Integrated Profiling by Gc-Ms And in Silico Evaluation of The Bioactive Components of The Ethanolic Extract of Capparis Spinosa L.: Pharmacokinetic, Toxicological and Molecular Docking Perspectives

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Abstract
Background: The caper plant (*Capparis spinosa*) is a medicinal plant known for various pharmacological properties that largely reflect its rich chemical composition. This research sought to determine the chemical components of the plant's ethanolic extract by gas chromatography-mass spectrometry (GC-MS) and to assess the physicochemical characteristics, pharmacokinetic profile, itoxicity., andl anti-inflammatoryl potential of the most abundant compounds in the extract through (in silico) analysis.
Methods: Aerial parts of (C. spinosa) were collected from Babylon Governorate, Iraq, and extracted using 95% ethanol via maceration for 24 hours. GC-MS analysis was performed using an Agilent system. The major chemical constituents were evaluated using SwissADME to predict physicochemical and pharmacokinetic properties, ProTox-3 to assess toxicity, and CD-Dock2 to conduct molecular docking studies with the cyclooxygenase-2 (COX-2) enzyme. Results: GC-MS analysis revealed the presence of several volatile phytochemicals, with the most chromatographically abundant compounds being: dodecenol(Z) isomers (34.63%, 20.31%, 14.47%), cis-vaccenic acid (15.87%), and N-hexadecanoic acid (9.74%). Furthermore, the computational analysis showed physicochemical properties consistent with Lipinski's five-part rule for the studied compounds. The SwissADME program predicted high gastrointestinal absorption and acceptable drug profiles if taken orally. The ProTox-3 program showed relatively low acute toxicity for most of the studied compounds. Molecular simulations also showed moderate interaction with the active site of the cyclooxygenase enzyme (COX-2), with hexadecanoic acid exhibiting the strongest binding affinity among the studied chemical substituents. In conclusion, Investigations utilizing gas chromatography-mass spectrometry (GC-MS) and computational methods revealed that the ethanolic extract of C. spinosa is abundant in biologically significant fatty acids and long-chain alcohols that demonstrate encouraging pharmacological effects and anti-inflammatory capabilities. These results support further experimental studies to validate the identified compounds as potential natural therapeutic agents.

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1. Introduction

Medicinal flora represent the paramount supply of bioactive chemical entities in pharmaceutical investigation, which have structural variety and extensive activity. Herbal medicines form a crucial component of primary health care for about 80% of the world's population, directly or indirectly, and are the source of many of the medicines currently approved for use. Therefore, investigations of medicinal plants are gaining importance for the discovery of new therapeutic agents which have better efficacy

