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Integrative Network Pharmacology Analysis of Gas Chromatography-Derived Bioactive Phytochemicals for Cardiovascular and Inflammatory Diseases

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Abstract

Cardiovascular and inflammatory diseases remain the leading causes of global morbidity and mortality. To identify potential therapeutic candidates for these complex conditions, this study employs an integrative network pharmacology and *in silico* approach to evaluate bioactive phytochemicals derived from *Allium odorum* L., *Xanthoxylum acanthopodium* DC., *Elsholtzia griffithii* Hook.f, *Ocimum canum* L., and *Allium ascalonicum* L. From compounds initially identified via gas chromatography, 23 terpenes and 8 terpenoids were selected for investigation. Utilizing SwissTargetPrediction, PharmMapper, BindingDB, and the STITCH database, 113 unique target genes were successfully mapped to 31 of these bioactive compounds. The resulting compound-target network, evaluated via network analyzer, comprised 71 nodes and 134 edges. A protein-protein interaction (PPI) network was constructed from the STRING database for 41 target genes and analyzed using the CytoHubba plugin in Cytoscape. Degree-based topological analysis identified 10 key hub genes, ALB, CASP3, TP53, MAPK14, ESR1, MAPK1, APP, NOS3, MAPK8, and PPARG, that are critically implicated in cardiovascular and inflammatory pathways. Subsequent molecular docking analysis confirmed strong binding affinities between top-ranked bioactive ingredients, particularly the terpene α -bisabolene and the terpenoid geranyl acetate, and these core hub targets. These findings underscore the utility of network pharmacology in elucidating the multitarget mechanisms of plant-derived compounds, offering a strong computational foundation for discovering and converting novel therapeutic interventions for cardiovascular and inflammatory diseases.

Keywords: Cardiovascular disease, Gas chromatography, Inflammatory diseases, Network Pharmacology.

Introduction

Cardiovascular diseases (CVDs), a class of heart and blood vessel disorders encompassing coronary heart disease, cerebrovascular disease, and rheumatic heart disease, are the prominent source of death, accounting for approximately 17.9 million deaths yearly. Heart attacks and strokes make up over 80% of CVD deaths, with one-third diagnosed before the age of 70 years (Mc et al. 2019). Inflammation triggers the early stages of atherosclerosis, and higher levels of inflammatory cytokines are linked with greater CVD risk (Ridker et al. 2017). Network pharmacology is a new strategy that uses biological networks to link disease features, bioactive compounds, and therapeutic targets, aiming to enhance treatment options (Chandran et al. 2015). Advances in bioinformatics and systems biology now allow evaluation of active compounds and pathways involved in drug action. Network pharmacology's focus has shifted from one-target, one-drug to network-target, multi-component therapeutics (Wu et al. 2022, Dong et al. 2021, and Li et al. 2017). Analytical profiling techniques can now integrate with network pharmacology to understand diverse disease mechanisms (Li et al. 2021, Lotfi et al. 2018 and Chandran et al. 2017). In this study, we focus on several ethnomedicinal aromatic spices from Manipur, including *Allium odorum* L., *Xanthoxylum acanthopodium* DC., *Elsholtzia griffithii*, *Ocimum canum*, and *Allium ascalonicum* L., which are widely used in North-east Indian cuisine and traditional medicine. Manipur, known for its biodiversity and herbal traditions, values spices for their flavors, colors, preservatives, and health benefits. There is increasing interest in exploring and conserving medicinal and edible wild plants (Chen et al. 2016). Integrative network pharmacology analysis of gas chromatography-derived bioactive phytochemicals can reveal the molecular mechanisms underlying their therapeutic roles across various diseases (Sharma et al. 2022).

A. odorum L is an important perennial herb and locally referred to as "Maroi nakupi" (Chinese chives), and it is a member of the Alliaceae family. This herb was traditionally used

in folk medicine as a diuretic and wormicide for infants with tapeworms, threadworms, and roundworms. For those with urinary problems, it can be served either boiled or steamed in water (Singh et al. 2015). The leaf decoction is used for urinary disorders, and the paste is applied to the head to improve hair growth (Usharani et al. 2015). *Z. acanthopodium* is commonly known as prickly ash, toothache tree, lemon pepper tree, yellow wood, suterberry, and in Manipur, it is locally known as 'Mukthubi'. The plant's fruits, seeds, and leaves have historically been used to treat cholera, chronic fever, dyspepsia, dysentery, toothache, stomach discomfort, and hair diseases (Singh et al. 2015 and Devi et al. 1995). The plant extract is used in the preparation of insecticides. *Elsholtzia griffithii*, also known as 'Lomba,' is used as a spice in the indigenous sauce 'Ametpa,' the indigenous dish 'Eromba,' and as an ingredient in the indigenous salad 'Singju' in Manipur (Yumnam et al. 2012). The dried inflorescence is used to treat chronic diarrhea, menstrual irregularities, tonsillitis, and fever. A decoction of dried chameleon root inflorescences is traditionally used to treat tonsillitis in Manipur. *E. griffithii* is a lesser-known spice under the family Lamiaceae, used by the northeastern people. It remains an under-exploited species. The species has potential as a potent aromatic plant as well. *Ocimum canum*, also known as 'Mayangton,' belonging to the family Lamiaceae, is an important spice used in Manipur. Leafy shoot paste is good for fever problems (local external application on the forehead (Sharma et al. 2013). For pyorrhea, a decoction of leafy shoots is used as a mouthwash. For fever, cough, and colic, leaf juice is administered with honey. Malaria and emaciation are treated with the seeds. *Allium ascalonicum*, also known as 'Meitei tilhou macha,' is a small bulbous herb used as a spice in Manipur. Bulb is cooked and eaten in post-natal complications. In summary, the present study aims to systematically analyze and characterize the bioactive phytochemicals of these five aromatic spices using gas chromatography coupled with a network pharmacology framework. By doing so, we seek to

