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Phytochemical Profiling and Insilco Analysis of Isopropyl Myristate, Oleic Acid, Squalene, and N-Hexadecanoic Acid Identified from Different Parts of *Lantana camara* plant

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Abstract

Background: Lantana camara is a medicinal plant known for its anti-inflammatory, antioxidant, and metabolic regulating activities. The phytochemical composition and bioactivity regarding peroxisome proliferator-activated receptors (PPARs) are still inadequately investigated. The objective of this work was to examine the elemental composition, phytochemical profile, and molecular interaction potential of bioactive compounds derived from various sections of L. camara (leaves, flowers, seeds) in relation to (PPARγ) and (PPARα) receptors.

Methods: The elemental composition was assessed using Energy Dispersive X-ray (EDX) analysis, whereas phytochemical ingredients were evaluated by Gas Chromatography–Mass Spectrometry (GC-MS). Molecular docking and MM/GBSA computations assessed the binding affinity of the discovered drugs for PPARγ (PDB ID: 1I7I) and PPARα (PDB ID: 6LXA).

Results: EDX analysis identified critical elements, such as K, Si, Cu, Cl, and S, differing between plant parts. GC-MS identified isopropyl myristate, oleic acid, octadecatrienoic acid, and squalene as the principal chemicals, exhibiting organ-specific distribution. Molecular docking revealed that squalene and oleic acid exhibited the highest binding affinity and thermodynamic stability for both PPARγ and PPARα, as indicated by docking scores and MM/GBSA ΔG_bind values.

Conclusion: Lantana camara possesses bioactive chemicals that can modulate PPAR receptors, underscoring its potential for applications in anti-inflammatory and metabolic regulation. These findings establish a basis for additional experimental validation and pharmacological advancement of L. camara ingredients.

التحليل الكيميائي النباتي والدراسة الحاسوبية (In Silico) لمركبات أيزوبروبيل ميرستات، وحمض الأوليك، والسكوالين، وحمض الهيكساديكانويك المحددة من أجزاء مختلفة لنبات *Lantana Camara*

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الخلاصة

يُعد نبات *Lantana camara* من النباتات الطبية المعروفة باحتوائه على مركبات ذات أهمية حيوية، إلا أن التركيب الكيميائي الحيوي له وإمكانات تفاعله الجزيئي مع مستقبلات منشط البروتين المرتبط بالبيروكسيسوم (PPARs) ما زالت غير مدروسة بشكل كافٍ. هدفت هذه الدراسة إلى تحليل التركيب العنصري، والتوصيف الكيميائي النباتي، وتقييم قابلية الارتباط الجزيئي لمركبات نشطة حيوياً مستخلصة من أجزاء مختلفة من نبات L. camara (الأوراق، الأزهار، والبذور) تجاه مستقبلات PPARγ وPPARα . تم تحديد التركيب العنصري باستخدام تقنية مطيافية الأشعة السينية المشتتة للطاقة(EDX) ، في حين جرى تحليل المكونات الكيميائية الحيوية بواسطة مطيافية الكروماتوغرافيا الغازية–مطياف الكتلة. (GC-MS) كما أُجريت دراسات حاسوبية (In silico)شملت المحاكاة الجزيئية وحسابات MM/GBSA لتقييم تقارب الارتباط بين المركبات الرئيسة المحددة ومستقبلات PPARγ (PDB ID: 1I7I) وPPARα (PDB ID: 6LXA). أظهرت نتائج تحليل EDX وجود عناصر أساسية مثل البوتاسيوم والسيليكون والنحاس والكلور والكبريت، مع اختلاف توزيعاتها بين أجزاء النبات المختلفة. كما بين تحليل GC-MS أن المركبات الرئيسة تضمنت أيزوبروبيل ميرستات، وحمض الأوليك، وحمض الأوكتادكاترينويك، والسكوالين، مع تباين واضح في توزعها تبعًا للجزء النباتي. أشارت نتائج الدراسات الحاسوبية إلى أن مركبي السكوالين وحمض الأوليك أظهرا قابلية ارتباط ملحوظة تجاه مستقبلات PPARγ وPPARα، كما انعكس ذلك من خلال قيم Docking وMM/GBSA، مما يشير إلى إمكانية حدوث تفاعلات جزيئية مستقرة داخل جيوب الارتباط لهذه المستقبلات.تشير هذه النتائج إلى أن المركبات المستخلصة من نبات *Lantana camara* تمتلك قابلية ارتباط محتملة مع مستقبلات PPAR، إلا أن هذه النتائج تقتصر على التنبؤات الحاسوبية ولا تمثل دليلاً على النشاط الحيوي الوظيفي. وعليه، فإن الدراسات المستقبلية، بما في ذلك المحاكاة الديناميكية الجزيئية والتجارب الحيوية المختبرية، تبقى ضرورية للتحقق من الأهمية البيولوجية والفسيولوجية لهذه المركبات.