and less side effects. The caper tree Capparis spinosa L. (Capparaceae) is a medicinal plant which has been the subject of a great deal of scientific research because of its nutritional and traditional medicinal properties. The roots, flower, buds, fruits and seeds of the plant are used for medicinal purposes in treating inflammatory diseases, rheumatism, diabetes, hypertension, liver ailments and digestive disorder[2]. Many of the traditional uses of C. spinosa have been verified by modern pharmacological studies as having anti-inflammatory, antioxidant, antimicrobial, hepatoprotective, neuroprotective, anticancer, and antidiabetic properties[3]. The biological activity of C. spinosa is most likely due to its varied chemical composition. Several classes of secondary receptor have been examined in the past: phenolic acids, glucosinolates, terpenoids, alkaloids, tocopherols, fatty acids, flavonoids, sterols and volatile compounds. These compounds demonstrate pharmacological effects via multiple mechanisms, such as scavenging free radicals, modulating inflammatory cytokines, inhibiting lipid peroxidation, suppressing oxidative stress, and regulating intracellular signaling pathways linked to chronic inflammation and cancer development [2,4]. Gas chromatography-mass spectrometry (GC-MS) is among the most dependable methods forlthe qualitativel and semii-quantitative examination of volatile and semi-volatile chemicals in medicinal plants. This method integrates high-resolution chromatography with mass spectrometry, facilitating fast analysiss and identificationh of the physiologically active constituents of intricate plant extracts. GC-MS has emerged as an essential analytical instrument in phytochemical research, offering vital insights into the chemical constituents that contribute to the biological efficacy of medicinal flora [5]. Although describing the chemical constituents of plants provides important information about their structure, successful drug discovery requires further evaluation of pharmacokinetic behavior and pharmacodynamic properties prior to experimental biological testing. Computer simulation has enabled the rapid prediction of these properties, given the advancements in computational pharmacology, which have reduced the cost and time required for development and research, while improving candidate selection during the early stages of drug discovery and development [6]. The SwissADME program has become one of the most widely accepted platforms for predicting physicochemical properties, water solubility, bioavailability, gastrointestinal absorption, blood-brain barrier permeability, lipophilicity, and adherence to Lipinski's five-point rule. These predictions provide an early assessment of the suitability of compounds for oral administration as medicines and facilitate the prioritization of promising natural compounds for further pharmacodynamic evaluation [6]. Similarly, computational toxicology hasjemerged as an importantktool in modern drug discovery. The ProTox-3 platform predicts oral toxicity, molecular toxicity targets, toxicity classes, and toxicity endpoints using machine learning algorithms trained on experimentally validated datasets. These predictions provide a preliminary assessment of a compound's safety prior to *in vitro* safety testing [7]. One of the fundamental computational methods used to predict ligand-protein interactions is molecular docking, which plays a role in understanding the potential mechanisms of drug activity. Cyclooxygenase-2 (COX-2) plays a crucial role in prostaglandin synthesis and inflammatory responses, making it an important inflammatory biomarker. COX-2 overexpression has been associated with chronic inflammation, cardiovascular disorders, rheumatoid arthritis, osteoarthritis, and various cancers. Consequently, inhibiting COX-2 is a key therapeutic target in the development of novel anti-inflammatory agents. The CB-Dock2 platform is an important tool for the automated detection of cavities and molecular docking, providing predictions of ligand affinity and interaction patterns with target proteins [8]. Many studies focus on the biological activities of the caper plant (Capparis spinosa). However, studies integrating the characterization of phytochemicals with computational analyses of pharmacokinetics, toxicity, and molecular interactions remain relatively limited, particularly for plant materials. Therefore, this study also applies GC-MS analysis to samples extracted from caper fruits (Capparis spinosa) collected in Babylon, Iraq, and evaluates the pharmacokinetic, toxicity, and molecular interaction characteristics of the dominant phytochemicals using software such as SwissADME, ProTox-3, and CB-Dock2. This integration of appropriate experimental equipment with modern computer systems and advanced information systems will enable the identification of potential samples and their inclusion in scientific databases for future biological and agricultural studies.

2. Materials and Methods

2.1. Collection of plantimaterials

In April 2026 the aerial parts of the spiny caper plant were collected from Babylon Governorate in Iraq. Collected parts were rinsed with distilled water and left to air dry in the shade at room temperature until they were completely dry. The dried plants were then powdered with an electric grinder and kept in tightly sealed containers until being extracted.

2.2. Preparation of the ethanolic extract

About 50g of plant material was extracted by soaking in 100mL of 95% ethanol for 24j hours at roomttemperature, with intermittent stirring. The mixture was filtered after extraction on Whatman No 1 filter paper for the removal of plant debris. Heat sensitive phytochemicals were retained by concentrating the filtrate under reduced pressure by rotary evaporation at temperature below 45 °C. The concentrated crude extract was then poured into amber-coloureddglass bottles and kept at 4 °C for further phytochemical analysis and computation.