provide molecular insight into their roles in the prevention and management of cardiovascular and inflammatory diseases.

Materials and methods

Collection and Preparation of Plant Samples

Fresh samples of *Allium odorum* L (leaves), *Xanthoxylum acanthopodium* DC (leaves), *Elsholtzia griffithii* Hook.f (inflorescence), *Ocimum canum* L (flower and leaves), and *Allium ascalonicum* L (leaves) were collected from Imphal West District, Manipur, and authenticated at IBSD, Imphal. Plant parts were placed in 15 mL vials with screw-top caps and silicone septa, each containing one-third of the sample. Roots and stems were trimmed to 2 cm and placed in the vials.

Headspace SPME-GC-MS

The SPME fiber was conditioned, and a blank run confirmed the absence of contaminants. One-third of the sample was filled in a 15 mL vial with a septum cap, exposed to the SPME fiber for 20 minutes, and then injected into the GC-MS instrument for 2 minutes. Analysis was performed using a Trace 1300 GC with TG-5MS column and mass detector (TSQ DUO, triple Quadrupole), with a 1:20 split ratio, helium at 1 mL/min, and a temperature program from 40°C to 250°C at 5°C/min, holding for 20 minutes. Relative VOCs were represented by peak area %. Compounds were identified by comparing mass spectra to the 2017 NIST GC-MS Libraries.

Retrieval of Bioactive Phytochemicals

Gas chromatography identified bioactive phytochemicals, and 3D structures and SMILES (simplified molecular input line entry system) data were obtained from the PubChem library (<https://pubchem.ncbi.nlm.nih.gov/>) (Gfeller et al. 2013). Further, the chemicals were classified into terpenes and terpenoids.

Target prediction of active compounds

The prediction of potential targets for the bioactive compounds involved the utilization of the following tools: SwissTargetPrediction (<http://www.swisstargetprediction.ch>) (Cao et al. 2022), where targets with a probability value ≥ 0.1 were selected; (Wang et al. 2017) Phrammapper (<https://www.lilab-ecust.cn/phrammapper/>) (Li et al. 2021), where targets with a normalized fit score > 0.9 were chosen; (Gilson et al. 2016) BindingDB (<https://www.bindingdb.org/rwd/bind/index.jsp>), Patil et al. 2022. Targets with a maximum similarity index of 0.7 were chosen (Szkłarczyk et al. 2016), and the STICH database (<http://stitch.embl.de/>) (Stelzer et al. 2016).

Potential Target screening of cardiovascular and Inflammatory diseases

To select potential targets from GeneCards (<https://www.genecards.org/>), keywords such as "cardiovascular diseases", "anti-inflammatory", and "inflammatory disorders" were used (Liu et al. 2022). Targets with a relevance score ≥ 15 were included (Pinero et al. 2020) from DisGeNET (<https://www.disgenet.org>) (Chen et al. 2023), the keywords "cardiovascular diseases" and "inflammation" retrieved targets with a GDA score > 0.06 (Shannon et al. 2003).

Identification of overlapping targets between bioactive compounds and selected diseases

To identify overlapping targets between bioactive compounds and selected diseases, a Venn diagram was generated using an online tool (<https://www.biotoools.fr/misc/venny>).

Construction of Compound -Target Network

To enhance our understanding of the interconnectedness among overlapping targets and bioactive compounds, a Compound-Target Network was constructed using Cytoscape v3.10.0 (Szkłarczyk et al., 2019).

PPI network and identification of hub genes

Overlapping targets were uploaded to STRING (<https://string-db.org/>) to obtain protein–protein interactions (Tabassum et al. 2022). Hub genes were identified using CytoHubba in Cytoscape based on degree (Ge et al. 2020).

Functional and Pathway enrichment analysis

The ShinyGO 0.77 web server (<http://bioinformatics.sdstate.edu/go>) was used for enrichment analysis of biological processes and KEGG pathways (Adnan et al. 2033). Common intersecting targets were input, and the species were set to human. Bar charts of enriched terms were obtained from the chart section (Morris et al. 2009).

