarius). Lastly, molecular docking was conducted for cis-vaccenic acid, (E)-9-octadecenoic acid, the cyclohepta[b]furan-2-one scaffold, and URS-20(30)-en-3-ol against both the thymidylate kinase enzyme and the active sites of *E. coli* DNA gyrase. The results from the molecular docking studies showed a strong correlation with the biological data. Moreover, these compounds exhibited good, proposed absorption, distribution, metabolism, and excretion–toxicity (ADMET) profiles. Our study highlights the potential of P. tomentosa, Z. coccineum, P. undulata, and O. baccatus for future medical applications and the development of new pharmaceuticals derived from desert flora.

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Abbreviations

P. tomentosa Pergularia tomentosa L
Z. coccineum Zygophyllum coccineum
P. undulata *Pulicaria* undulata
O. baccatus Ochradenus *baccatus*
FRAP Ferric reducing ability of plasma
TAC The total antioxidant
DNA Deoxyribonucleic acid
TMPK Thymidylate kinase
PDB Protein Data Bank
ADMET absorption, distribution, metabolism, and excretion–toxicity

1. Introduction

Deserts, often characterized by extreme aridity and harsh environmental conditions, are commonly misperceived as barren wastelands devoid of life [1]. However, contrary to this belief, desert ecosystems support a wide variety of plant species that have adapted to thrive under such challenging circumstances [2]. These resilient plants have developed unique mechanisms for water conservation and heat tolerance, enabling them to combat various environmental stressors, including pests and diseases [2]. Additionally, many of these desert plants possess significant medicinal properties [3,4]. Indigenous communities have recognized and utilized the medicinal potential of desert plants for centuries [5]. These traditional healers have accumulated a wealth of knowledge about the therapeutic applications of specific desert plant species, passing down this wisdom from generation to generation [6]. In recent years, scientific investigations shed the light on the chemical constituents and pharmacological activities of these plants, confirming their medicinal value and opening up new avenues for drug discovery and development [7,8].

Wadi Sannor, located in the Beni-Suef Governorate, is home to a unique cave system that provides a rare opportunity to study plant life in challenging subterranean conditions [9,10]. The plants collected from this environment have adapted to thrive in darkness, with limited nutrients and fluctuating microclimates [11]. Research into these plants highlights their unique survival strategies and potential medicinal properties [12]. These plants, which exhibit specialized growth patterns and metabolic pathways, offer insights into plant physiology and ecology, contributing to both conservation efforts and potential applications in various fields [13–15].

Pergularia tomentosa, Zygophyllum coccineum, Pulicaria undulata, and *Ochradenus baccatus* are among these hardy desert plants that are notable for their traditional applications and therapeutic qualities [16]. For example, *P. tomentosa,* or the Milkweed vine, has long been used to treat respiratory, skin, and gastrointestinal disorders [17–19]. Studies show the plant contains alkaloids, terpenoids, and flavonoids with anti-inflammatory and antioxidant properties [20–22]. Similarly, *Z. coccineum* has been used for diabetes and hypertension, with research confirming its bioactive compounds' therapeutic potential [23]. The presence of these bioactive constituents supports the traditional use of Z. coccineum and highlights its potential in the development of natural remedies [24]. *P. undulata*, or desert fleabane, and *O. baccatus*, known as yellow salsify, also exhibit significant medicinal properties due to the presence of bioactive substances like sesquiterpene lactones and flavonoids, which support their traditional uses [25–27]. *P. undulata* is recognized for its extensive use in traditional Arabian medicine [28], as an antipyretic, analgesic, and anti-inflammatory agent [29,30]. *O. baccatus* has been employed to alleviate respiratory problems, gastrointestinal disorders, and skin conditions [31,32]. Overall, these desert plants from Wadi Sannor, showed unique adaptations and bioactive compounds.

Although desert plants possess great medicinal potential due to their phytochemical richness, they are still underexplored. This study focuses on the chemical composition and medicinal potential of *P. tomentosa, Z. coccineum, P. undulata*, and *O. baccatus* from Wadi Sannor, Beni-Suef Governorate, Egypt. Additionally, molecular docking was performed for compounds like cis-vaccenic acid and (E)-9-octadecenoic acid against thymidylate kinase enzyme and *E. coli* DNA gyrase, providing further insights into their therapeutic potential. This research aims to explore these plants' chemical and biological properties and their potential applications in modern medicine.

2. Materials and methods

2.1. Plant samples

In March 2021, samples of *Pergularia tomentosa, Zygophyllum coccineum*, *Pulicaria undulata*, and *Ochradenus baccatus* were collected from Wadi Sannor in the Beni-Suef Governorate of Egypt (28° 37′ 23″ N, 31° 17′ 11″ E). The samples were documented, and voucher specimens for each plant were deposited in the herbarium of Beni-Suef University, Egypt, under the numbers 317–320. The collected specimens were identified by the Botany and Microbiology Department of the same institution.

Plant samples of *P. tomentosa, Z. coccineum*, *P. undulata*, and *O. baccatus* were collected from Wadi Sannor, Beni-Suef Governorate, Egypt, in March 2021 (Fig. 1.).

2.2. Preparation of the plant extracts

Once air-dried at 60 °C and powdered (50 g each), the plant samples underwent maceration in 70 % ethanol (Piochem, Egypt) (500 ml) for three days with regular agitation. The solvent was then evaporated under reduced pressure using a BIOBASE-RE100-Pro rotary evaporator. The extracts of *P. tomentosa*, Z. coccineum, P. undulata, and *O. baccatus* were subsequently stored at −20 °C for further analysis [33].

2.3. Phytochemical screening

Phytochemical analyses were carried out on all extracts from *P. tomentosa, Z. coccineum, P. undulata*, and *O. baccatus* using standard methods outlined by Brain and Turner (1975).

2.3.1. Detection of anthraquinones (Borntrager's test)

Approximately 0.2 g of extract was heated with 10 % HCl (Piochem, Egypt) in a water bath for a few minutes. After filtering and allowing it to cool, an equal volume of $CHCl_3$ (Piochem, Egypt) was added to the filtrate. A few drops of 10 % NH_3 (Piochem, Egypt) were then added, and the mixture was heated. The presence of anthraquinones is indicated by the formation of a pink color.

2.3.2. Detection of flavonoids (Lead acetate test)

The extracts were treated with a few drops of lead acetate (Alpha Chemika, India). The appearance of a yellow precipitate indicates the presence of flavonoids.

2.3.3. Detection of steroids (Liebermann-burchard test)

2 ml of acetic anhydride (Alpha Chemika, India) was added to 0.5 g of the extracts, followed by 2 ml of H2SO4 (Piochem, Egypt). A color change from violet to blue or green in certain samples suggests the presence of steroids.

2.3.4. Detection of terpenoids (Salkowski's test)

To create a layer, 0.2 g of the extract was mixed with 2 ml of chloroform (Piochem, Egypt), followed by the careful addition of 3 ml of concentrated H_2SO_4 (Piochem, Egypt). The formation of a reddish-brown layer indicates the presence of terpenoids.

2.3.5. Detection of phenols (Ferric chloride test)

Several drops of a 5 % ferric chloride solution (Qualikems, India) were added to the extracts. A bluish-black color indicates the presence of phenols.

2.3.6. Detection of saponins (Froth test)

About 0.2 g of extract was mixed with 5 ml of distilled water and shaken. The formation of stable, creamy foam indicates the presence of saponins.

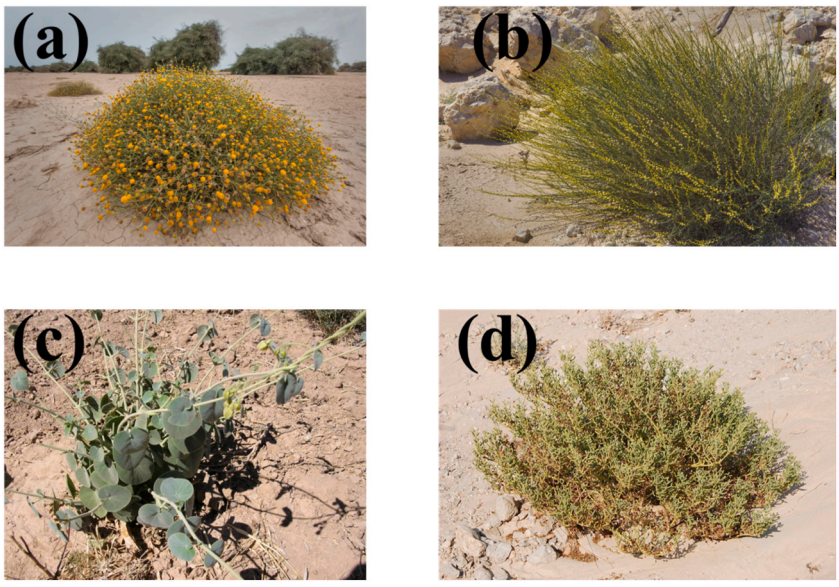

Fig. 1. The plant samples collected from Wadi Sannor, Beni-Suef Governorate, Egypt (A) *Pulicaria undulata*, (B) *Ochradenus baccatus*, (C) *Pergularia tomentosa* L and (D) *Zygophyllum coccineum.*

2.4. GC-MS analysis of plant extracts

This detailed Analysis was conducted using a state-of-the-art DB5-MS column, with dimensions of 30 m × 0.25 mm ID, supplied by J&W Scientific, USA, utilizing helium at a 1 mL/min flow rate as the carrier gas for optimal separation and detection of compounds. To accurately identify the major chemical constituents represented by the principal peaks in the chromatograms, the research team referred to the authoritative WILEY and NIST (National Institute of Standards and Technology, Gaithersburg, MD, USA) spectral libraries, ensuring a rigorous and comprehensive identification process [34].