2.3. GC-MSianalysiss

The chemical examination of the ethanolic extract was conducted utilizing gas chromatography-mass spectrometry (GC-MS) from Agilent. A microliter of the prepared sample was administered at a 1:30 ratio, with the syringe temperature held at 250 degrees Celsius prior to injection. The sample was diluted with 1 ml of high-purity ethanol suitable for HPLC, utilizing helium as an inert gas at a steady flow rate of 1.0 ml/min and a column pressure of 10 psi. The oven's temperature setting was established at 100 degrees Celsius with a duration of 3 minutes. The temperature increased at a pace of 5 degrees per minute until it reached 210 degrees Celsius, maintained for 5 minutes, followed by a rise of 10

degrees per minute to 280 degrees Celsius, also sustained for 5 minutes. Regarding mass spectrometry, the spectra were acquired over a scanning range of 1 to 2000 m/z, and the compounds were identified by juxtaposing thelobtained massspectra with those in the NationallInstitute of Standardssand Technology (NIST.) mass spectrometry library, utilized for large-scale identification of plant chemical compounds in GC-MS analyses.

2.4. Selection of Major Phytochemical Components

Chromatographic analysis revealed several volatile compounds. The compounds that showed the highest chromatographic abundance were selected for computational studies. These included Z-dodecenol isomers, n-hexadecanoic acid, and cis-vaccinic acid, which represent the main biologically active components detected in the ethanolic extract.

2.5. Physicochemical and ADME Prediction

To predict the physicochemical properties and pharmacokinetic behavior of selected plant compounds using the swissADME platform. The PubChem database was used to obtain SMILES codes sent to swissADME for the analysis of the following molecular indices: molecular formula, molecular weight, hydrogen bond donors (HBD), hydrogen bond acceptors (HBA), topological polar surface area (TPSA), spin-coupled bonds, agreed distribution coefficient (LogP), gastrointestinal absorption, blood-brain barrier permeability, water solubility, Lipinski's five-point rule, and bioavailability index. These criteria were used to assess the suitability of specific plant compounds for oral medicinal use and to predict their pharmacokinetic suitability. The SwissADME platform is one of the most widely used platforms for early prediction of absorption, distribution, metabolism, and excretion processes in natural product research.

2.6. Toxicity Prediction

To predict the toxic properties of the selected compounds, the ProTOX-3 platform was used, which provided an initial estimate of the compound's safety prior to experimental toxicity assessment. The computational assessment via this platform included: the lethal oral dose (LD50), toxicity class, predictive accuracy, structural similarity, and toxicological targets.

2.7. Molecular Docking Analysis

The CB-Dock2 platform was used to perform molecular docking to evaluate the anti-inflammatory properties of selected chemical compounds. The crystal structure of human cyclooxygenase-2 (COX-2) from the protein bank ID IKR5 was selected as the target receptor. CB-Dock2 detected the most likely binding cavities, and docking calculations were performed using the AutoDock Vina algorithm, expressing electron affinity as a Vina index (kcal/mol). The cavity size and reacting amino acid residues were recorded. Cycloxib was used as a reference inhibitor to compare docking performance. CB-Dock2 demonstrated accuracy in identifying binding sites and predicting binding positions by incorporating template-based cavity detection.

3. Result

3.1. GC-MS Phytochemical Analysis

Gas chromatography-mass spectrometry (GC-MS) analysis of the ethanolic extract of caper plant (Capparis spinosa LL.) revealed thirteen chemical compounds representing a variety of volatile plant compounds, including long-chain alcohols, fatty acids, esters, hydrocarbons, and heterocyclic compounds. These compounds were identified based on retention time, molecular formula, molecular mass, similarity to the instrument database, and the percentage of chromatographic peak area. The fiveecompoundsswith the highest chromotogrphic peak area, represented the major fraction offthe detected profile, are shown in Table 1.

Table 1: Main phytochemicals identified in the ethanolic extract of Caper spinosa by GC-MS analysis.