Molecular Docking Analysis

The 3D structures of selected target proteins were retrieved from the Protein Data Bank. Binding site grid coordinates were defined in BIOVIA Discovery Studio Visualizer 2021, and charges and hydrogens were assigned using AutoDock MGLTools v1.5.7. (Eberhardt et al. 2021). Molecular docking was performed with AutoDock Vina v1.1.2 (Kareti et al. 2020), and the results were visualized with BIOVIA Discovery Studio Visualizer 2021.

Results

The GC-MS chromatogram for all the plants is shown in **Figure 1**. Major compounds for each plant sample are listed in **Tables 1–6**. A total of 23 terpenes and 8 terpenoids were identified using gas chromatography, with details provided in **Table 7**. Overall, 113 unique target genes for 31 bioactive compounds were identified using SwissTargetPrediction, PharmMapper, BindingDB, and the STITCH database. No target genes were identified for o-Cymene; it was not used for further analysis. Additionally, 1446 and 1321 gene targets associated with cardiovascular and inflammatory diseases were obtained from GeneCards and DisGeNET, respectively. Consequently, we identified 41 overlapping targets between the bioactive compounds and both cardiovascular and inflammatory diseases. The Venn diagram of the

overlapping targets of bioactive compounds and those associated with cardiovascular and inflammatory diseases is shown in **Figure 2**. A network connecting 41 common gene targets and 30 bioactive compounds was built using Cytoscape, as shown in **Figure 3**. Using the "network analyzer" feature, we determined that the compound-target network comprises 134 edges and 71 nodes. By analyzing the network topology, the top 10 bioactive ingredients were ranked by degree, as shown in **Table 8**. Nodes with higher degrees in the network have more biological functions. We chose these top 10 targets for further molecular docking analysis.

We used the STRING database to construct a protein-protein interaction (PPI) network for 41 target genes, as shown in **Figure 4**. The network contains 38 nodes and 201 edges. Using the CytoHubba plugin in Cytoscape, we analyzed the network by degree. Table 9 shows the top 10 HUB genes ranked by degree. We chose these top 10 hub genes for further molecular docking analysis. Functional enrichment analysis of biological processes and KEGG pathways was done using ShinyGO v0.77 web server. In the biological processes category, we identified terms closely associated with inflammation. In the KEGG pathway analysis, most inflammatory pathway terms were identified. **Figure 5** shows a bar plot representing the top 20 Biological Processes and KEGG pathways.

Auto Dock Vina was used to perform molecular docking between the top 10 compounds obtained by the compound-target network and top 10 hub genes ALB (PDBID: 1AO6), CASP3 (PDBID: 3DEI), TP53 (PDBID: 3DCY), MAPK14 (PDBID: 1M7Q), MAPK8 (PDBID: 1UKI), MAPK1 (PDBID: 7AUV), ESR1 (PDBID: 1A52), APP (PDBID: 1AAP), NOS3 (PDBID: 1M9R), and PPARG (PDBID: 2PRG) which are obtained through PPI network. The molecular docking results, including binding energies in kcal/mol, are displayed as a heat map (**Figure 6**). Only two compounds, 24798703 and 1549026, showed optimal binding affinity below -7. **Table 10** illustrates the amino acid interactions of these two compounds with their targets; the bolded amino acid residues are the matching residues reported in the literature and

the PDB (Du et al. 2022 and Batool et al. 2022). The compound 24798703 (α -Bisabolene) demonstrated strong binding affinity with several targets, including ALB, ESR1, MAPK1, NOS3, MAPK8, and PPARG. The compound 1549026 (Geranyl acetate) showed good binding towards NOS3. **Figure 7** depicts the 3D and 2D key amino acid interactions of these two compounds towards the targets.

Discussion

In recent years, natural product research has attracted substantial attention for several reasons. Pharmacology plays a crucial role in the study and treatment of cardiovascular diseases and inflammatory diseases (Roth et al. 2020). Cardiovascular diseases cover various health conditions that affect the heart and blood vessels. They stand as a significant cause of mortality worldwide. Heart failure, stroke, coronary artery disease, and hypertension are a few examples of cardiovascular diseases (Chen et al., 2018). Inflammatory diseases encompass various medical conditions characterized by abnormal inflammation in the body. Examples of common inflammatory diseases include rheumatoid arthritis, inflammatory bowel disease, asthma, and psoriasis (Noor et al. 2022). These conditions present substantial healthcare challenges. However, network pharmacology provides a robust framework for comprehending the intricate molecular mechanisms at play, facilitating the discovery of novel therapeutic targets and compounds (To et al. 2022).