2.5. Metabolites analysis

Nelson's method [35] was used to measure total soluble sugar content, while soluble proteins were quantified using the Folin-Lowry method [36]. The Folin-Ciocalteu and $AlCl_3$ colorimetric assays were employed to determine total phenolic and flavonoid content [37].

Fatty acid profiles were analyzed as described by Hassan et al. [38]. Plant material was treated with a chloroform-ethanol mixture (2:1 v/v) at 25 °C, and the resulting mixture was centrifuged at 16,000 rpm for 30 min. The clear liquid layer was analyzed using GC-MS (Hewlett Packard 6890 with MSD 5975 mass spectrometer, fitted with an HP-5 MS column). Fatty acids were identified using the NIST 05 and Golm Metabolome Databases (available at http://gmd.mpimp-golm.mpg.de). For the detection and quantification of phenolic compounds, we employed UHPLC-MS/MS, adhering to the procedure described by Xavier and colleagues [39].

2.6. Antimicrobial activity

2.6.1. Microbial strains

The antimicrobial activity of the extracts (70 % Ethanol) from selected plants was evaluated against seven microorganisms, including four Gram-positive bacteria: *Staphylococcus epidermidis* (RCMB 9241, ATCC 12228), *Staphylococcus saprophyticus* (RCMB 010028, ATCC 15305), *Enterococcus faecalis* (RCMB 010052) and *Streptococcus salivarius* (ATCC 13415). And three Gram-negative bacteria: *Escherichia coli* (RCMB 010052, ATCC 25922), *Salmonella enterica serovar typhimurium* (RCMB 006(1), ATCC 14028), *Pseudomonas aeruginosa* (ATCC 27853). The Regional Center for Mycology and Biotechnology (RCMB) at Al-Azhar University in Egypt provided these bacterial specimens for the research.

2.6.2. Antimicrobial assay

The antimicrobial activity of the plant extracts was evaluated using the agar well diffusion method, following the guidelines set by the National Committee for Clinical Laboratory Standards (NCCLS) [40]. The extracts were prepared in a solution of 5 mg/mL dimethyl sulfoxide (DMSO, Merck), with control agents included for comparison. Gentamicin (10 μg/ml) served as the positive control, while 5 % DMSO was used as the negative control. Mueller-Hinton agar was used as the culture medium. Each well, with a diameter of 6 mm, was filled with 100 μl of either plant extract or control solution. The plates were incubated at 37 °C for 24 h under aerobic conditions. The antimicrobial activity was determined by measuring the diameters of the inhibition zones in millimeters. Gentamicin was also applied as a standard filter disk for comparison as the positive control.

2.7. Antioxidant activity

The in vitro antioxidant activity of the plant extracts was evaluated using the DPPH (2,2-diphenyl-1-picrylhydrazyl) and FRAP (Ferric reducing antioxidant power) assays [41]. Approximately 0.2 g of each plant sample was extracted with 70 % ethanol, followed by centrifugation at 14,000 rpm for 20 min. For the antioxidant assessment, 0.1 mL of the suitably diluted extract was mixed with 0.25 mL of either DPPH or FRAP solution. The FRAP solution consisted of 10 mM TPTZ (2,4,6-tripyridyl-s-triazine) and 20 mM $FeCl_3$, prepared in an acetate buffer (0.25 M, pH 3.6). The mixtures were incubated at room temperature, and the absorbance was measured at 517 nm for DPPH and 600 nm for FRAP using spectrophotometric analysis.

2.8. Anti-lipid peroxidation

Lipid oxidation levels were assessed using the thiobarbituric acid reactive substances (TBARS) method, with an egg yolk mixture as the lipid source [42]. The plant extracts were mixed with an egg yolk solution (0.5 ml, 10 % by volume) and ferrous sulfate at a concentration of 15 mM. Thirty minutes later, 1.5 ml of a 10 % solution of trichloroacetic acid (TCA) was introduced to the mix. Subsequently, this blend was placed into a vessel containing 1.5 ml of 0.67 % thiobarbituric acid (TBA) and subjected to heat for 30 min. The development of the colored complex was determined by spectrophotometrically measuring the absorbance at 535 nm.

2.9. Statistical analysis

Statistical analysis were performed using a one-way analysis of variance (ANOVA) to compare multiple groups and determine the statistical significance of the observed differences. Post-hoc comparisons between the groups were carried out using Tukey's test to identify specific pairwise differences. A significance threshold of $\boldsymbol{P < 0.05}$ was set to indicate statistically significant differences, ensuring that any variation between the groups was not due to random chance.

2.10. ADMET approach

In silico reports of the four compounds cis-Vaccenic acid (Pergularia tomentosa), (E)-9-Octadecenoic acid (Zygophyllum coccineum), cyclohepta[b]furan-2-one (Pulicaria undulata) scaffold and URS-20(30)-en-3-ol (Ochradenus baccatus) were directed for their proposed ADMET profile and physicochemical character evaluation. It was calculated using SwissADMET and pkCSM descriptor algorithm procedures [43].

2.11. Molecular docking

Molsoft software was used to check the molecular interactions between cis-Vaccenic acid (Pergularia tomentosa), (E)-9-Octadecenoic acid (Zygophyllum coccineum), cyclohepta[b]furan-2-one (Pulicaria undulata) scaffold and URS-20(30)-en-3-ol (Ochradenus baccatus) with Thymidylate kinase enzyme and E. coli DNA gyrase active sites. Molsoft expects how small molecules, such as drug candidates or substrates can bind to a receptor of known 3D structure. Molsoft is a suit of automated docking tools, which permits flexible ligand docking. The protein target needed to be prepared and modeled according to the format requirements of the docking algorithms used. Thus the crystal structures of the receptors were downloaded from the Brookhaven Protein Databank Thymidylate kinase (PDB: 4QGG) [44] and E. coli DNA gyrase (PDB: 5MMN) [45], using Molsoft program. The protein was prepared for docking by polar hydrogens addition to the protein atoms. The protein active site was detected by placing a grid over the center of co-crystallized ligand. Before a protein was prepared for docking simulations, all the necessary grid maps were calculated prior to docking.

3. Results

3.1. Phytochemical screening

Table 1.

3.2. GC-MS analysis of the plant extracts

GC-MS was used to analyze the volatile compounds in the 70 % ethanol extracts of the selected plants. The results identified thirteen, thirty-seven, fifty-two, and seventeen chemical components in P. tomentosa, Z. coccineum, P. undulata, and *O. baccatus*, respectively (Fig. 2(a–d), Table 1(a-d)). The extracts of the four plants contained a variety of chemical compounds, including fatty acids, hydrocarbons, esters, sterols, alkaloids, aldehydes, and terpenes. The major chemical constituents in the Pergularia tomentosa L. extract were cis-vaccenic acid (38.49 %), n-hexadecanoic acid (24.96 %), octadecanoic acid (10.33 %), (E)-9-octadecenoic acid (8.99 %), and 2-hydroxy-3-[(9E)-9-octadecenoyloxy]propyl(9E)-9-octadecenoate (3.37 %). In Zygophyllum coccineum, the main components were (E)-9-octadecenoic acid (18.18 %), hexadecenoic acid (13.98 %), oleic acid (7.35 %), octadecanoic acid (6.75 %), 3-O-methyl-d-glucose (5.53 %), and 2-furancarboxaldehyde, 5-methyl-ethyl (4.05 %). For Pulicaria undulata, the major components included 2H-cyclohepta[b]furan-2-one, 3,3a,4,7,8,8a-hexahydro-7-methyl-3-methylene-6-(3-oxobutyl) [3aR-(3aα,7α,8aα)] (26.66 %), followed by 2H-cyclohepta[b]furan-2-one, 3,3a,4,7,8,8a-hexahydro-7-methyl-3-methylene-6-(3-oxobutyl)-, [3aR-(3aα,7α,8aα)] (12.92 %), hexadecenoic acid (6.48 %), p-menthane, 2,3-dibromo-8-phenyl- (5.58 %), ethyl 9,12,15-octadecatrienoate (5.1 %), and methyl eugenol (3.70 %). In Ochradenus baccatus, the major components were URS-20(30)-en-3-ol (32.81 %), olean-12-en-3-ol acetate, (3α) (14.04 %), trans-13-octadecenoic acid (11.00 %), and α-amyrin (9.16 %) (see Table 2).

3.3. Metabolites analysis

The amino acid analysis revealed that *O. baccatus* exhibited the highest levels of most amino acids, including glycine, arginine, ornithine, glutamine, asparagine, isoleucine, methionine, serine, phenylalanine, glutamic acid, aspartate, and cystine. In contrast, Z. coccineum showed higher concentrations of histidine, leucine, threonine, and valine, while P. undulata was richest in lysine and alanine. P. tomentosa L. had the lowest levels of all amino acids except for tyrosine. Therefore, *O. baccatus* was the richest in amino acid content, while P. tomentosa L. had the lowest (Table 3).