Peak Area (%)	Molecular Weight (g/mol)	Compound	Retention Time (min)	Peak No.
9.742	256	n-Hexadecanoic acid	13.303	3
34.625	184	Z-4-Dodecenol	15.236	6
14.465	184	3-Dodecen-1-ol, (Z)	15.349	7
20.305	184	3-Dodecen-1-ol, (Z)	15.414	8
15.869	254	cis-Vaccenic acid	15.510	9

The results showed that (Z)-4-dodecenol was the most abundant compound in the extract, representing 34.625% of the total peak area. It was followed by 3-dodecen-1-ol (Z), which appeared in two separate peaks, with 20.305% and 14.465%. cis-vaccenic acid and n-hexadecanoic acid represented 15.869% and 9.742%, respectively. The remaining compounds appeared in low percentages, none exceeding 1% of the total peak area.

Figure 1 illustrates the chromatogram obtained by GC-MS analysis, showing the distribution of the chromatographic peaks of the separated compounds according to their retention times. A clear difference in peak intensity was observed depending on the relative abundance of each compound.

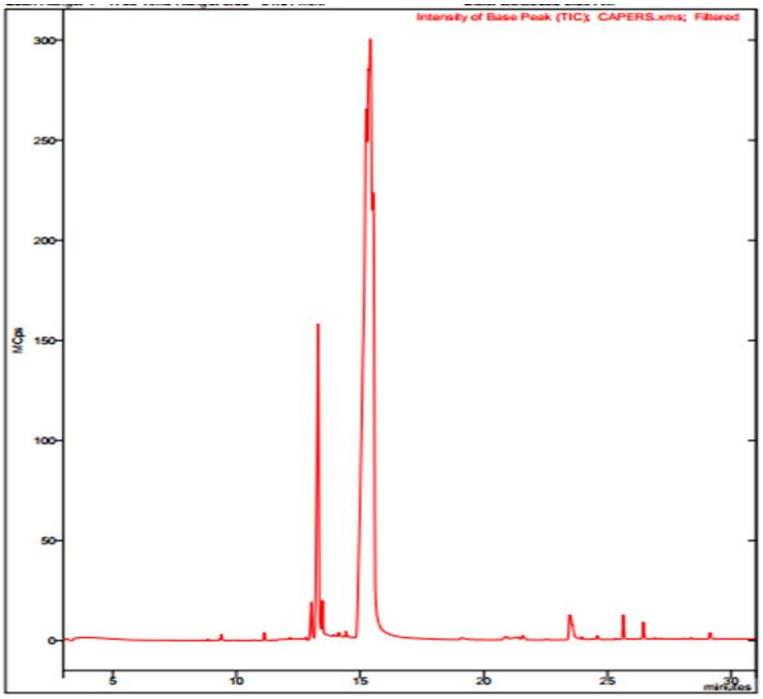


Fig 1: GC-MS chromatogram of the ethanolic extract of Capparis spinosa L.

The outcomes suggested that the ethanolic extract of Caper plant was rich with a lots of chemical constituents, mainly long-chain alcohols and unsaturated fatty acids. Many reports indicate that these compounds have potential pharmacological activities such as antioxidant, anti-inflammatory and antimicrobial properties. This helps to identify the compounds that are going to be used in computational analysis for further studies such as pharmacological studies, toxicity prediction, and molecular docking studies.