الكلمات المفتاحية: *Lantana camara* ، GC-MS؛ EDX، الإرساء الجزيئي، PPARγ، PPARα، المواد الكيميائية النشطة بيولوجيًا.

Introduction

Lantana camara L. (synonyms: *Camara vulgaris*, *Lantana scabrida*; common names: Sleeper weed, wild sage) is a perennial ornamental shrub of the family *Verbenaceae,* widely distributed across tropical and subtropical regions, including the Americas, India, Australia, and parts of Africa (1). The plant serves as a vital nectar source for pollinators which includes butterflies and moths while its ecological value extends beyond its beautiful flower colors which display yellow and orange and red and purple hues (2). The plant grows quickly through its vegetative stage which helps stop soil erosion while it builds up pasture organic matter and withstands different environmental settings (3). The morphology of the plant shown in the figure (1).

Figure (1): Represent the main part of Lantana camara.

The different sections of plants serve as sources for creating bio pesticides and fragrances and food additives and household products including brooms and furniture. The substance requires careful handling because its leaves and unripe fruits contain toxic triterpenoids including lantadene A and B which cause liver damage and stomach problems and skin problems and additional harmful reactions [(4)].

Many researcher conduct studied about *L. camara* plants that they discovered multiple bioactive compounds through phytochemical analysis which include alkaloids and flavonoids and triterpenoids and saponins and glycosides and steroids and fatty acids and fixed oils [(5,6,7,8)]. The compounds Isopropyl Myristate, Oleic Acid, Squalene and N-Hexadecanoic Acid show special interest because they have known pharmacological effects. Studies of leaf and flower extracts showed they contain effective antimicrobial compounds which combat *Pseudomonas aeruginosa* and *Bacillus subtilis* and *Escherichia coli* bacterial pathogens. The leaf extracts demonstrated protective properties against gastric ulcers when researchers tested them on animals but the flower extracts displayed mosquito-repelling abilities which indicate their potential medical applications [(9)].

Materials and Methods

Plant Materials

Fresh flowers, leaves, and seeds of *Lantana camara* were collected form botanical home of Mustansiriyah university\ college of pharmacy during the flowering season (march month). The plant materials were authenticated by a qualified botanist, and voucher specimens were preserved for future reference. The collected samples were cleaned, shade-dried at room temperature, and separately ground into fine powders using a mortar and pestle prior to extraction.

Many Researches has investigated the biological properties of these compounds but scientists still need to understand how these compounds interact with their target proteins at a molecular level. The research team needs these findings to confirm drug potential and to develop new medications. The existing knowledge gap affects major compounds including Isopropyl Myristate and Oleic Acid and Squalene and N-Hexadecanoic Acid because these substances have lipid-modulating [(10)] and antioxidant [(11)] and antimicrobial [(12)] anti-inflammatory [(13)] properties but scientists have not performed sufficient mechanistic studies.

The research uses an integrated method which combines GC-MS with EDX to study the complete phytochemical and elemental composition of *L. camara* leaves and flowers and seeds before performing in silico molecular docking of essential compounds against particular target proteins. The method allows scientists to forecast protein compound binding strength and identify vital protein contacts which help them understand how compounds affect biological systems. The research establishes a strong method to evaluate *L. camara* pharmacological value through its analysis of chemical properties against docking simulation results which will guide upcoming experimental work and therapeutic applications.

Chemicals and Materials

Fresh flowers, leaves, and seeds of *Lantana camara*; ethanol; mortar and pestle; filter paper; funnels; beakers; volumetric flasks; spatula; sensitive balance.

Extraction procedure

The extraction of Lantana camara flowers, leaves and seeds used maceration [(14)] because this method provides easy access at a budget-friendly price [(15)]. The method of cold extraction helps maintain heat-sensitive bioactive compounds including fatty acids and triterpenoids and flavonoids [(16)]. The method produces a complete chemical profile of the entire sample which becomes available for subsequent GC-MS analysis and molecular docking research. The Fresh flowers, leaves, and seeds of *L. camara* were collected, dried at room temperature, and ground separately into fine powders using a mortar and pestle. For the extraction, 25.48 g of flower powder, 25 g of leaf powder, and 4 g of seed powder were placed in separate beakers. Ethanol was added to each beaker, 250 mL for flowers and leaves and 50 mL for seeds, and the mixtures were left to macerate at room temperature for 14 days. The extracts underwent filtration through filter paper and funnels which produced volumetric flasks containing the collected filtrates for upcoming tests. Overall step of maceration shown in figure (2).