Fatty acid analysis revealed that *O. baccatus* had the highest levels of most fatty acids, including myristic (C14:0), palmitic (C16:0), heptadecanoic (C17:0), stearic (C18:0), arachidic (C20:0), docosanoic (C22:0), heptadecenoic (C17:1), oleic (C18:1), linoleic (C18:2),

Table 1
Phytochemical analysis of all ethanolic extracts of *Pulicaria undulata, Ochradenus baccatus, Pergularia tomentosa and Zygophyllum coccineum.*

Test	*P. undulata*	*O. baccatus*	*P. tomentosa*	*Z. coccineum*
Flavonoids	+ve	+ve	+ve	+ve
Phenols	+ve	+ve	+ve	+ve
Steroids	+ve	-ve	+ve	+ve
Terpenoids	+ve	-ve	+ve	+ve
Anthraquinones	-ve	-ve	-ve	-ve
Saponins	+ve	+ve	+ve	+ve

Table 2
Most abundant chemical components of 70 % ethanol extracts of *Pergularia tomentosa* L, *Zygophyllum coccineum, Pulicaria undulata*, and *Ochradenus baccatus*.

No.	Chemical class	Compounds	RT	Area (%)	Molecular formula	MW
2 (a) chemical constituents of 70 % ethanol extract **of *P. tomentosa***						
1	1,2-diacylglycerols	Glycerol 1,2-diacetate	13.10	2.49	$C_7H_{12}O_5$	176
2	long-chain fatty acids	n-Hexadecanoic acid	26.98	24.96	$C_{16}H_{32}O_2$	256
3	long-chain fatty acids	cis-Vaccenic acid	30.25	38.49	$C_{18}H_{34}O_2$	282
4	long-chain fatty acids	Octadecanoic acid	30.70	10.33	$C_{18}H_{36}O_2$	284
5	long-chain fatty acids	9-Octadecanoic acid (Z).	32.13	2.27	$C_{18}H_{34}O_2$	282
6	Fatty acid derivatives	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	35.01	2.14	$C_{21}H_{40}O_4$	356
7	1,3-Dielaidin	2-Hydroxy-3-[(9E)-9-octadecenoyloxy] prpoylm (9E)-9-octadecenoate.	38.82	3.37	$C_{39}H_{72}O_5$	620
2 (b) chemical constituents of 70 % ethanol extract **of *Z. coccineum***						
1	Aryl-aldehydes	2-Furancarboxaldhyde-5-methyl.	4.85	4.05	$C_6H_6O_2$	110
2	Apocynaceae	Proceroside.	6.24	2.75	$C_{29}H_{40}O_{10}$	548
3	Benzofurans	2,3-Dihydro-benzofuran.	10.28	2.39	C_8H_8O	120
4	Hexopyranose	4-o-Hexopyranosylhexopyranose.	17.04	2.02	$C_{12}H_{22}O_{11}$	342
5	D-aldohexose	3-o-Methyl-d-glucose	21.10	5.53	$C_7H_{14}O_6$	194
6	Inositol	Momeinositol.	21.14	2.76	$C_7H_{14}O_6$	194
7	long-chain fatty acids	Hexadecanoic acid.	26.97	13.98	$C_{16}H_{32}O_2$	256
8	long-chain fatty acids	9-Octadecenoic acid, (E)-	30.23	18.18	$C_{18}H_{34}O_2$	282
9	Fatty acid	Oleic Acid	30.32	7.35	$C_{18}H_{34}O_2$	282
10	long-chain fatty acids	Octadecanoic acid.	30.68	6.75	$C_{18}H_{36}O_2$	284
11	Alkaloids	Ethyl iso-allocholate	42.48	3.03	$C_{26}H_{44}O_5$	436
2 (c) chemical constituents of 70 % ethanol extract of *P. undulata*						
1	alk-2-enylbenzenes	Methyleugenol	14.53	3.70	$C_{11}H_{14}O_2$	178
2	long-chain fatty acids	Hexadecanoic acid.	26.98	6.48	$C_{16}H_{32}O_2$	256
3	Benzyl Halides	p-Menthane, 2,3-dibromo-8-phenyl	27.78	5.58	$C_{16}H_{22}Br_2$	372
4	Naphthol	1-Naphthalenepropanol, à-ethenyldecahydro-à,5,5,8a-tetrame thyl-2-methylene.	28.55	2.49	$C_{20}H_{34}O$	290
5	Polyunsaturated fatty acid	Methyl 3-cis,9-cis,12-cis-octadecatrienoate	29.36	2.94	$C_{19}H_{32}O_2$	292
6	Polyunsaturated fatty acid	Ethyl 9,12,15-octadecatrienoate	29.43	5.10	$C_{20}H_{34}O_2$	306
7	Sesquiterpene lactone	2H-Cyclohepta[B]furan-2-one, 3,3A,4,7,8,8A-Hexahydro-7-methyl-3-methylene-6-(3-oxo butyl)	30.26	26.66	$C_{15}H_{20}O_3$	248
8	Betulin	LUP-20(29)-ene-3,28-diol, (3á)-	42.20	3.23	$C_{30}H_{50}O_2$	442
2 (d) chemical components of 70 % ethanol extract **of *O. baccatus***						
1	long-chain fatty acids	Hexadecanoic acid.	26.97	5.43	$C_{16}H_{32}O_2$	256
2	long-chain fatty acids	trans-13-Octadecenoic acid	30.23	11.00	$C_{18}H_{34}O_2$	282
3	Sterol	Stigmasterol	32.75	3.62	$C_{29}H_{48}O$	412
4	Chelsterols	Stigasta-5,22-dien-3-ol.	32.89	2.20	$C_{29}H_{48}O$	412
5	Amyrin	Olean-12-en-3-ol, acetate, (3β)-	38.89	14.04	$C_{32}H_{52}O_2$	468
6	Heptatriacotanol	1-Heptatriacotanol	41.92	4.04	$C_{37}H_{76}O$	536
7	Sterols	URS-20(30)-en-3-ol.	42.20	32.81	$C_{30}H_{50}O$	426

linolenic (C18:3 ω−3), and eicosenoic (C20:1). In contrast, P. undulata showed higher levels of tricosanoic (C23:0), pentacosanoic (C25:0), palmitoleic (C16:1), and tetracosenoic (C24:1). Z. coccineum and P. tomentosa L. had the lowest fatty acid content. Therefore, *O. baccatus* demonstrated the highest overall fatty acid levels (Table 4).

Six organic acids were identified and quantified in the extracts tested: oxalic acid, malic acid, succinic acid, citric acid, isobutyric acid, and fumaric acid. The results indicated that *O. baccatus* exhibited the highest concentrations of all the organic acids (Table 5).

The results indicated that *O. baccatus* had the highest concentration of total sugars, showcasing superior levels for most sugars, whereas *P. tomentosa* L exhibited the lowest sugar content (Fig. 3).

The findings revealed that *O. baccatus* contained the highest levels of total sugars and was especially rich in various phenolic compounds, such as p-coumaric acid, caffeic acid, chicoric acid, rosmarinic acid, naringenin, luteolin, apigenin, rutin, quercetin, and chlorogenic acid. In contrast, *P. tomentosa* L had the lowest sugar content, as shown in Table 6.

The highest total phenolic content was in *O. baccatus,* then in *Z. coccineum*, then in *P. tomentosa*, and the lowest in *P. undulata.* The highest polyphenol quantity was observed in *O. baccatus*, then *P. undulata* and *Z. coccineum,* and the lowest levels were found in *P. tomentosa* L (Fig. 4a). The total flavonoid content was found to be the highest in *O. baccatus*, *P. tomentosa* L, then in *Z. coccineum*, and the lowest in *P. undulata.* They concluded that the highest flavonoid quantity was observed in *O. baccatus*, then *P. undulata*, then *P. tomentosa,* and the lowest in *Z. coccineum* (Fig. 4-b).