3.2. In Silico Prediction of Physicochemical and Pharmacokinetic Properties

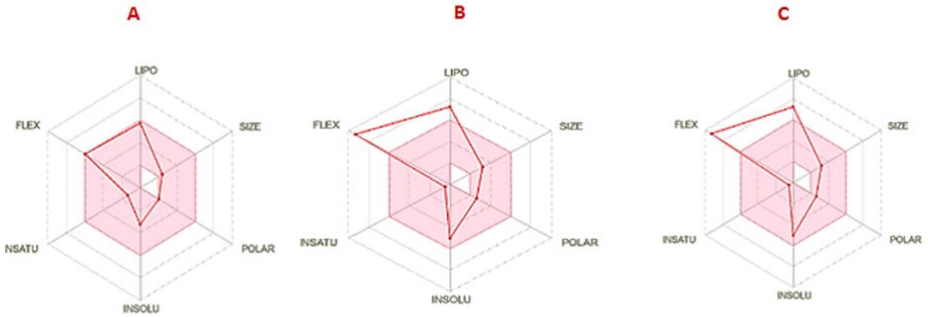
Based on the GC-MS analysis results, three main compounds—3-dodecen-1-ol (Z), n-hexadecanoic acid, and cis-vaccenic acid—were selected for computational evaluation using the SwissADME platform to study their physicochemical properties and suitability as drug candidates.

The results showed that all three compounds exhibited suitable physicochemical properties, with molecular weights ranging from 184.32 to 256.42 g/mol and total surface area polarity (TSAP) values between 20.23 and 37.30 Å². All compounds also showed a low number of hydrogen bond donors and acceptors, while consensus LogP values ranged from 3.41 to 5.54, reflecting moderate to high lipophilicity in the selected compounds, as detailed in Table 2.

Tables 2: Physical and chemicallpropertiessand pharmacodynamic predictions of selected compoundss using the SwissADME platform.

Consensus LogP	Rotatable Bonds	HBD	HBA	TPSA (Å²)	Molecular Weight (g/mol)	Molecular Formula	Compound
3.41	10	1	1	20.23	184.32	$C_{12}H_{24}O$	3-Dodecen-1-ol, (Z)
5.54	14	1	2	37.30	256.42	$C_{16}H_{32}O_2$	n-Hexadecanoic acid
5.27	13	1	2	37.30	254.41	$C_{16}H_{30}O_2$	cis-Vaccenic acid

To give a visual representation of how well these properties meet the requirements of oral bioavailability, Figure (2) shows the bioavailability radar plot of the selected compounds, where most values are within or close to the ideal range of pharmacokinetic properties With slight differences related to the degree of lipophilia.



A: 3-Dodecen-1,ol (Z), B: n-Hexadecanoic acid, C: cis-Vaccenic acid

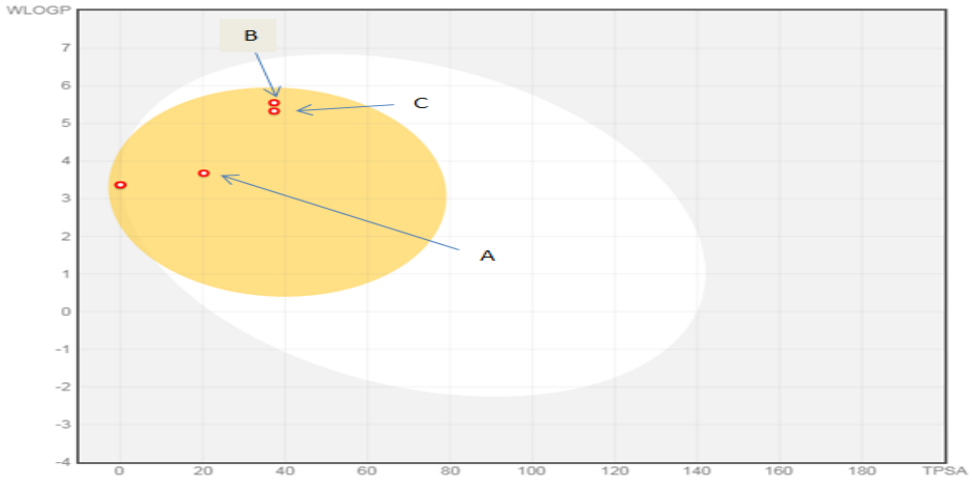
Fig 2: Bioavailability radar chart for selected compounds generated by the SwissADME platform.