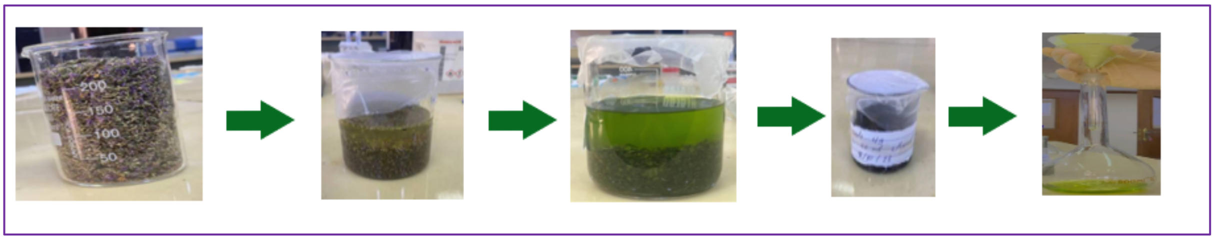


Figure (2): Steps of extraction that represent the cold method.

Characterization Methods

The GC-2030 Gas Chromatograph with Mass Spectrometry (GC-MS) operated as a Nexis instrument to determine the chemical makeup of extracted substances. The analysis process started with sample injection followed by three minutes at 60°C before the system raised its temperature at 10°C per minute until it reached 240°C for 10 minutes of maintenance. The complete analysis required 24 minutes to complete [17]. The research team conducted Energy Dispersive X-ray (EDX) analysis to detect vital mineral elements such as potassium and copper through additional elemental analysis of the extracted materials [18].

Molecular Structure of the highly yield extraction compounds

The following figure represent the final extraction compounds as shown in figure (3).

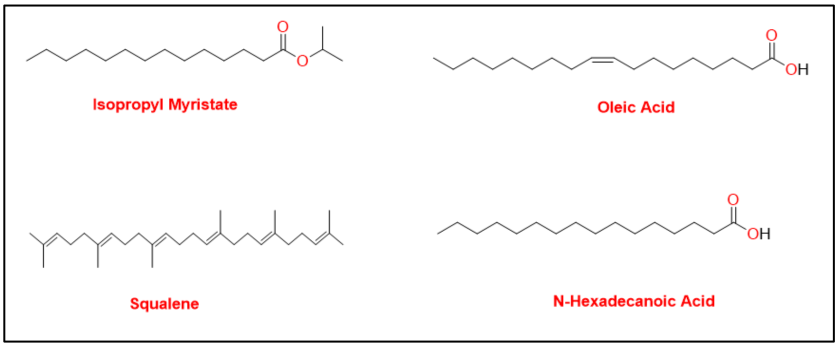
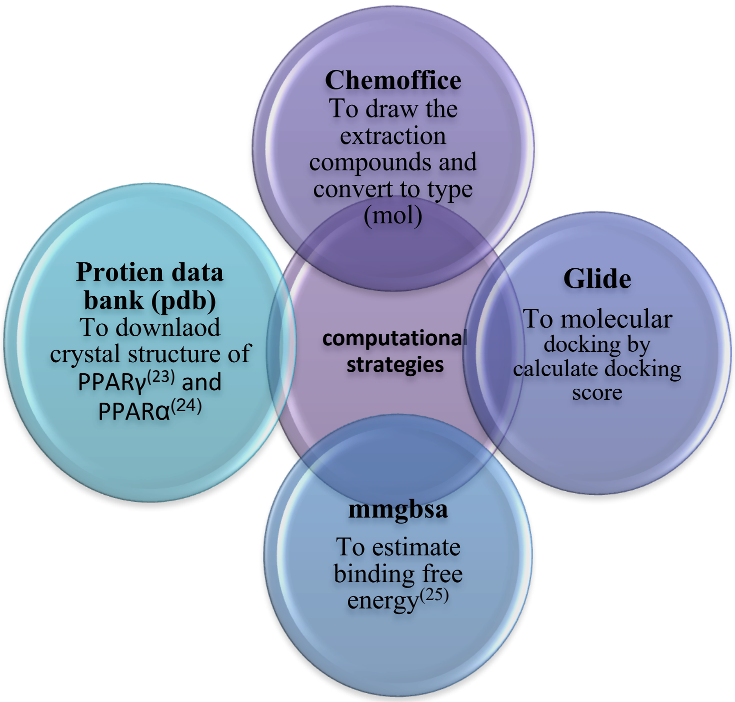


Figure (3): Represent The main extraction compounds with high yields.

In Silico Molecular Docking Study

The major bioactive compounds identified in the GC-MS analysis, namely Isopropyl Myristate, Oleic Acid, Squalene, and n-Hexadecanoic Acid, were selected. The 3D structures of these compounds were prepared using the ligand structure preparation (LigPrep) [19] module of the Schrödinger suite, which optimized geometries and added hydrogen atoms. The Protein Data Bank provided the target protein structure which underwent preparation through the Protein Preparation Wizard tool that performed bond order assignment and hydrogen bond optimization and water molecule removal and energy minimization [20]. The receptor grid defined the active site and from point of main ligands in pdb code [21]. Glide used to perform docking operations through Extra Precision (XP) modes [22]. The docking results produced binding scores and interaction profiles which scientists used to evaluate the pharmacological value of the compounds [23]. The overall computational study represents in scheme (1).