3.4. Antimicrobial activity

The antimicrobial activity shown in Table 7 was tested against seven pathogens: four Gram-positive bacteria (*Staphylococcus saprophyticus, Staphylococcus epidermidis, Enterococcus faecalis, and Streptococcus salivarius*) and three Gram-negative bacteria

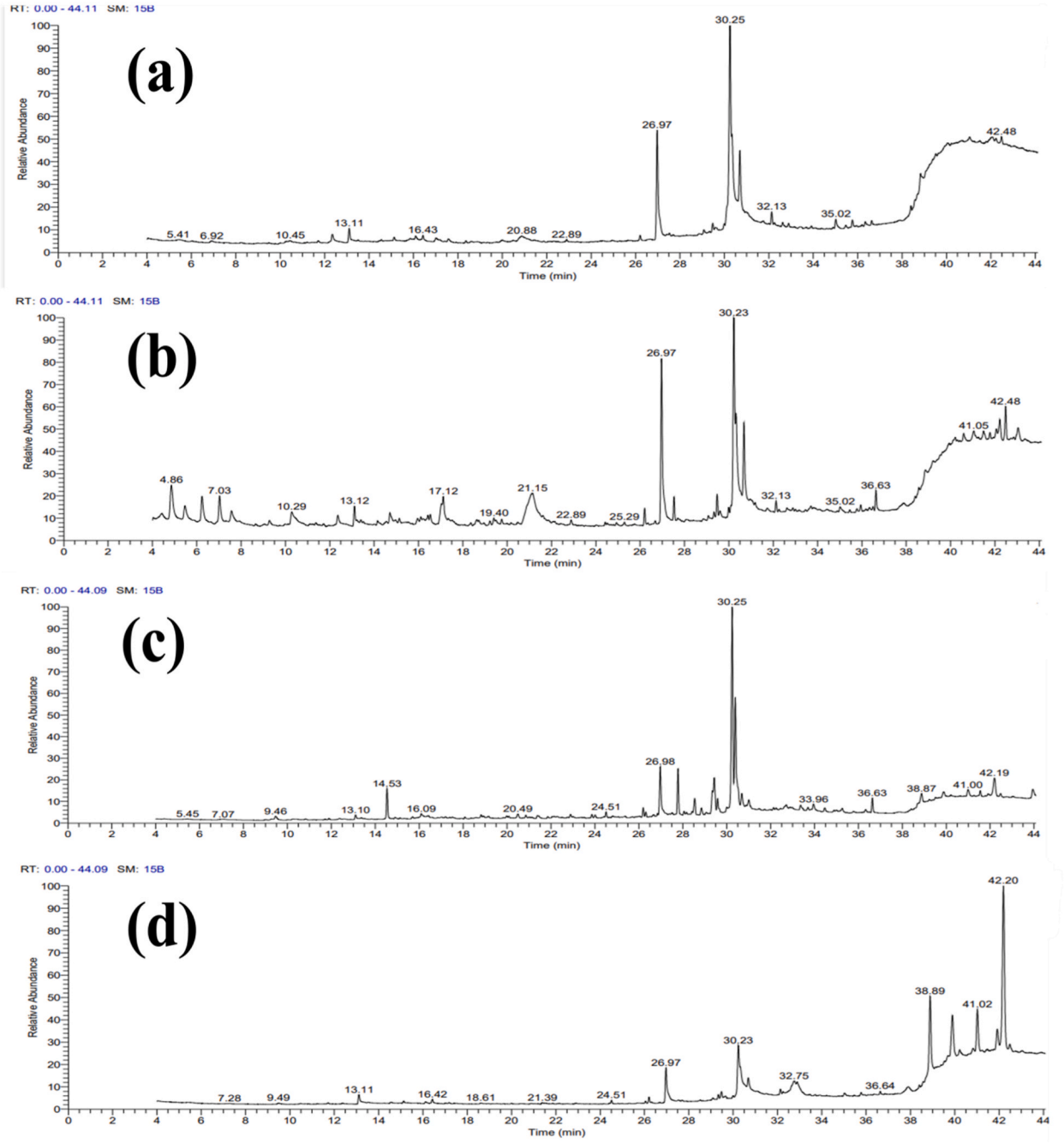

Fig. 2. GC resulted in chromatograms of 70 % ethanol extracts of four plants: (a) *Pulicaria undulata,* (b) *Ochradenus baccatus,* (c) *Pergularia tomentosa and* (d) *Zygophyllum coccineum*.

(*Escherichia coli, Salmonella typhimurium,* and *Pseudomonas aeruginosa*). The extracts against the Gram-positive bacteria demonstrated that *Z. coccineum* exhibited the highest activity, while *P. undulata* showed the lowest activity. For the Gram-negative bacteria, *P. tomentosa* exhibited the highest activity against *Escherichia coli* and *Salmonella typhimurium*, whereas *Z. coccineum* showed the highest activity against *Pseudomonas aeruginosa*.

3.5. Antioxidant activity

The extract of *O. baccatus* displayed the highest total antioxidant capacity including FRAP assay and DPPH radical scavenging capacities, whereas the extract of *Z. coccineum* exhibited the highest superoxide-anion-scavenger activity (Fig. 5).

Table 3
Amino acid concentrations (mg/g DW) across four plant species: Pergularia tomentosa L., Zygophyllum coccineum, Pulicaria undulata, and Ochradenus baccatus. Values are presented as means ± S.E.

Amino acids	*P. tomentosa* L	*Z. coccineum*	*P. undulata*	*O. baccatus*
Glycine	59.690 ± 1.47 b	51.810 ± 1.09 a	51.630 ± 1.04 a	65.840 ± 1.57 c
Lysine	4.417 ± 0.30 a	5.164 ± 0.29 a	5.193 ± 0.11 a	4.817 ± 0.16 a
Histidine	1.757 ± 0.08 b	2.207 ± 0.29 b	0.890 ± 0.07 a	1.456 ± 0.20 ab
Alanine	12.470 ± 0.39 c	8.955 ± 0.18 a	14.31 ± 00.47 d	10.770 ± 0.24 b
Arginie	0.690 ± 0.06 ab	1.254 ± 0.26 b	0.591 ± 0.05 a	1.168 ± 0.04 ab
Ornithine	0.469 ± 0.03 a	0.454 ± 0.02 a	0.510 ± 0.08 a	1.127 ± 0.20 b
Glutamine	0.555 ± 0.06 a	1.791 ± 0.41 a	0.968 ± 0.30 a	2.073 ± 0.68 a
Asparagine	0.359 ± 0.04 a	1.733 ± 0.04 b	1.210 ± 0.03 b	3.189 ± 0.24 c
Isoleucine	0.255 ± 0.04 a	0.229 ± 0.05 a	0.135 ± 0.02 a	1.263 ± 0.02 b
Leucine	0.241 ± 0.03 ab	0.303 ± 0.04 b	0.120 ± 0.02 a	0.232 ± 0.03 ab
Methionine	0.164 ± 0.01 a	0.304 ± 0.06 a	0.135 ± 0.03 a	0.305 ± 0.09 a
Threonine	0.474 ± 0.25 a	0.724 ± 0.27 a	0.571 ± 0.25 a	0.706 ± 0.20 a
Valine	1.027 ± 0.03 b	1.094 ± 0.02 b	0.999 ± 0.02 b	0.870 ± 0.03 a
Serine	0.446 ± 0.13 a	0.272 ± 0.07 a	0.364 ± 0.14 a	0.513 ± 0.18 a
Phenylalanine	1.003 ± 0.27 a	0.937 ± 0.36 a	1.155 ± 0.34 a	1.408 ± 0.39 a
GlutamIic acid	1.157 ± 0.02 a	1.453 ± 0.03 b	1.431 ± 0.03 b	1.639 ± 0.03 c
Aspartate	0.160 ± 0.01 a	0.180 ± 0.01 a	0.191 ± 0.01 a	0.261 ± 0.02 b
Cystine	0.365 ± 0.20a	0.324 ± 0.17 a	0.157 ± 0.08a	0.384 ± 0.17a
Tyrosine	0.767 ± 0.03c	0.641 ± 0.02b	0.316 ± 0.01a	0.640 ± 0.02b

Different letters (a-d) indicate significant (Tukey test $p > 0.05$) differences between different plants species.

Table 4
Fatty acids concentrations (mg/g DW) across four plant species: *Pergularia tomentosa, Zygophyllum coccineum, Pulicaria undulata*, and *Ochradenus baccatus.* Values are shown as means ± S.E.

Fatty acids	P. tomentosa	Z. coccineum	P. undulata	*O. baccatus*
Myristic (C14:0)	0.800 ± 0.01 a	0.970 ± 0.02 b	1.250 ± 0.01 c	2.160 ± 0.02 d
Palmitic (C16:0)	32.05 ± 0.57 a	27.09 ± 1.72a	49.190 ± 1.29 b	77.530 ± 0.39 c
Heptadecanoic (C17:0)	0.077 ± 0.01 a	0.091 ± 0.01 ab	0.125 ± 0.01 b	0.226 ± 0.015 c
Stearic (C18:0)	2.627 ± 0.24 a	2.380 ± 0.21 a	5.052 ± 0.07 b	5.909 ± 0.12 c
Arachidic (C20:0)	1.492 ± 0.04 a	1.701 ± 0.06 ab	2.567 ± 0.31 bc	3.221 ± 0.27 c
Docosanoic (C22:0)	0.726 ± 0.06 a	1.001 ± 0.08 a	1.559 ± 0.12 b	2.050 ± 0.17 b
Tricosanoic (C23:0)	0.057 ± 0.01 a	0.064 ± 0.01 a	0.070 ± 0.01 a	0.066 ± 0.01 a
Pentacosanoic (C25:0)	0.006 ± 0.01 a	0.006 ± 0.01 a	0.007 ± 0.01 a	0.007 ± 0.01 a
Palmitoleic (C16:1)	0.185 ± 0.03 a	0.208 ± 0.03 a	0.223 ± 0.04 a	0.205 ± 0.03 a
Heptadecenoic (C17:1)	0.220 ± 0.03 a	0.194 ± 0.03 a	0.191 ± 0.03 a	0.224 ± 0.02 a
Oleic (C18:1)	58.810 ± 6.68 a	61.90 ± 09.99 a	67.950 ± 10.9a	70.710 ± 5.8a
Linoleic (C18:2)	0.029 ± 0.01 a	0.025 ± 0.01 a	0.025 ± 0.01 a	0.029 ± 0.01 a
Linolenic (C18:3 ω−3)	0.023 ± 0.01 b	0.022 ± 0.00 a	0.0215 ± 0.00 a	0.025 ± 0.01 b
Eicosenoic (C20:1)	1.434 ± 0.16 a	1.298 ± 0.14 a	1.301 ± 0.15 a	1.458 ± 0.14 a
Eicosenoic (C20:1)	0.086 ± 0.01a	0.076 ± 0.01 a	0.075 ± 0.02 a	0.087 ± 0.01 a
Tetracosenoic (C24:1)	0.017 ± 0.00 a	0.017 ± 0.00 a	0.018 ± 0.00 a	0.018 ± 0.00 a

Different letters (a-d) indicate significant (Tukey test $p > 0.05$) differences between different plants species.