The SwissADME platform was utilized to assess the pharmacokinetic characteristics and drug development potential of the compounds. The findings indicated that all drugs demonstrated significant gastrointestinal absorption, and the platform forecasted their capacity to traverse the blood-brain barrier. Moreover, the findings demonstrated that the compounds do not serve as substrates for P-glycoprotein, displaying differing levels of water solubility; 3-dodecen-1-ol (Z) exhibited great solubility, whereas the fatty acids showed moderate solubility. Moreover, the compounds exhibited strong adherence to Lipinski's Rule of Five and achieved advantageous bioavailability ratings, as illustrated in Table 3.

Table 3: Predicted pharmacokinetic and drug similarity properties for the selected phytochemicals using Swiss ADME.

Bioavailability Score	Lipinski	Water Solubility	P-gp Substrate	BBB Permeant	GI Absorption	Compound
0.55	Yes (0)	Soluble	No	Yes	High	3-Dodecen-1-ol, (Z)
0.85	Yes (1)	Moderately soluble	No	Yes	High	n-Hexadecanoic acid
0.85	Yes (0)	Moderately soluble	No	Yes	High	cis-Vaccenic acid

The cooked egg technique was employed to investigate the possibilities of intestinal absorption and infiltration into the central nervous system. The findings indicated that the chosen compounds were situated in the area linked to elevated intestinal absorption, with an anticipated ability to traverse the blood-brain barrier, suggesting they have pharmacokinetic characteristics appropriate for oral administration, as depicted in Figure (3).



A: 3-Dodecen-1,ol (Z), B: n-Hexadecanoic acid, C: cis-Vaccenic acid

Fig 3: A BOILED-EGG diagram illustrating anticipated gastrointestinal absorption (HIA) and blood-brain barrier permeability (BBB) of certain phytochemicals produced using SwissADME.

3.3. Toxicological Prediction

To obtain a preliminary safety assessment of thelselected compoundss, a predictive analysis was performedlusing the ProTox-3 platform. This platform employs machine learning models to predict acute toxicity and classify compounds according to the Globally Harmonized System (GHS), as well as to estimate median lethal dose (LD_{50}) values and other toxicity indicators.

The results showed differences among the compounds in LD_{50} values and toxicity classification. However, all compounds presented acceptable preliminary toxicity profiles and did not show high toxicity predictions that would limit their use in preliminary drug discovery studies. The results also showed limited variation in the probability of association with some toxicity targets, while the prediction accuracy remained within acceptable limits for the model used, as shown in Table 4.

Table 4: Predicted toxicity profile of the selected compounds using ProTox-3

Toxicity Targets	Prediction Accuracy (%)	Average Similarity (%)	Toxicity Class	LD50 (mg/kg)	Compound
Androgen receptor, Amine oxidase A	70.97	81.36	4	1016	3-Dodecen-1-ol, (Z)
Androgen receptor, Amine oxidase A, Glucocorticoid receptor, Prostaglandin G/H Synthase 1, Progesterone receptor	100	100	4	900	n-Hexadecanoic acid
Androgen receptor, Amine oxidase A, Prostaglandin G/H Synthase 1, Progesterone receptor	100	100	2	48	cis-Vaccenic acid

LD_{50}: Median lethal dose; Toxicity class according to the Globally Harmonized System (GHS); Average similarity and Prediction accuracy were obtained from the ProTox-3 prediction Model.

These results indicate that the selected compounds have an adequate level of predictive safety, which justifies their continued evaluation through molecular docking studies.