Network pharmacology is becoming a more efficient method for developing new drugs, thanks to tremendous advances in systems biology. This work examined the potential targets of bioactive chemicals derived from GC for treating cardiovascular and inflammatory illnesses using a systems biology approach. This approach involved identifying and predicting targets for selected compounds and diseases, constructing networks, enriching KEGG pathways, and performing molecular docking. We identified 41 common targets shared by the selected bioactive compounds and both cardiovascular and inflammatory diseases. From the compound-

target pathway, we shortlisted the top 10 bioactive compounds that had the most targets, and from the PPI network, we shortlisted the top 10 hub genes, i.e., ALB, CASP3, TP53, MAPK14, ESR1, MAPK1, APP, NOS3, MAPK8, and PPARG, which were further used for molecular docking analysis. The functional and pathway enrichment analyses revealed that the intersecting gene targets shared between cardiovascular and inflammatory diseases are involved in several biological processes. These activities include regulation of the inflammatory response, lipid responses, positive regulation of the phosphorus metabolic process, regulation of responses to external and abiotic stimuli, regulation of programmed cell death, and other processes. These suggest that the gene targets play essential roles in the pathogenesis of cardiovascular and inflammatory diseases. In addition, the term "cellular response to organic cyclic compound" implies that these compounds may alter cellular state or activity and have potential therapeutic effects for cardiovascular and inflammatory diseases by influencing cellular responses (Zhou et al. 2021). The KEGG pathway analysis revealed several pathways and diseases associated with cardiovascular and inflammatory diseases. The notable pathways and diseases include arginine and proline metabolism, prolactin signaling pathway, IL-17 signaling pathway, TNF signaling pathway, Sphingolipid signaling pathway, fluid shear stress, atherosclerosis, and platelet activation (Yu et al. 2021, Jia et al. 2021, Goa et al. 2021, Liu et al. 2021, De et al. 2014 and Oh et al. 2021).

Molecular docking revealed that α -Bisabolene exhibited binding affinity for the targets ALB, ESR1, MAPK1, NOS3, MAPK8, and PPARG. Also, the compound Geranyl acetate showed binding affinity towards NOS3. It is well known that albumin (ALB) possesses physiological properties, including antioxidant, anti-inflammatory, anticoagulant, and antiplatelet aggregation activities (Noor et al. 2022). ESR1 (estrogen receptor 1) is important for bone growth and the normal function of the cardiovascular system. Mutations in ESR1 are associated with cancer and inflammatory response (Wang et al. 2021). MAPKs (mitogen-activated protein

kinases) are known to stimulate the production of inflammatory cytokines, such as interleukins and TNF- α (Tumor Necrosis Factor-Alpha), and to actively participate in inflammation (Marfella et al. 2006 and Vetuschi et al. 2018). NOS3 (nitric oxide synthase 3) is responsible for producing nitric oxide (NO). Nitric oxide promotes angiogenesis, inflammation, and cell proliferation. PPARG (peroxisome proliferator-activated receptor gamma) plays an inhibitory role in atherosclerosis and has anti-inflammatory effects (Vetuschi et al. 2018). These targets, along with the compounds α -Bisabolene (Terpene) and Geranyl acetate (Terpenoid), can play a key role in the treatment of cardiovascular and inflammatory diseases. This study emphasizes the importance of network pharmacology in accelerating the development of effective drugs for cardiovascular and inflammatory diseases.

The application of network pharmacology to cardiovascular and inflammatory diseases has significant potential. The present study has provided important information regarding potential therapeutic targets and bioactive compounds. Using a systems biology approach, we identified overlapping gene targets and related pathways for cardiovascular and inflammatory diseases and explored their molecular bases. Significant roles of key hub genes, including ALB, CASP3, TP53, MAPK14, ESR1, MAPK1, APP, NOS3, MAPK8, and PPARG, were identified in these diseases. Further molecular docking analysis was performed to validate the binding affinity of specific compounds to targets, such as α -Bisabolene (Terpene) and Geranyl acetate (Terpenoid), which showed therapeutic significance. This study highlights the significance of network pharmacology in accelerating the discovery and development of efficacious medications for cardiovascular and inflammatory diseases, thereby paving the way for more customized and accurate medical interventions in the future.

Conclusion

The therapeutic potential of phytochemicals identified by gas chromatography from five medicinal plant species was explored using an integrative network pharmacology and

molecular docking approach. In total, 31 bioactive compounds were screened, including 23 terpenes and 8 terpenoids, and 113 unique target genes were identified across multiple target prediction databases. The network analysis revealed significant interactions among compounds, targets, and key bioactive components involved in disease modulation. The protein-protein interaction analysis showed that the major hub genes ALB, CASP3, TP53, MAPK14, ESR1, MAPK1, APP, NOS3, MAPK8, and PPARG are closely related to cardiovascular and inflammatory pathways. Molecular docking studies showed strong binding affinities between compounds such as α -Bisabolene and Geranyl acetate and these key targets, supporting their potential therapeutic importance. Overall, the findings provide mechanistic insights into the multitarget actions of these phytochemicals and highlight the value of network pharmacology as an effective strategy for identifying novel plant-derived candidates for the management of cardiovascular and inflammatory diseases.