3.6. Anti-lipid peroxidation

Z. coccineum had the strongest inhibition of lipid peroxidation while *P. tomentosa* L had the lowest inhibition of lipid peroxidation (Fig. 6).

Table 5
Organic acid concentrations (mg/g DW) across four plant species: *Pergularia tomentosa* L, *Zygophyllum coccineum, Pulicaria undulata*, and *Ochradenus baccatus.* Values are shown as means ± S.E.

Organic acids	*P. tomentosa*	*Z. coccineum*	*P. undulata*	*O. baccatus*
Oxalic	1.800 ± 0.07 a	2.940 ± 0.10 b	1.95 ± 00.06 a	3.082 ± 0.11 b
Malic	13.490 ± 0.55 a	12.550 ± 0.52 a	13.610 ± 0.56 a	27.640 ± 1.15 b
Succinic	9.044 ± 0.24 b	1.430 ± 0.05 a	7.960 ± 0.80 b	9.205 ± 1.01 b
Citric	3.887 ± 0.13 ab	3.055 ± 0.10 a	4.350 ± 0.15 b	9.115 ± 0.33 c
Isobutyric	3.482 ± 0.199 ab	2.245 ± 0.101 a	3.051 ± 0.183 a	4.849 ± 0.549 b
Fumaric	0.305 ± 0.01 b	0.222 ± 0.01 a	0.294 ± 0.01 b	0.491 ± 0.02 c

Different letters (a-d) indicate significant (Tukey test $p > 0.05$) differences between different plants species.

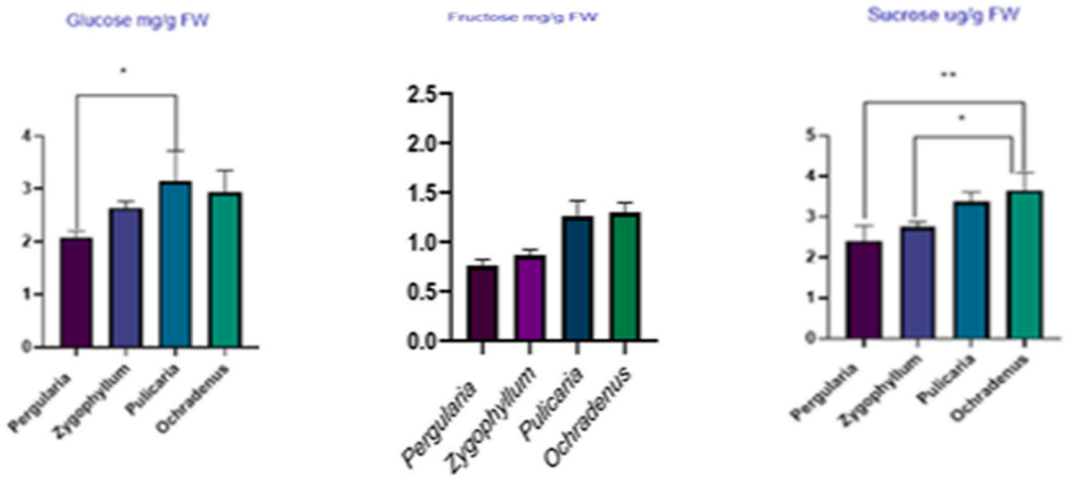

Fig. 3. Sugar content in Pergularia tomentosa, Zygophyllum coccineum, Pulicaria undulata, and Ochradenus baccatus, including: (a) glucose, (b) fructose, and (c) sucrose.

Table 6
Phenolic acids concentrations (mg/g DW) across four plant species: Pergularia tomentosa L., Zygophyllum coccineum, Pulicaria undulata, and Ochradenus baccatus. The values are presented as means ± S.E.

Phenolic acids	*P. tomentosa*	*Z. coccineum*	*P. undulata*	*O. baccatus*
Gallic acid	3.090 ± 0.32 a	2.87 ± 00.17 a	2.870 ± 0.29 a	2.910 ± 0.43 a
Caffeic acid	3.043 ± 0.84 a	2.538 ± 0.90 a	3.190 ± 1.00 a	4.034 ± 1.19 a
***p*-Coumaric acid**	4.536 ± 0.59 a	5.019 ± 0.75 a	5.429 ± 0.74 a	6.400 ± 0.84 a
Chicoric acid	2.765 ± 0.05 a	3.423 ± 0.07 b	3.405 ± 0.07 b	3.991 ± 0.09 c
Rosmarinic acid	1.102 ± 0.42 a	1.051 ± 0.36 a	0.731 ± 0.17 a	1.357 ± 0.39 a
Protocatechuic acid	2.376 ± 0.38 b	2.025 ± 0.32 ab	0.995 ± 0.16 a	2.151 ± 0.31 ab
Quercetin	0.161 ± 0.01 a	0.187 ± 0.01 ab	0.218 ± 0.01 b	0.270 ± 0.01 c
Naringenin	2.360 ± 0.08 a	2.286 ± 0.07 a	2.901 ± 0.10 b	2.934 ± 0.12 b
Kaempferol	2.224 ± 0.08 a	2.120 ± 0.07 a	2.698 ± 0.09 b	2.688 ± 0.11 b
Luteolin	0.013 ± 0.00 a	0.0137 ± 0.00 ab	0.016 ± 0.00 b	0.019 ± 0.00 c
Apigenin	0.008 ± 0.00 a	0.009 ± 0.00 ab	0.010 ± 0.00 bc	0.012 ± 0.00 c
Naringenin	0.046 ± 0.00 a	0.071 ± 0.00 b	0.049 ± 0.00 a	0.075 ± 0.00 b
Rutin	0.365 ± 0.01 a	0.368 ± 0.02 a	0.370 ± 0.01 a	0.730 ± 0.03 b
Chlorogenic acid	0.535 ± 0.02 b	0.332 ± 0.01 a	0.512 ± 0.02 b	0.875 ± 0.02 c

Different letters (a-d) indicate significant (Tukey test $p > 0.05$) differences between different plants species.

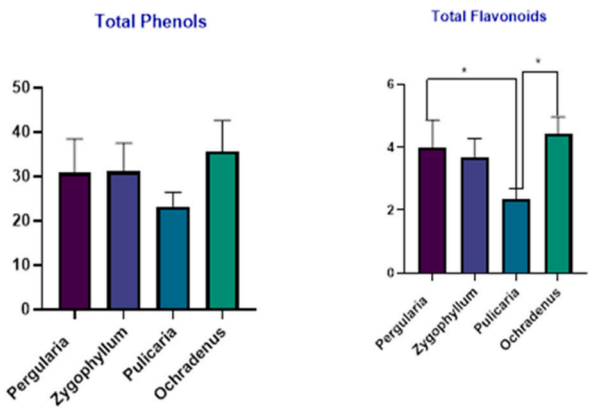

Fig. 4. Content of e total phenolic content analysis (a) and total flavonoids content analysis (b) of the four plants species: *Pergularia tomentosa, Zygophyllum coccineum, Pulicaria undulata*, and *Ochradenus baccatus*.

Table 7
The anti-microbal ctivity of the ethanoic extracts of the four plants species (*Pergularia tomentosa, Zygophyllum coccineum, Pulicaria undulata*, and *Ochradenus baccatus*) and **Gentamicin** against pathogenic bacteria and fungi. ($p < 0,05$) with each Column.

	Gentamicin	*P. tomentosa*	*Z. coccineum*	*P. undulata*	*O. baccatus*
S. saprophyticus	22.0 ± 0.5a	10.79 ± 0.20b	10.6 ± 0.33b	9.73 ± 0.158b	10.08 ± 0.26b
S. pidermidis	23.00 ± 0.57a	12.52 ± 0.31b	12.77 ± 0.39b	11.94 ± 0.23b	12.70 ± 0.34b
E. faecalis	18.00 ± 0.8a	14.00 ± 0.337b	15.93 ± 0.57b	8.122 ± 0.16c	13.44 ± 0.41b
S. salivarius	23 ± 0.2a	8.1 ± 0.17b	9.18 ± 0.33b	6.34 ± 0.11b	7.34 ± 0.23b
E. coli	20 ± 0.58a	14.94 ± 0.33b	14.99 ± 0.47b	13.89 ± 0.25b	8.9 ± 0.24c
S. typhimurium	16 ± 0.3a	7.45 ± 0.18b	2.12 ± 0.07d	5.64 ± 0.11c	7.34 ± 0.21b
P. aeruginosa	17 ± 0.1a	11.84 ± 0.25b	12.42 ± 0.41b	10.4 ± 0.19b	8.35 ± 0.24c

Different letters (a-d) indicate significant (Tukey test $p > 0.05$) differences between different plants species.