3.4. Moleculari Dockingi Analysis

A molecularrdocking research was conducted utilizing the CB-Dock2 platform to examine the interaction potential of the chosen drugs with the cyclooxygenase-2 (COX-2)

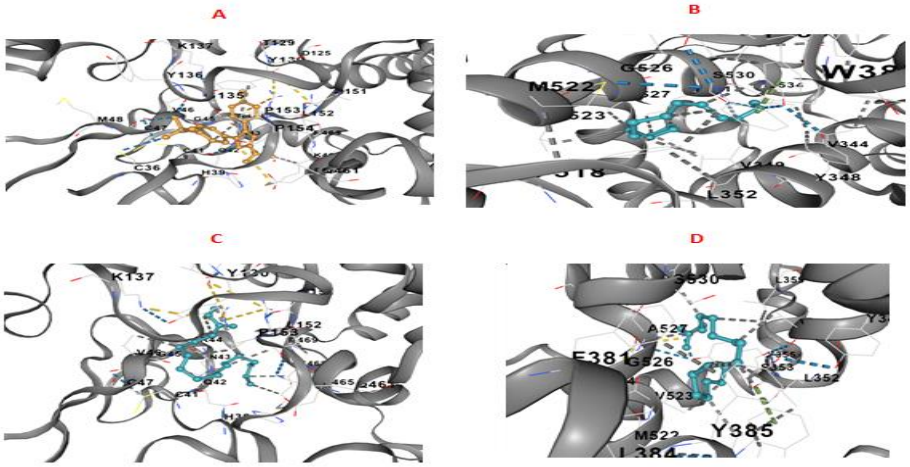
enzyme.

The results revealed that all the compounds were bound to the active site of the enzyme with negative value of Vina score, which means that the compounds can form stable complexes with the target protein. The results also showed variations in the number of amino acid residues with which the compounds interact and in the size of the protein lumen that is received by each compound. This is due to the different binding patterns of each compound in the active pocket of the enzyme as shown in Table 5.

Table 5: Molecular docking results of the selected phytochemicals against Cyclooxygenase-2 (COX-2, PDB ID: IKR5)

No. of Contact Residues	Cavity Volume (Å³)	Vina Score (Kcal/mole)	Best Cavity	Compound
59	3164	−9.0	C4	Celecoxib
31	3934	−6.4	C2	n-Hexadecanoic acid
35	3934	−6.0	C2	3-Dodecen-1-ol, (Z)
44	4765	−5.8	C1	cis-Vaccenic acid

To demonstrate the binding locations of the chemicals in the active site of the COX-2 enzyme, three-dimensional models of the studied compounds were presented. These models show the positioning of each compound within the active pocket, along with the different binding directions and surrounding interactions, as illustrated in Figure (4).



A: Celecoxib, B: 3-Dodecen-1,ol (Z), C: n-Hexadecanoic acid D: cis-Vaccenic acid

Fig 4: Predicted binding poses of the selected phytochemical compounds within the active site of Cyclooxygenase-2 (COX-2) generated using CB-Dock2.

4. Discussion

GC-MS analysis of the ethanolic extract of the caper plant (Capparis spinosa L.) revealed thirteen chemical compounds belonging to different classes, including fatty acids, alcohols, esters, and unsaturated compounds. This chemical diversity confirms that the caper plant is a rich source of bioactive secondary compounds, consistent with recent studies that have shown that this plant contains a wide range of phenolic compounds, flavonoids, fatty acids, and other biologically active compounds [2,3, 7, 10].

Based on the GC-MS results, three compounds were selected for computational analysis based on their relative abundance and the clarity of their mass spectrum. SwissADME results showed that the selected compounds possess suitable physicochemical properties in terms of molecular weight, number of hydrogen bonds, surface polarity, and lipophilicity index (LogP), properties directly related to their absorption and bioavailability. All compounds also met Lipinski's empirical rule, indicating suitable initial properties for their development as potential pharmaceutical compounds [6, 17].