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Author contribution

Nameirakpam Bunindro Singh: Conceptualization, experimental design, data acquisition, and manuscript drafting. Thokchom Biona: Experimental work, sample collection, and initial data analysis. Kshetrimayum Vimi: Investigation, laboratory work, and data compilation. Keithellakpam Ojit Singh: Formal analysis, visualization, and manuscript review. Shankarrao Patil: Methodology validation, resources, and critical review. Sanjai Srinivasan: Formal analysis, validation, and manuscript review. Nanaocha Sharma: Study supervision, manuscript review and editing, and correspondence.

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Data availability

All data generated or analyzed during this study are included in this published article.

Declaration

The authors declare no competing interests

ABBREVIATIONS

ALB: Albumin; **APP:** Amyloid Precursor Protein; **CASP3:** Caspase 3, apoptosis-related cysteine peptidase; **CVD:** Cardiovascular Disease; **ESR1:** Estrogen Receptor 1; **GC-MS:** Gas Chromatography-Mass Spectrometry; **KEGG:** Kyoto Encyclopedia of Genes and Genomes; **MAPK8:** Mitogen-Activated Protein Kinase 8; **MAPK14:** Mitogen-Activated Protein Kinase 14; **MAPK1:** Mitogen-Activated Protein Kinase 1; **NOS3:** Nitric Oxide Synthase 3; **NO:** Nitric oxide; **PPARG:** Peroxisome Proliferator-Activated Receptor Gamma; **PPI:** Protein-Protein Interaction; **SPME:** Solid-Phase Microextraction; **SMILES:** Simplified Molecular-Input Line-Entry System; **STRING:** Search Tool for the Retrieval of Interacting Genes/Proteins; **STITCH:** Search Tool for Interactions of Chemicals; **TP53:** Tumor Protein p53; **VOC:** Volatile Organic Compound; **3D:** Three-Dimensional; **2D:** Two-Dimensional.

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Table 1: Major Volatile Organic Compounds Present in the leaves of *A. odorum*

RT ^a	Compound	RSI ^b	RA ^c %	Mol. Wt
7.75	Disulfide, methyl 2-propenyl	954	72.82	120
12.47	Diallyl disulphide	818	12.53	146
3.86	Disulfide, dimethyl	948	11.17	94
6.21	Leaf alcohol	876	0.83	100
8.15	Methyl isopropyl disulphide	831	0.42	122
13.09	(E)-1-Allyl-2-(prop-1-en-1-yl) disulfane	862	0.38	146
12.87	1-Allyl-2-isopropyldisulfane	854	0.3	148
4.85	3-Hexenal	891	0.13	98
10.35	trans-1,4-Hexadiene	918	0.13	82
16.93	cis-3-Hexenyl valerate	863	0.07	184
14.22	Trisulfide, methyl 2-propenyl	807	0.06	152
9.27	Dimethyl trisulfide	871	0.05	126
10.85	o-Cymene	928	0.05	134
12.79	Tricyclo[3.2.1.0(2,,4)]oct-6-en e, 8-methylene-, (1à,2à,4à,5à)-	920	0.03	118
6.13	Cyclobutanone, 2-methyl-2-oxiranyl	821	0.02	126
7.04	(E)-Allyl(prop-1-en-1-yl)sulfane	807	0.02	114
13.52	Acetoacetic acid, 1-thio-, S-allyl ester	847	0.02	158
17.94	Butane, 2,3-dimethyl-2-nitro-	852	0.02	131
6.58	Acetoacetic acid, 1-thio-, S-allyl ester	836	0.01	158
6.95	(E)-Allyl(prop-1-en-1-yl)sulfa ne	817	0.01	114
14.32	Acetoacetic acid, 1-thio-, S-allyl ester	871	0.01	158
16.56	2,6-Dimethyl-1,3,6-heptatriene	811	0.01	122
16.83	cis-3-Hexenyl valerate	856	0.01	184
17.14	2-Methyl-6-methylene-octa-1,7 -dien-3-ol	837	0.01	152
46.38	3'-Amino-6-methoxyaurone	894	0.01	267
47.96	8-Isopropyl-5-methyl-5,6,7,8-t etrahydro-2,4- quinazolinedione	864	0.01	222
48.82	Urea, propyl-	839	0.01	102
56.24	Semioxamazide	838	0.01	103
61.69	1,3,5-Trioxepane	824	0.01	104
62.52	3(2H)-Benzofuranone, 6-methoxy-2-[(3-methoxyphe nyl)methylene]-, (E)-	857	0.01	282
Total area %			99.17	

RT^a: Retention time; **RSI^b:** Reversed search index on TG-5MS capillary column, **RA^c%:** Relative area (peak area relative to the total peak area).