Scheme 1. Computational protocol of the desired compounds [24,25].

Docking protocol validation and active site definition

The docking protocol was validated by re-docking the co-crystallized native ligand into the binding pocket of PPARγ (PDB ID: 1I7I) and PPARα (PDB ID: 6LXA). The redocked poses were compared with the experimental crystallographic conformations, and the root mean square deviation (RMSD) values were calculated to assess the reliability of the docking protocol. RMSD values below 2.0 Å confirmed the accuracy and reproducibility of the docking methodology. The receptor grid was generated based on the coordinates of the native ligand present in the crystal structure. The grid box was centered on the ligand-binding pocket with dimensions sufficient to encompass the active site residues involved in ligand recognition and binding. Grid parameters were defined to ensure adequate sampling of the binding cavity without imposing artificial constraints. Additionally, known reference ligands of PPARγ and PPARα were docked under identical conditions to provide benchmarking controls. The docking scores and binding interactions of the reference ligands were compared with those of the investigated phytochemicals, allowing evaluation of the relative binding affinity and biological relevance of the studied compounds

Results and discussion

Qualitative result of elements from EDX-8000 Instrument

The EDX analysis system analyzed Lantana camara plant components to obtain their elemental composition which supported the GC-MS profiling results. The analysis showed in table (1) and reflect that plants contain vital elements which include K, Si, Cu, Cl and S while their concentrations differ between plant sections because of their biological functions.

The element potassium (K) appeared in high amounts throughout all samples because it functions as a metabolic enzyme activator and photosynthetic process participant in leaves and flowers. The highest concentration of Silicon (Si) appeared in seeds which indicates that this element serves as a protective agent that helps maintain seed extract stability. Copper (Cu) appears in every sample and seeds contain the highest amount of this essential redox-active trace element which could explain the antimicrobial and antioxidant effects described for L. camara. The chemical element chlorine (Cl) appeared in flower and leaf samples but sulfur (S) only appeared in leaf tissue because it serves as a precursor for sulfur-based compounds in plant metabolism.

Table (1): shown the result of the element from different part of plant.

Plant part	Si	K	Cl	CU	S	Sample Image
Flowers	36.16%	33.22%	17.29%	13.31%	-	
Leaves	14.822	33.26%	20.97%	9.17%	21.764	
Seeds	59.62%	21.56%	-	18.80%	-	

The EDX results confirm the phytochemical findings from GC-MS through their elemental analysis. The method of elemental analysis fails to show pharmacological activity but it does reveal which bio-relevant elements exist in the extract which can affect its stability and its ability to produce synergistic effects. The combination of GC-MS and EDX analysis techniques confirms which plant components should be studied through molecular docking and enhances the chemical description of L. camara which shows promise as a pharmaceutical material.

Qualitative result of compounds from GC-MASS Instrument

The GC-MS analysis of Lantana camara showed that bioactive compounds distributed differently between leaves and flowers and seeds as shown in table (2) and figures (4-7). The research identified four main compounds which dominated the entire sample composition: Isopropyl Myristate, Oleic Acid, Octadecatrienoic Acid and Squalene. The highest amount of Isopropyl Myristate occurred in seeds while leaves contained a middle range of this compound and flowers contained the smallest amount. The highest concentration of Oleic Acid appeared in leaves followed by seeds which contained moderate amounts while flowers contained no trace of this compound. The analysis showed Octadecatrienoic Acid existed mainly in flowers but we found it only in small amounts in leaves and not at all in seeds. Squalene was highly concentrated in leaves, low in flowers, and not detected in seeds. The research findings show that different plant parts contain specific bioactive compounds which accumulate in leaves and flowers for fatty acids and antioxidants but seeds contain mostly fatty acid derivatives.

Table (2): represent the result of main compounds extraction from the plant

Compounds	**Part of plant**								
	Leaves			**Flowers**			**Seeds**		
	R.T. (minutes)	**Area%**	**Height%**	**R.T. (minutes)**	**Area%**	**Height%**	**R.T. (minutes)**	**Area%**	**Height%**
Methoxyacetaldehyde diethyl acetate	**-**	**-**	**-**	**-**	**-**	**-**	**3.92**	**17.99**	**16.34**
Caryophyllene	**12.17**	**11.94**	**11.40**	**12.17**	**1.26**	**3.51**			
Neophytadine	**16.35**	**4.26**	**5.69**	**-**					
Isopropyl Myristate	**16.66**	**21.68**	**22.54**	**16.66**	**3.38**	**9.35**	**16.67**	**31.30**	**26.30**
n-hexadecanoic acid	**18.51**	**6.39**	**6.68**	**18.6**	**12.34**	**16.4**	**18.51**	**5.25**	**5.71**
Oleic Acid	**20.48**	**22.03**	**16.31**	**-**	**-**	**-**	**20.49**	**8.24**	**10.44**
Octadecatreienoic acid	**20.63**	**2.46**	**3.17**	**20.85**	**56.33**	**22.71**	**-**	**-**	**-**
D-lactamide,methylether	**-**	**-**	**-**	**23.17**	**3.48**	**6.72**	**-**	**-**	**-**
Squalene	**25.65**	**18.69**	**20.68**	**25.64**	**1.52**	**4.59**	**-**	**-**	**-**