In the SwissADME tests, all three compounds were found to have good gastrointestinal absorption, with moderate to good water solubility and bioavailability. Most of the pharmacokinetic parameters were within acceptable limits for absorption and permeability as suggested by Bioavailability Radar and BUILD-Egg plots, which make the drugs potential precursor molecules in the drug development process. The results, however, must be further confirmed by *in vitro* and clinical studies.[15,14 ,6]

In terms of toxicity assessment, the compounds were chosen based on their initial toxicity profile, the results of which were obtained from the ProTox-3 platform, indicating acceptable toxicity with minor differences in LD_{50} values and toxicity class, and no high toxicity markers. The findings correspond with the capability of the modern artificial intelligence tools to estimate the safety of natural compounds before moving into the laboratory studies, which helps in minimizing the time and cost at the initial phase of the drug development process.[7]

The molecular docking findings indicated that the chosen compounds successfully docked at the active site of cyclooxygenase-2 (COX-2), and the negative binding values demonstrated the stability of the ligand-protein complexes established during docking. In addition, through the 3-D model it was found that there were several interactions among the amino acids of the active site of the enzyme, such as hydrogen bond and hydrophobic interaction with the compounds, which may be responsible for increased binding stability and increase of the expected activity of the compounds.[18 ,16 ,14 ,8]

All these results suggest that coupling GC-MS chemical analysis techniques with computational prediction tools like SwissADME, ProTox-3 and CB-Dock2 is an effective method for screening the pharmacological potential of natural

compounds prior to their costly biological investigation. It has now emerged as one of the most common strategies adopted in drug discovery, especially when investigating plants containing multiple chemical compounds, such as capers, where the initial screening is not likely to be successful. [1, 15, 18].

Despite the promising results obtained by the study, it is based on chemical analyses and computer predictions, so it should be interpreted with caution until it is supported by *in vitro* and *in vivo* experiments to confirm biological activity and verify pharmacological and toxicological properties under real biological conditions [13,15].

5. Conclusion

This research revealed that the ethanolic extract of the caper plant (Capparis spinosa L.) encompasses an array of biochemical constituents detected using gas chromatography-mass spectrometry (GC-MS), such as 3-dodecen-1-ol (Z), n-hexadecanoic acid, and cis-vacenic acid. These findings suggest that the extract is a substantial reservoir of bioactive chemicals with therapeutic significance, aligning with contemporary research on the chemical makeup of this flora [2,3,13].

Computer analyses also showed that the selected compounds possess suitable physical, chemical, and pharmacological properties, with good compliance with most drug tolerability rules, high intestinal absorption, acceptable bioavailability, and expected toxicity profiles within acceptable limits, increasing the possibility of their use as precursor compounds in the development of future therapeutic agents [6,7,17].

The results of molecular docking showed a good binding affinity between the studied compounds and the active pocket of the cyclooxygenase-2 (COX-2) enzyme, with negative binding values and the formation of a series of bonds and interactions with amino acids within the active site, indicating that these compounds may have anti-inflammatory activity worthy of further study [14,16,18].

Overall, the results of the study confirm that the combination of chemical analysis using GC-MS and chemical informatics tools provides an effective approach to exploring candidate plant compounds, but definitive proof of biological activity requires future laboratory, cellular and animal studies before considering therapeutic applications [15].

6. Recommendations

In light of the results of this research, the subsequent recommendations are proposed:

1. Conduct *in vitro* studies to verify the anti-inflammatory activity of the selected compounds, particularly 3-dodecen-1-ol (Z), n-hexadecanoic acid, and cis-vacenic acid, to confirm the results of molecular docking and computational predictions.
2. Conduct *in vivo* studies to evaluate the therapeutic efficacy and pharmacovigilance of the active compounds before considering their development as potential drugs.
3. Isolation and purification of the key compounds identified using GC-MS, and individual study of their biological properties compared to the effects of the whole-plant extract.
4. Expansion of future studies to include target proteins and other biological pathways associated with inflammation, oxidative stress, and chronic diseases, with the aim of exploring additional therapeutic applications of caper compounds.
5. Adoption of an approach that combines chemical analysis, chemoinformatics techniques, and experimental biological studies to accelerate the discovery and development of candidate natural compounds for promising pharmaceutical applications.

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