Table 2: Major Volatile Organic Compounds Present in the leaves of *X. Acanthopodium*

RT^a	Compound	RSI^b	RA^c %	Mol. Wt
10.38	α -Sabinene	895	47.17	136
9.27	α -Pinene	873	14.33	136
9.64	β -Thujene	901	9.38	136
12.45	Linalool	919	7.02	154
9.99	α -Terpinolene	911	5.54	136
10.26	o-Cymene	916	3.58	134
16.85	Linalyl acetate	931	3.14	196
10.92	α -Ocimene	936	1.29	136
7.63	α -Pinene	932	0.95	136
9.76	4-Hexen-1-ol, acetate, (Z)-	895	0.91	142
11.23	γ -Terpinene	917	0.46	136
5.71	3-Hexen-1-ol, (Z)-	935	0.41	100
13.64	trans-Alloocimene	923	0.35	136
8.44	Benzaldehyde	918	0.31	106
13.28	1,3-Cyclohexadiene, 1,3,5,5-tetramethyl	923	0.26	136
10.13	Cyclopenta[c]pyran-1,3-dione, 4,4a,5,6-tetrahydro-4,7-dimethyl	885	0.25	180
21.22	Caryophyllene	919	0.2	204
20.24	Geranyl acetate	919	0.17	196
8.91	1-ethenyl-2-hexenyl-, [1 α ,2 α (E)]-(η)-	863	0.16	150
8.75	β -Terpinene	944	0.15	136
23.76	Calamenene	905	0.12	202
Total area %			96.15	

RT^a: Retention time; **RSI^b:** Reversed search index on TG-5MS capillary column, **RA^c%:** Relative area (peak area relative to the total peak area).

Table 3: Major Volatile Organic Compounds Present in *E. griffithii* inflorescence

RT ^a	Compound	RSI ^b	RA ^c %	Mol. Wt
18.11	α -Citral	906	48.96	152
17.26	Tricyclo[3.2.1.0(2,,4)]oct-6-en e, 8-methylene-, (1à,2à,4à,5à)-	948	44.27	118
21.93	Caryophyllene	959	3.41	204
10.83	o-Cymene	950	0.73	134
22.77	Humulene	904	0.39	204
15.46	3-Heptyne, 5-methyl-	871	0.21	110
12.78	Tricyclo[3.2.1.0(2,,4)]oct-6-ene, 8-methylene-, (1à,2à,4à,5à)-	948	0.13	118
9.83	à-Pinene	891	0.11	136
23.44	Germacrene D	943	0.1	204
10.26	1,3,8-p-Menthatriene	929	0.09	134
14.94	trans-Verbenol	862	0.08	152
25.90	10-Pentadecen-5-yn-1-ol, (E)-	935	0.08	222
9.75	5-Hepten-2-one, 6-methyl-	913	0.06	126
14.37	6-Octenal,7-methyl-3-methylene-	878	0.05	152
14.53	photocitral A	969	0.05	152
13.52	Tricyclo[3.2.1.0(2,4)]octane, 8-methylene-, (1à,2à,4à,5à)-	857	0.04	120
15.83	2-Heptanone,6-methyl-5-methylene-	939	0.03	140
24.43	5,6-Decadien-3-yne,5,7-diethyl-	916	0.02	190
26.50	3-Hexyne, 2-methyl-	937	0.02	96
5.41	1-Nonyne, 7-methyl-	836	0.01	138
6.92	5-Hexen-2-one, 5-methyl-3-methylene-	863	0.01	124
7.19	trans-4,4-Dimethyl-2-hexene	865	0.01	112
10.05	4-Pentene-2-ol, 2-methyl	884	0.01	100
11.70	6-Methyl-1,5-heptadiene	824	0.01	110
12.15	Ethanone, 2-(formyloxy)-1-phenyl-	913	0.01	164
12.97	Monochloromethyl isopentanoate	858	0.01	150
13.20	photocitral B	936	0.01	152
16.04	Cyclobutaneethanol, à-methylene-	879	0.01	112

16.24	6-(3-Methyl-3-cyclohexenyl)- 2-methyl-2,6-heptadienol	886	0.01	220
16.55	2,6-Dimethyl-1,3,6-heptatriene	874	0.01	122
16.85	2-Methyl-6-methylene-octa-1,7-dien-3-ol	851	0.01	152
18.39	4-Pentene-2-ol, 2-methyl	887	0.01	100
19.77	2-Heptanone, 6-methyl-5-methylene-	869	0.01	140
21.02	à-Bourbonene	912	0.01	204
21.13	3,4-Nonadien-6-yne, 5-ethyl-3-methyl-	936	0.01	162
23.30	5,6-Decadien-3-yne, 5,7-diethyl-	910	0.01	190
23.83	Dihydro-cis-à-copaene-8-ol	909	0.01	222
24.22	Germacrene D	922	0.01	204
27.11	10-Pentadecen-5-yn-1-ol, (E)-	963	0.01	222
27.57	5,10-Pentadecadiyn-1-ol	917	0.01	220
Total area %			99.04	

RT^a: Retention time; **RSI^b**: Reversed search index on TG-5MS capillary column, **RA^c%**: Relative area (peak area relative to the total peak area).