3.6.1. *In-silico ADMET profile*

In silico reports of the four natural compounds cis-Vaccenic acid (Pergularia tomentosa), (E)-9-Octadecenoic acid (Zygophyllum coccineum), cyclohepta[b]furan-2-one (Pulicaria undulata) scaffold and URS-20(30)-en-3-ol (Ochradenus baccatus) were conducted for the proposed ADMET profile and evaluation of their physicochemical character (Table 8). It was predicted using SwissADMET and pkCSM descriptor algorithm procedures [46] and matched to the rule of five described by Lipinski [47]. The molecules that accomplish at least three rules were expected to have good absorption properties: (i) No more than 10 hydrogen bond acceptors, (ii) No more than five hydrogen bond donors, (iii) Not more than 5 for logP, (iv) Molecular weight less than 500. In the current work, our compounds do not violate any rule.

3.6.2. *Docking studies*

The mechanism of anti-bacterial drugs generally includes the inhibition of cell wall synthesis, inhibition of protein synthesis, inhibition of nucleic acid (DNA) synthesis and anti-metabolism [48]. In general, the antibiotics inhibit these routes by interacting with specific cell proteins which are responsible for specific activity. Thymidylate kinase (TMPK), a nucleotide 50-monophosphate kinase, contains an evolutionarily conserved essential enzyme which catalyzes the biosynthetic pathway that generates dTTP used for DNA synthesis of bacterial cells [49]. Since antibiotics e.g. ciprofloxacin acts by inhibiting the DNA gyrase which is necessary to separate the bacterial DNA resulting in the cell division inhibition therefore, we took the TMPK and E. coli DNA gyrase as target proteins to explore the molecular interactions between natural ligands and target proteins which are responsible for the antibacterial activity of our compounds.

Molsoft software was used for molecular docking investigations. The Protein Data Bank (PDB) IDs for Thymidylate kinase (PDB: 4QGG) and E. coli (PDB: 5MMN) were used in each experiment, respectively. With the two targeted proteins used the calculated binding affinities explained that the two compounds cis-Vaccenic acid (Pergularia tomentosa) and (E)-9-Octadecenoic acid (Zygophyllum coccineum), exhibited the highest antibacterial activities where they showed the highest binding energies when molecularly docked when compared to the other two compounds cyclohepta[b]furan-2-one (Pulicaria undulata) scaffold and URS-20(30)-en-3-ol (Ochradenus baccatus).

cis-Vaccenic acid exhibited −91.76 kcal/mol and form 4 H-bonds with TMPK (PDB: 4QGG) (Fig. 8A) while against E. coli (PDB: 5MMN) it showed −96.27 kcal/mol and form 7 H-bonds (Fig. 8A). (E)-9-Octadecenoic acid exhibited −92.36 kcal/mol and form 4 H-bonds with TMPK (Fig. 7B) while against E. coli it showed −97.04 kcal/mol and form 7 H-bonds also (Fig. 8B). On the other hand, cyclohepta[b]furan-2-one scaffold (−65.76 kcal/mol) and URS-20(30)-en-3-ol (−59.14 kcal/mol) formed 3 H-bonds each with TMPK (Fig. 8C & D) respectively. While against E. coli cyclohepta[b]furan-2-one scaffold showed −65.84 kcal/mol and form 5 H-bonds (Fig. 8C). Also, URS-20(30)-en-3-ol exhibited −54.71 kcal/mol and form 4 H-bonds (Fig. 8D). These results explained the high

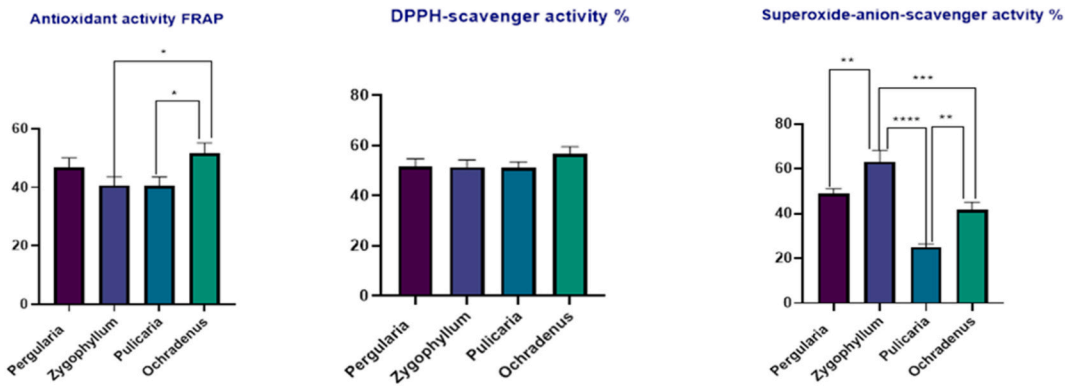

Fig. 5. Antioxidant analysis of four plant species: *Pergularia tomentosa, Zygophyllum coccineum, Pulicaria undulata*, and *Ochradenus baccatus*, including (a) FRAP assay, (b) DPPH radical scavenging capacities, and (c) superoxide-anion-scavenger activity %.

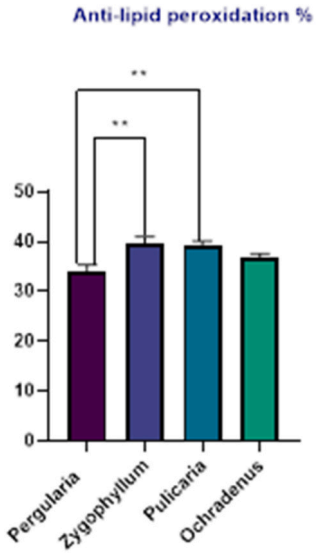

Fig. 6. Anti-lipid peroxidation analysis of ethanolic extracts of the four plants species (*Pergularia tomentosa, Zygophyllum coccineum, Pulicaria undulata*, and *Ochradenus baccatus*).

Table 8
ADMET profile for cis-Vaccenic acid, (*E*)-9-Octadecenoic acid, cyclohepta[b]furan-2-one scaffold and URS-20(30)-en-3-ol.

Parameter	cis-Vaccenic acid	(E)-9-Octadecenoic acid	cyclohepta[b]furan-2-one	URS-20(30)-en-3-ol
Physicochemical properties				
Molecular Weight	282.468	282.468	248.322	426.729
LogP	6.1085	6.1085	2.8097	8.0248
Rotatable Bonds	15	15	3	0
Acceptors	1	1	3	1
Donors	1	1	0	1
Surface Area	125.209	125.209	107.894	192.398
TPSA	37.30	37.30	43.37	20.23
Molar Refractivity	89.94	89.94	70.53	135.14
Volume	318.84	318.84	243.86	461.60
Lipinski	Yes; 1 violation: MLOGP>4.15	Yes; 1 violation: MLOGP>4.15	Yes	Yes; 1 violation: MLOGP>4.15
Water solubility	Moderately soluble	Moderately soluble	Soluble	Poorly soluble
Absorption				
GI absorption	High	High	High	Low
Distribution				
BBB Permeability	No	No	Yes	No
Metabolism				
CYP1A2 inhibitor	Yes	Yes	No	No
CYP2C19 inhibitor	No	No	No	No
CYP2C9 inhibitor	Yes	Yes	No	No
CYP2D6 inhibitor	No	No	No	No
CYP3A4 inhibitor	No	No	No	No

antibacterial activities for both cis-Vaccenic acid/(E)-9-Octadecenoic acid and the lower antibacterial activities of both cyclohepta[b] furan-2-one scaffold and URS-20(30)-en-3-ol.

4. Discussion

The analysis of bioactive compounds present in the 70 % ethanol extracts of Pergularia tomentosa, Z. coccineum, *P. undulata*, and *O. baccatus* provided valuable insights into the chemical composition of these plants. The results revealed the presence of diverse classes of chemical compounds, including fatty acids, esters, sterols, terpenes, alkaloids, hydrocarbons, and aldehydes. Identifying and characterizing these major chemical constituents in the selected plant extracts contribute to the understanding of the chemical diversity and ecological roles of these desert plants. Exploring the chemical profiles of plants found in extreme environments, such as deserts, can provide valuable insights into their adaptations and survival strategies. The identification of specific compounds may also aid in the classification and taxonomy of these plant species.

The results indicate variations in the levels of different amino acids among these plants. *O. baccatus* exhibited the highest levels of

most of the amino acids analyzed, including ornithine, glycine, arginine, isoleucine, methionine, glutamine, serine, phenylalanine, glutamic acid, aspartate, cystine, and asparagine. These findings suggest that *O. baccatus* is particularly rich in these essential and non-essential amino acids. Amino acids are the building blocks of proteins and play crucial roles in various physiological processes [50]. For example, glycine is involved in the synthesis of collagen and plays a role in maintaining healthy skin, joints, and muscles [51]. Arginine and ornithine are important for the urea cycle and play a role in detoxification and ammonia elimination [52]. Lutamine and asparagine are essential for maintaining the integrity of the gastrointestinal tract and supporting immune function [53]. The high levels of these amino acids in *O. baccatus* suggest potential nutritional and health benefits associated with its consumption.