The bioactive compounds in Lantana camara exist in distinct patterns which indicate their possible functions throughout various plant sections. The high concentration of Oleic Acid in leaves suggests it functions as a natural PPARγ agonist which helps regulate metabolism and reduces inflammation. The seed contains Isopropyl Myristate which functions as either an energy storage compound or a structural lipid. Octadecatrienoic Acid exists primarily in flowers where it functions as an antioxidant protector for reproductive tissues. Squalene which occurs naturally in leaf tissue provides skin protection and immune system regulation so leaves contain useful therapeutic substances. The chemical composition of specific plant parts enables researchers to develop extraction methods which focus on particular compounds: leaves contain fatty acids and squalene while flowers contain polyunsaturated acids and seeds contain fatty acid esters. The research results establish a basis to conduct additional bioactivity tests which could lead to drug development using compounds from Lantana camara plants.

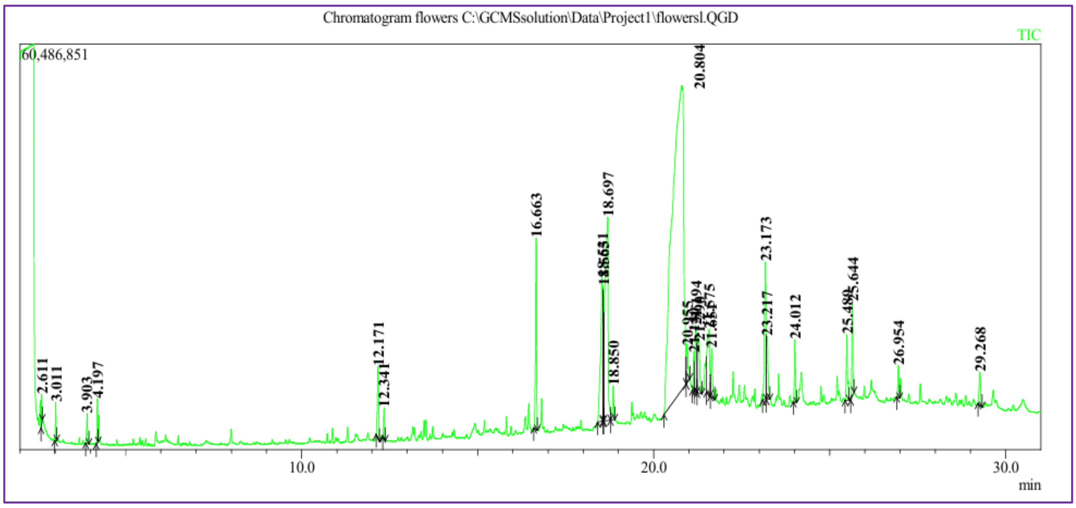