Table 4: Major Volatile Organic Compounds Present in the fruits of *O. canum*

RT ^a	Compound	RSI ^b	RA ^c %	Mol. Wt
13.86	Camphor	900	16.79	152
10.39	D-sylvestrene	898	12.8	136
10.98	á-Ocimene	919	12.43	136
21.27	Caryophyllene	916	5.75	204
9.27	(-)-β-Pinene	899	5.09	136
12.12	Terpinolene	906	4.39	136
8.04	Camphene	940	3.87	136
17.33	α-Citral	905	3.05	152
16.19	cis-Geraniol	934	2.93	154
12.5	Linalool	913	2.84	154
16.52	Citral	865	2.54	152
10.25	o-Cymene	910	1.92	134
16.91	Geraniol	934	1.91	154
21.61	trans-à-Bergamotene	946	1.65	204
10.63	à-Pinene	912	1.57	136
13.7	ALLO-OCIMENE	913	1.51	136
9.63	β-Thujene	905	1.35	136
13.32	1,3-Cyclohexadiene, 1,3,5,5-tetramethyl	899	1.29	136
11.25	ç-Terpinene	904	1.27	136
23.78	5,6-Decadien-3-yne, 5,7-diethyl	919	1.11	190
24.19	2,5-Heptadiene	942	1.05	204
9.99	Terpinolene	902	0.89	136
20.11	à-Cubebene	911	0.82	204
22.1	4,7,-Cycloundecatriene, 1,5,9,9-tetramethyl-, Z,Z,Z	921	0.68	204
22.77	(1R,2S,6S,7S,8S)-8-Isopropyl-1-methyl-3-methylenetricyclo[4.4.0.02,7]decane-rel	921	0.68	204
5.69	Leaf alcohol	934	0.57	100
23.18	Zonarene	899	0.44	204
15.32	Estragole	932	0.42	148
22.28	Cadina-1(6),4-diene	918	0.37	204
14.71	p-Menth-1-en-4-ol	906	0.35	154
22.65	ç-Murolene	929	0.3	204
23.1	Cubenene	910	0.3	190

11.65	Cyclopropane, pentyl-	904	0.27	112
21.46	10,10-Dimethyl-2,6-dimethylenebicyclo[7.2.0]undecane	888	0.26	204
7.44	β -Thujene	935	0.25	136
10.06	α -Ocimene	842	0.25	136
14.84	3-Heptyne, 5-methyl-	922	0.22	110
9.76	3-Hexen-1-ol, acetate, (E)-	824	0.2	142
11.9	Terpinolene	882	0.19	136
15.63	Acetic acid, octyl ester	922	0.16	172
20.44	5,6-Decadien-3-yne, 5,7-diethyl	864	0.16	190
21.99	Germacrene D	900	0.16	204
14.41	endo-Borneol	918	0.15	154
15.1	α -TERPINYL FORMATE	890	0.15	182
5.58	2-Hexenal	911	0.14	98
7.29	Tricyclene	931	0.14	136
11.17	β -Terpinene	901	0.14	136
11.56	1,3-Cyclopentadiene, 5,5-dimethyl-1-propyl	863	0.14	136
19.41	α -Cubebene	934	0.14	204
22.58	1-Isopropyl-4,7-dimethyl-1,2,3,4,5,6-hexahydronaphthalene	907	0.14	204
13.08	2,6-Dimethyl-1,3,5,7-octatetraene, E,E	927	0.13	134
21	α -Gurgujene	890	0.13	204
23.39	5,6-Decadien-3-yne, 5,7-diethyl	929	0.12	190
21.1	(1R,9R,E)-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-4-ene	881	0.11	204
12.91	Cyclohexene, 1,5,5-trimethyl-3-methylene	836	0.1	136
24	Cubenene	946	0.1	204
24.27	α -Calacorene	960	0.1	200
Total area %			96.98	

RT^a: Retention time; **RSI^b:** Reversed search index on TG-5MS capillary column, **RA^c%:** Relative area (peak area relative to the total peak area).

Table 5: Major Volatile Organic Compounds Present in the leaves of *O. canum*

RT ^a	Compound	RSI ^b	RA ^c %	Mol. Wt
13.8	Camphor	904	27.79	152
10.36	D-sylvestrene	875	17.02	136
5.72	Leaf alcohol	908	7.28	100
8.05	Camphene	950	6.53	136
17.3	α -Citral	898	5.01	152
9.77	4-Hexen-1-ol, acetate, (Z)-	911	3.7	142
10.25	o-Cymene	893	3.62	134
16.49	cis-Verbenol	866	3.43	152
12.12	Terpinolene	921	3.25	136
9.27	α -Pinene	909	2.98	136
7.64	(-)- α -Pinene	902	2.43	136
10	Terpinolene	903	1.42	136
10.93	α -Ocimene	928	1.23	136
21.25	Caryophyllene	938	0.9	204
9.19	5-Hepten-2-one, 6-methyl-	897	0.76	126
11.24	ζ -Terpinene	925	0.75	136
16.15	cis-Geraniol	922	0.75	154
7.47	β -Thujene	931	0.64	136
12.47	Linalool	912	0.64	154
6.03	Cyclopropane, propyl-	879	0.51	84
16.88	Geraniol	927	0.46	154
10.63	Tricyclo[3.2.1.0(2,4)]octane,8-methylene-, (1 α ,2 α ,4 α ,5 α)-	915	0.44	120
13.66	trans-allo-Ocimene	927	0.43	136
14.72	(-)-Terpinen-4-ol	913	0.43	154
14.84	Isoneral	901	0.41	152
23.78	cis-Calamenene	876	0.39	202
13.31	trans-allo-Ocimene	916	0.38	136
5.62	Cyclopropane, 1,1-diethyl-	850	0.3	98
13.91	Photocitral A	989	0.3	152
7.31	Tricyclene	907	0.21	136
14.41	endo-Borneol	926	0.2	154
15.32	Estragole	899	0.2	148
14.94	Butanoic acid, 3-hexenyl ester,(E)-	936	0.19	170