Z. coccineum exhibited higher levels of certain amino acids, including histidine, leucine, threonine, and valine. Histidine synthesizes histamine, a neurotransmitter involved in various physiological processes [54]. Leucine, threonine, and valine are essential amino acids that play important roles in protein synthesis and muscle maintenance [55]. *P. undulata* also relatively higher levels of lysine and alanine. Lysine is an essential amino acid that plays a role in protein synthesis, collagen formation, and calcium absorption [56]. Alanine is a non-essential amino acid that contributes to glucose metabolism and participates in the formation of other amino acids [57]. *P. tomentosa* exhibited the lowest levels for most of the detected amino acids. Tyrosine is a non-essential amino acid that produces neurotransmitters and hormones, such as dopamine and thyroid hormone [58]. The lower levels of other amino acids in *P. tomentosa* L compared to the other plant species may indicate its relatively lower nutritional value regarding amino acid content. Overall, the presence of these amino acids in suggests potential nutritional value of targeted species.

O. baccatus demonstrated the highest levels of most fatty acids. Fatty acids are essential components of lipids and play crucial roles in various physiological processes [59]. Myristic, palmitic, and stearic acids are saturated fatty acids that contribute to the structure and stability of cell membranes [60]. Oleic, linoleic, and linolenic acids are unsaturated fatty acids important for maintaining cardiovascular health and supporting the immune system [61]. *P. undulata* exhibited higher levels of specific fatty acids, including tricosanoic (C23:0), palmitoleic (C16:1), and tetracosenoic (C24:1). Tricosanoic and pentacosanoic acids are long-chain saturated fatty acids that are less commonly found in plant sources [62]. Palmitoleic acid is a monounsaturated fatty acid associated with anti-inflammatory properties and potential health benefits [63]. Tetracosenoic acid is a monounsaturated fatty acid involved in various physiological processes [64]. Oxalic acid is a dicarboxylic acid found in various plant sources, known for its sour taste [65]. It is commonly used as a food additive and has been associated with antioxidant and chelating properties [66]. Malic acid is a dicarboxylic acid involved in the Krebs cycle, which plays a role in cellular energy production [67]. Succinic acid is another dicarboxylic acid involved in metabolic processes and has potential therapeutic applications, including antioxidant and anti-inflammatory properties [68]. Citric acid, a tricarboxylic acid, is widely used as a flavoring agent and preservative in the food and beverage industry [69],and it is also a key component of the Krebs cycle, essential for cellular respiration [70]. Isobutyric acid is a short-chain fatty acid naturally produced during the metabolism of certain amino acids [71]. Fumaric acid, a dicarboxylic acid involved in the Krebs cycle, has been investigated for its potential therapeutic applications, particularly in supporting immune function [72]. The analysis results indicate variations in sugar and phenolic acid levels among the tested plants, with *O. baccatus* showing the highest content and P. tomentosa L the lowest. Total sugars are an important component of the human diet and play a vital role in providing energy for various physiological processes [73]. The high sugar content in *O. baccatus* suggests that it can serve as a rich source of carbohydrates, which not only provide energy but also enhance the taste and palatability of foods [74]. In addition to sugars, the analysis measured the levels of various phenolic acids in the tested plants. Phenolic acids are a diverse group of compounds known for their antioxidant properties and potential health benefits [75]. *O. baccatus* exhibited the highest concentrations of several phenolic acids, including caffeic acid, *p*-coumaric acid, chicoric acid, rosmarinic acid, quercetin, naringenin, luteolin, apigenin, rutin, and chlorogenic acid. These compounds are recognized for their antioxidant, anti-inflammatory, and antimicrobial properties, among other health benefits [76]. The high levels of these phenolic acids in *O. baccatus* suggest its potential as a rich source of bioactive compounds. Total phenolic content is an important parameter used to assess the presence of phenolic compounds known for their antioxidant and potential health-promoting effects [77]. Flavonoids, a subclass of phenolic compounds, are known for their antioxidant and anti-inflammatory properties [78]. The results indicate variations in antimicrobial activity among the tested plant species. *Z. coccineum* exhibited the highest antimicrobial activity against Gram-positive bacteria, while *P. undulata* displayed the lowest. P. tomentosa L showed the highest activity against Gram-negative bacteria, specifically *Escherichia coli* and *Salmonella typhimurium*, while *Z. coccineum* demonstrated the highest activity against *Pseudomonas aeruginosa*. These findings suggest that the tested plant species possess varying antimicrobial properties, likely due to bioactive compounds with antimicrobial potential.

The antioxidant capacity of the plant extracts was assessed using various assays. *O. baccatus* displayed the highest values in the FRAP assay and DPPH radical scavenging capacities, indicating its strong antioxidant potential. *Z. coccineum* exhibited the highest superoxide anion scavenger activity. These results suggest that *O. baccatus* and *Z. coccineum* possess notable antioxidant properties, which may contribute to their potential health benefits. Furthermore, the anti-lipid peroxidation activity of the plant extracts was evaluated. *Z. coccineum* exhibited the strongest inhibition of lipid peroxidation, indicating its potential as a protective agent against oxidative damage. In contrast, P. tomentosa L showed the lowest inhibition of lipid peroxidation.

According to ADMET data (Table 8), we can adopt that our compounds cis-Vaccenic acid, (*E*)-9-Octadecenoic acid, cyclohepta[b] furan-2-one scaffold showed high GIT absorption in human which indicates easier to cross different biological membranes [76]. So, they may show a significantly good bioavailability through GIT. Compound URS-20(30)-en-3-ol exhibited low GIT absorption. Concerning BBB penetrability, our compounds cis-Vaccenic acid, (*E*)-9-Octadecenoic acid and URS-20(30)-en-3-ol cannot reach CNS so no side effects while the other compound can penetrate CNS. It is well known that CYP3A4, the major drug-metabolizing enzyme, couldn't be inhibited by our compounds.

The data obtained from molecular docking is highly correlated with that obtained from biological activities. cis-Vaccenic acid exhibited high antibacterial and high binding affinity toward TMPK (PDB: 4QGG) with −91.76 kcal/mol and form 4 H-bonds with

Arg36 (1.79 Å and 1.79 Å) and *Arg48* (1.72 Å and 1.88 Å) Moreover, the remaining structure occupies the hydrophobic pocket formed by *Phe66, Glu62, Arg105, Gln101, Phe159, Tyr100, Glu11, Arg92* and *Arg70* (Fig. 7A) while against *E. coli* (PDB: 5MMN) it showed −96.27 kcal/mol and form 7 H-bonds with *Arg76* (2.50 Å, 2.52 Å, 2.56 Å, 2.64 Å and 2.65 Å), and *Arg136* (1.51 Å and 2.76 Å). Moreover, the remaining structure occupies the hydrophobic pocket formed by *Gly164, Gly77, Thr165, Ile78, Met166, Val167, Val120, Val43, Asn46, Ala47, Glu50* and *Asp73* (Fig. 8A). (*E*)-9-Octadecenoic acid exhibited −92.36 kcal/mol against TMPK and form 4 H-bonds with *Arg36* (1.62 Å and 1.67 Å) and *Arg48* (1.88 Å and 2.64 Å) (Fig. 7B) while against *E. coli* it showed −97.04 kcal/mol and form 7 H-bonds with *Arg76* (2.50 Å, 2.52 Å, 2.59 Å, 2.67 Å and 2.68 Å), and *Arg136* (1.62 Å and 2.75 Å) (Fig. 8B).

On the other hand, cyclohepta[b]furan-2-one scaffold against TMPK showed −65.76 kcal/mol and formed 3 H-bonds with *Arg70* (1.85 Å and 2.41 Å) and *Ser69* (1.74 Å) (Fig. 7C). URS-20(30)-en-3-ol against TMPK exhibited −59.14 kcal/mol and formed 3 H-bonds with *Arg48* (1.41 Å, 1.72 Å and 2.76 Å) (Fig. 7D). While against *E. coli* cyclohepta[b]furan-2-one scaffold showed −65.84 kcal/mol and form 5 H-bonds with *Thr165* (1.63 Å and 2.59 Å), *Asn46* (2.57 Å), *Gly77* (2.48 Å) and *Ile78* (2.20 Å) (Fig. 8C). Also, URS-20(30)-en-3-ol against *E. coli* exhibited −54.71 kcal/mol and form 4 H-bonds with *Arg76* (1.54 Å, 2.31 Å and 2.97 Å) and *Glu50* (1.86 Å) (Fig. 8D). These results explained the high antibacterial activities for both cis-Vaccenic acid/(*E*)-9-Octadecenoic acid and the lower antibacterial activities of both cyclohepta[b]furan-2-one scaffold and URS-20(30)-en-3-ol.