Figure (4): Spotlight on chart of GCM obtain after analysis of flowers

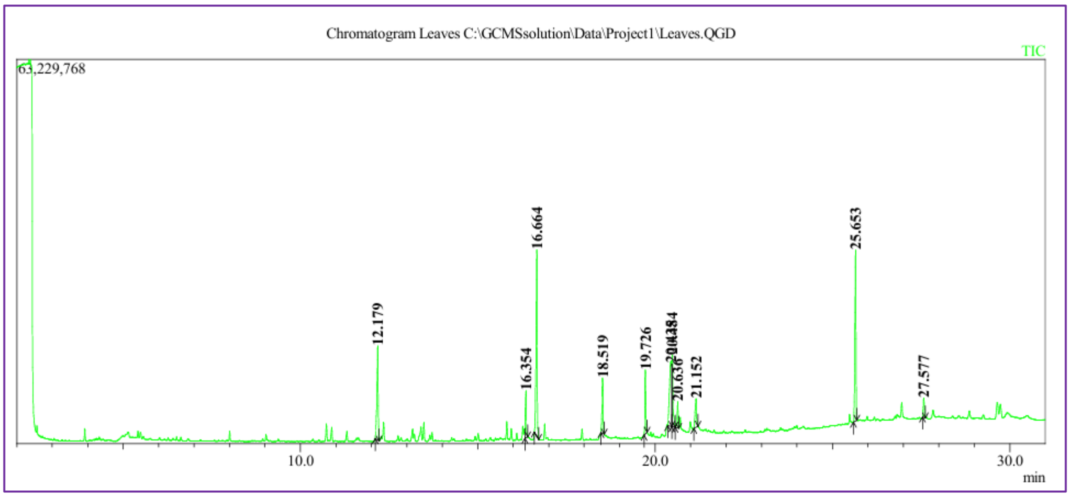


Figure (5): Spotlight on chart of GCM obtain after analysis leaves

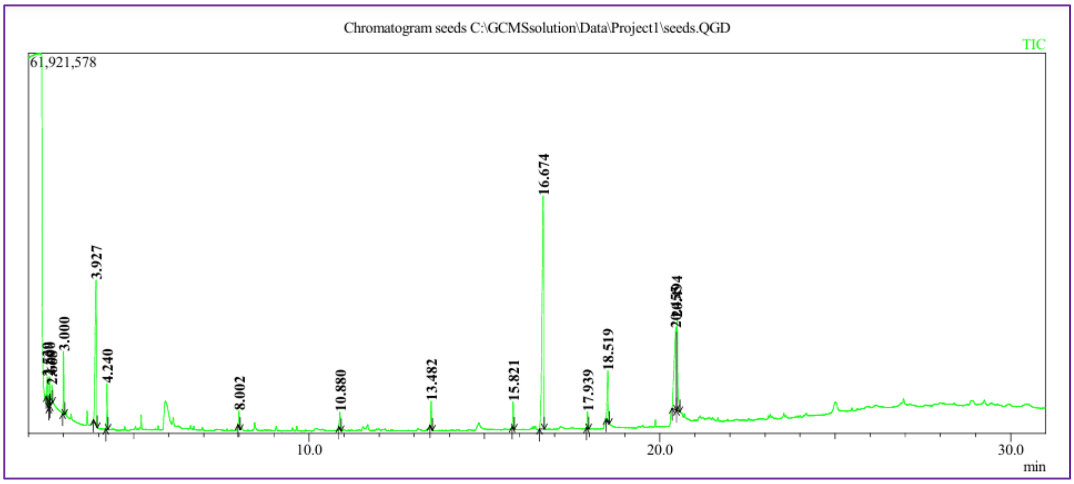


Figure (6): Spotlight on chart of GCM obtain after analysis of seeds

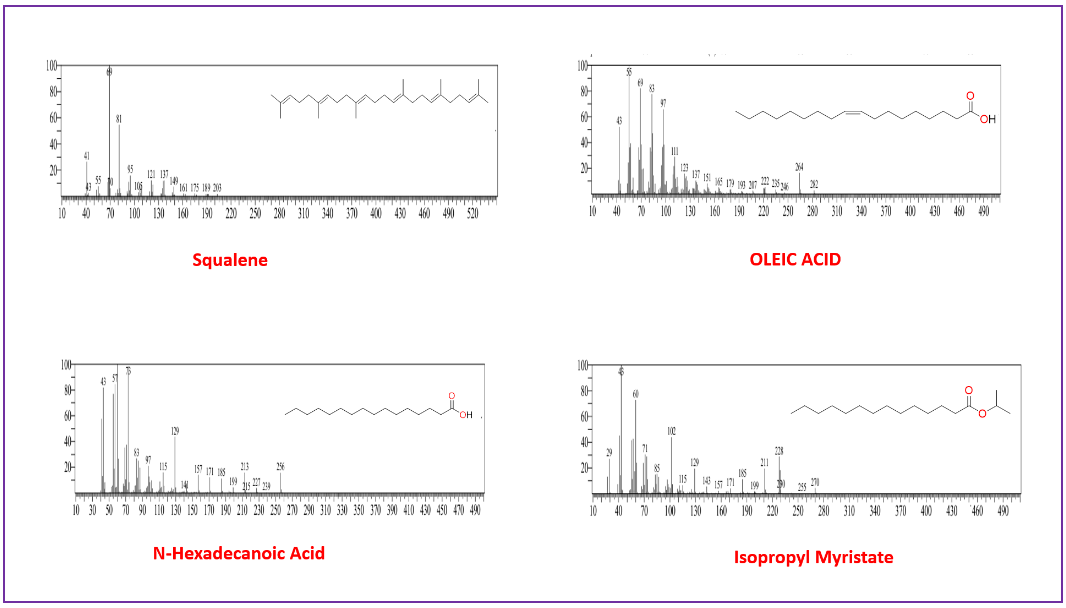


Figure (7): represent the mass peaks of our main extraction.

Analysis of docking final results

The validated docking protocol ensured reliable prediction of ligand–receptor interactions, as confirmed by acceptable RMSD values obtained from re-docking experiments. The docking study measured the binding potential of four Lantana camara bioactive compounds against PPARγ (1I7I) and PPARα (6LXA) through multiple assessment methods which included Docking score and Glide score and MMGBSA ΔG Bind and Prime Energy. Prime energy values were included solely as indicators of complex stability and were not interpreted as binding energies. These values reflect internal conformational energies rather than ligand–receptor binding strength. The results are summarized in Table (3).

Table (3): Insilco parameter for extraction compounds targeting PPARγ and PPARα.

No.	compounds	Docking score with different parameters							
		1I7I (PPARγ)				6LXA (PPARα)			
		Docking score	Glide emodel	MMGBSA dG Bind	Prime Energy	Docking score	Glide emodel	MMGBSA dG Bind	Prime Energy
1	Squelene	-7.07	-53.12	-71.31	-10639.1	-7.85	-39.23	-35.04	-11401.1
2	Oleic acid	-6.88	-54.69	-52.63	-10592.3	-7.29	-7.29	-57.85	-11390.2
3	N-Hexadecanoic Acid	-3.09	-47.29	-53.45	-10593.9	-8.18	-61.07	-55.60	-11383.7
4	Isopropyl Myristate	-3.37	-49.13	-54.63	-10593.1	-4.59	-4.59	-50.89	-11380.8

For PPARγ (1I7I), Although squalene exhibited slightly lower docking scores compared to other compounds, the differences were within a comparable range, suggesting similar binding tendencies rather than definitive superiority it achieved a docking score of -7.07 and MMGBSA ΔG Bind of -71.31 kcal/mol which shown in figure (9) that shows it binds tightly to the PPARγ active site, The observed discrepancies between docking scores and MM/GBSA binding energies may be attributed to the dominance of hydrophobic interactions. While docking scores primarily reflect pose fitting, MM/GBSA calculations account for overall thermodynamic contributions, including van der Waals interactions and solvation effects, which are particularly relevant for lipid-like compounds. The Glide score of -53.12 shows that the compound creates a strong bond with its target molecule. The docking results for oleic acid produced a score that was slightly lower than squalene at -6.88 but the MMGBSA energy of -52.63 kcal/mol showed that the compound had strong binding stability. The docking scores of N-Hexadecanoic Acid and Isopropyl Myristate were weaker at -3.09 and -3.37 respectively while their MMGBSA energies showed -53.45 and -54.63 kcal/mol which suggests they have moderate interactions because of their limited hydrophobic surface area and reduced hydrogen bonding capabilities.

The Prime energies track followed the same pattern as the other energies because squalene (-10639.1) and oleic acid (-10592.3) demonstrated the most stable conformations when they bound to the protein. The research data shows that squalene and oleic acid bind strongly to PPARγ receptors which makes them suitable for PPARγ activity control.

The compounds naturally attract to the lipophilic binding site of PPARγ because of their hydrophobic properties.

For PPARα (6LXA) as shown in figure (9), Squalene as demonstrated the highest docking affinity (-7.85) among all tested compounds because it produced a negative MMGBSA ΔG Bind value of -35.04 kcal/mol. The docking score of oleic acid showed a lower value than other compounds at -7.29 but its Glide score also reached the lowest value at -7.29 which indicates it binds with moderate strength. The MMGBSA ΔG Bind calculation produced a favorable result of -57.85 kcal/mol which shows that the complex maintains strong thermodynamic stability.

The docking results for N-Hexadecanoic Acid showed a moderate binding affinity of -8.18 but the MMGBSA ΔG Bind calculation produced a lower binding free energy of -55.60 kcal/mol. The docking geometry of this compound shows less favorability but the total binding free energy remains stable.

The docking affinity of Isopropyl Myristate proved to be the lowest at -4.59 while its MMGBSA energy reached -50.89 kcal/mol which shows that this compound does not bind well with PPARα. Interaction analysis revealed that the studied compounds predominantly occupied the hydrophobic ligand-binding pocket of PPARγ, interacting with key residues such as Tyr473, His323, and Ser289 mainly through hydrophobic contacts rather than hydrogen bonding. This interaction pattern is consistent with the lipidic nature of fatty acids and squalene, The study demonstrates Squalene shows its highest affinity for PPAR isoforms which suggests it can activate two distinct targets. The binding properties of oleic acid demonstrate potential through its ability to stabilize energy which could help modify the functional activity of PPARα. The docking scores together with MMGBSA energies indicate that hydrophobic compounds such as squalene and oleic acid bind more strongly to PPAR ligand-binding domains. The tight binding of squalene makes it suitable for development into a first compound which can target PPAR receptors for therapeutic purposes.

The natural fatty acid oleic acid maintains a moderate binding affinity while keeping its high MMGBSA stability which supports its function as a PPAR natural agonist.

The binding strength of compounds depends on their chain length and polar group content because Isopropyl Myristate with its short chain and polar groups tends to bind less strongly because it has fewer hydrophobic interactions.

The research results indicate that Lantana camara compounds have the ability to affect PPAR activity which could lead to new uses for anti-inflammatory and metabolic and lipid-regulating treatments. The result shows that Lantana camara extracts have pharmaceutical value because they function as natural PPAR modulators which makes them suitable for additional laboratory tests and we also create binding site surface as shown in figure (10).