5. Conclusion

In conclusion, this study examined the phytochemical composition, antimicrobial, and antioxidant activities of four desert plants from Wadi Sannor, Beni-Suef Governorate, Egypt: P. tomentosa, Z. coccineum, P. undulata, and *O. baccatus*. Phytochemical analysis identified key compounds in the ethanol extracts of these plants. P. tomentosa contained trans-13-octadecenoic acid and n-hexadecanoic acid. Z. coccineum included 9-octadecenoic acid, n-hexadecanoic acid, trans-13-octadecenoic acid, octadecanoic acid, and dodecanoic acid. P. undulata featured 2H-cyclohepta[b]furan-2-one and n-hexadecanoic acid, while *O. baccatus* contained lupeol, olean-12-en-3-ol acetate, trans-13-octadecenoic acid, and α-amyrin. Antimicrobial tests showed Z. coccineum had the highest activity against Gram-positive bacteria, and P. tomentosa was most effective against Gram-negative bacteria, indicating their potential as

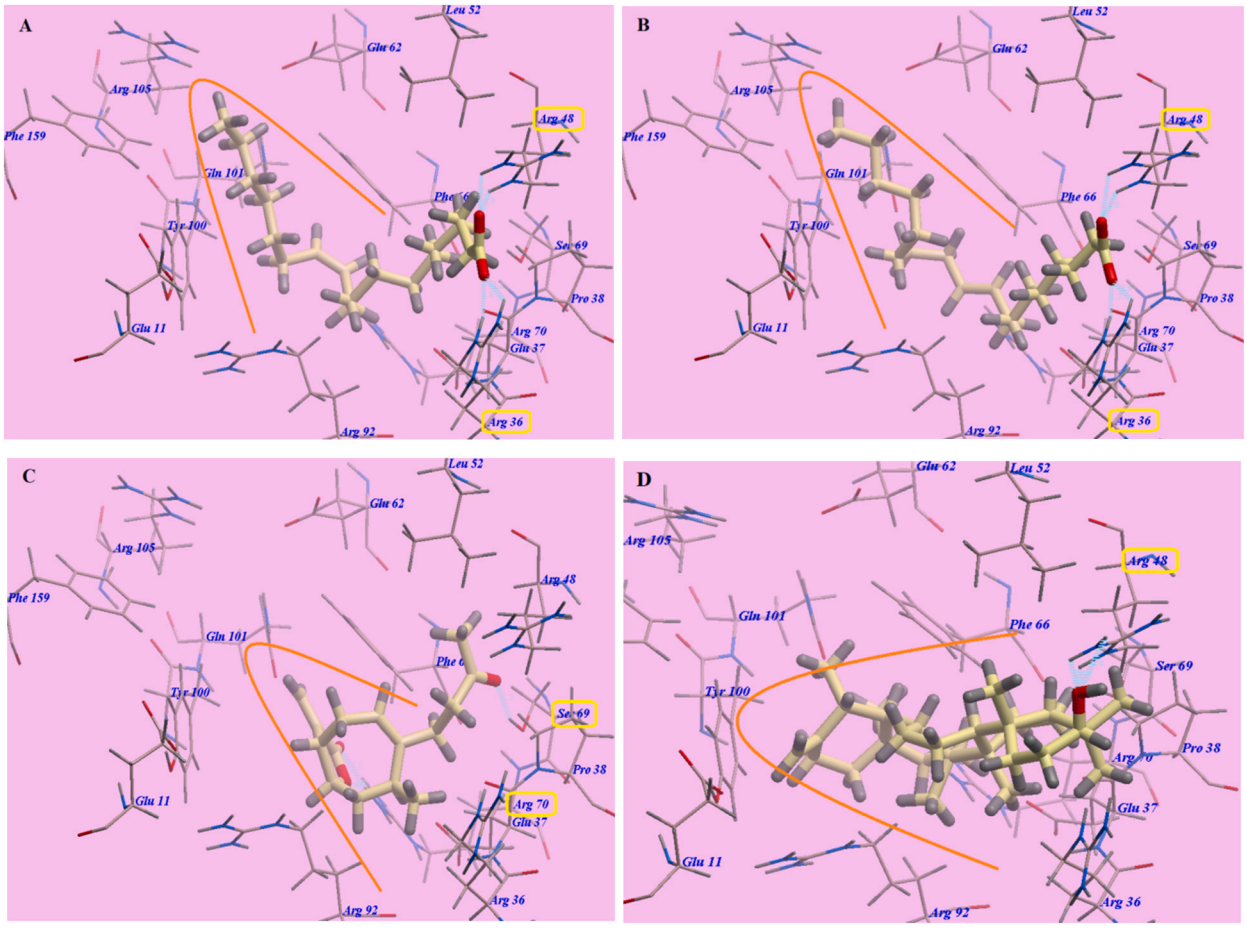

Fig. 7. Docking of our compounds in the active site of 4QGG **A)** cis-Vaccenic acid, **B)** (*E*)-9-Octadecenoic acid, **C)** cyclohepta[b]furan-2-one scaffold and **D)** URS-20(30)-en-3-ol.

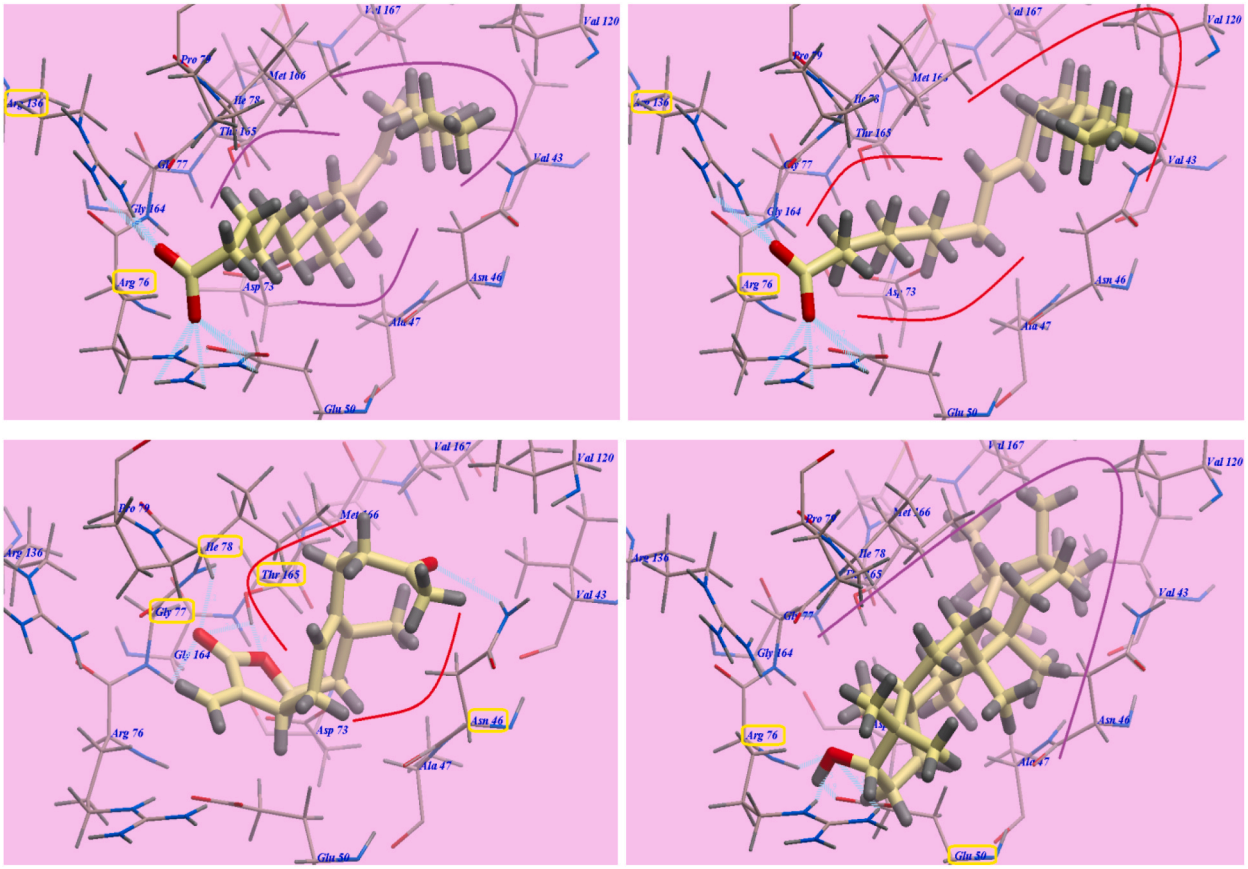

Fig. 8. Docking of our compounds in the active site of 5MMN **A)** cis-Vaccenic acid, **B)** (*E*)-9-Octadecenoic acid, **C)** cyclohepta[b]furan-2-one scaffold and **D)** URS-20(30)-en-3-ol.

natural antimicrobial agents. Antioxidant activity was highest in *O. baccatus*, evidenced by FRAP assay values and DPPH radical scavenging capacities, with Z. coccineum showing the highest superoxide-anion-scavenger activity. Molecular docking for cis-vaccenic acid, (E)-9-octadecenoic acid, cyclohepta[b]furan-2-one, and URS-20(30)-en-3-ol against thymidylate kinase and E. coli DNA gyrase active sites correlated well with biological data. These compounds also exhibited favorable ADMET profiles, including high GIT absorption and no CYP3A4 inhibition.

CRediT authorship contribution statement

Amany H. El-Zairy: Methodology. **Hussein S. Mohamed:** Writing – original draft. **Shimaa A. Ahmed:** Methodology. **Sayed A. Ahmed:** Writing – review & editing. **Mohammad K. Okla:** Resources. **Khaled El-Adl:** Formal analysis. **Hamada AbdElgawad:** Formal analysis. **Wael N. Hozzein:** Supervision.

Ethical approval

This article does not include any studies that use human or animal tissues.

Availability of data and materials

The data that support the findings of this study are available on request.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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