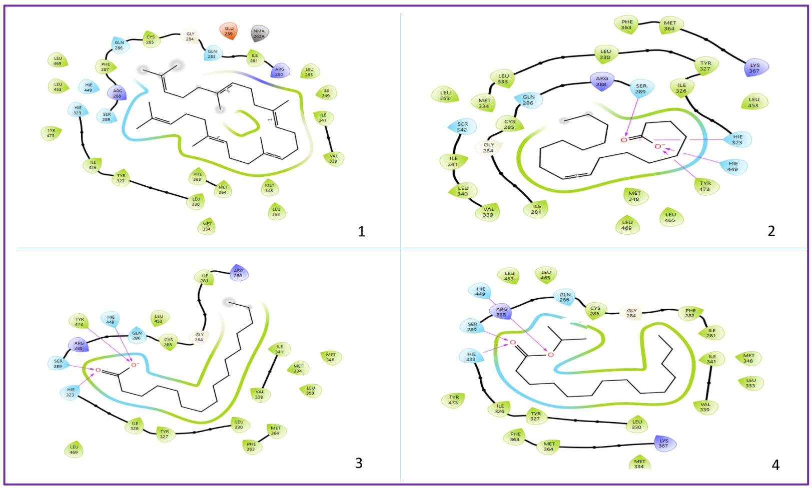


Figure (8): represent the 2D interaction of our four extraction on PPARγ with pdb (1I7I).

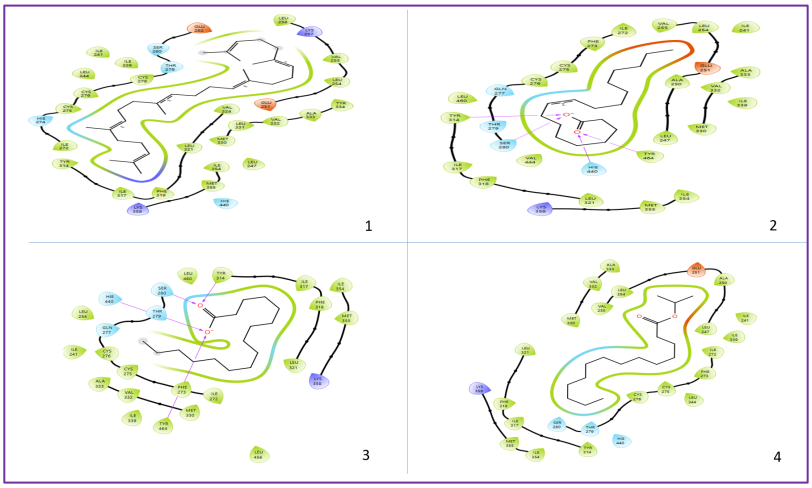


Figure (9): represent the 2D interaction of our four extraction on PPARα with pdb (6LXA).

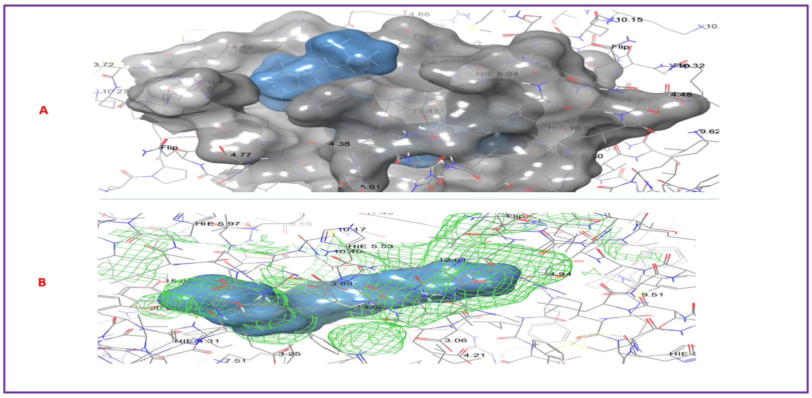


Figure (10): Represent binding site surface; A) For squalene on PPARγ using solid style for both ligand and active site. B) For N-Hexadecanoic Acid on PPARα using solid style for ligand with mesh style for active site

Conclusion

This study provides a comprehensive phytochemical and in silico investigation of bioactive compounds identified from different parts of Lantana camara. GC-MS and EDX analyses revealed the presence of lipidic compounds and essential elements, while molecular docking and MM/GBSA calculations suggested that squalene and oleic acid exhibit favorable binding affinity toward PPARγ and PPARα receptors. These findings indicate potential ligand–receptor interactions rather than confirmed biological activity. Nevertheless, the present study is subject to several limitations inherent to molecular docking approaches. The docking simulations were performed using a rigid receptor model and did not account for full solvation dynamics, entropy contributions, or receptor flexibility. In addition, PPARs are known to be promiscuous lipid-binding receptors, which may influence the interpretation of docking scores obtained for fatty acids and lipid-like compounds. Therefore, the computational results presented herein should be regarded as preliminary predictions. Future studies should focus on molecular dynamics simulations to assess binding stability over time, as well as experimental validation through in vitro functional assays, such as reporter gene assays or ligand-binding experiments, to confirm receptor activation and biological relevance.

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