21.6	trans-à-Bergamotene	935	0.19	204
20.11	à-Cubebene	925	0.18	204
24.19	trans-alpha-bisabolene	946	0.18	204
17.2	Photocitral B	895	0.15	152
15.57	cis-1,3,3-trimethylbicyclo[3.1.0]hexane-1-carboxaldehyde	934	0.14	152
15.9	Bicyclo[3.1.0]hexane,6-isopropylidene-	873	0.13	122
12.91	Cyclohexene,1,5,5-trimethyl-3-methylene-	863	0.12	136
14.33	3-Heptyne, 5-methyl-	878	0.11	110
7.14	3-Hexyne, 2-methyl-	922	0.1	96
8.99	1-Octen-3-ol	906	0.1	128
Total Area %			96.38	

RT^a: Retention time; **RSI^b**: Reversed search index on TG-5MS capillary column, **RA^c%**: Relative area (peak area relative to the total peak area).

Table 6: Major Volatile Organic Compounds Present in the leaves of *A. ascalonicum*

RT ^a	Compound	RSI ^b	RA ^c %	Mol. Wt
12.57	Disulfide, dipropyl	878	59.94	150
12.82	(Z)-1-(Prop-1-en-1-yl)-2-prop yldisulfane	867	11.98	148
7.51	Disulfide, methyl propyl	868	5.59	122
5.64	Leaf alcohol	869	2.73	100
5.53	2-Hexenal	870	2.04	98
5.91	trans-2-Hexenol	871	1.45	100
6.87	1,2,4-Thiadiazole-3,5-diamine	872	1.44	116
18.7	Trisulfide, dipropyl	873	1.34	182
15.39	Heptane, 3,4,5-trimethyl-	874	0.89	142
6.62	1-(1-Propenylthio)propane	875	0.84	116
7.74	(E)-1-Methyl-2-(prop-1-en-1-y l)disulfane	876	0.83	120
20.25	Methyl cis-cinnamate	877	0.6	162
9.43	Cyclotetrasiloxane, octamethyl	878	0.46	296
8.41	Propanethioic acid, S-propyl ester	879	0.33	132
5.4	2-Hexyn-1-ol	880	0.28	98
12.16	1-Allyl-2-isopropyl disulfane	881	0.28	148
24.75	2,2-Dimethyl-2-sila-1,3-dioxo cyclohexane	882	0.28	132
13.97	Isophthalic acid, di(2-isopropylphenyl) ester	883	0.22	402
5.09	(Z)-4-Methyl-2-hexene	884	0.2	98
23.71	trans-Calamenene	885	0.2	202
7.05	3-Hexyne, 2-methyl-	886	0.19	96
9.54	2(1H)-Pyrimidinone, 5-chloro-4,6-diphenyl	887	0.18	282
14.52	Isothiazole, 3,5-dimethyl-	888	0.17	113
44.34	Ethyl 4-([(E)-(2-nitrophenyl)methylidene]amino)benzoate	889	0.16	298
6.43	2-Hexanamine, 5-methyl-	890	0.15	115
7.2	1,2,4-Thiadiazole-3,5-diamine	891	0.15	116
50.57	1H-Indene, 2,4,5,6,7,7a-hexahydro-7a-methyl-3-(2-methylpropyl)-	892	0.15	192
52.72	4-Methyl-2,4-bis(p-hydroxyphenyl)pent-1-ene, 2TMS derivative	893	0.14	412
8.77	2-Cyclopenten-1-one, 2,3,5-trimethyl-4-methylene	894	0.12	136
10.27	Ethyne, fluoro-	895	0.12	44

16.38	Heptane, 3,4,5-trimethyl-	896	0.11	142
8.68	β -Terpinene	897	0.1	136
13.27	2-Pentenoic acid, 4-oxo-, methyl ester, (Z)-	898	0.1	128
18.95	7-Methyl-5,6,7,8-tetrahydro-2, 4-quinazolinedione	899	0.1	180
45.19	2-Propenoic acid, 3-bromo-, methyl ester, (Z)-	900	0.1	164
55.05	Imidazo[1,5-a]pyridine, 3-phenyl	901	0.1	194
Total area %			94.06	

RT^a: Retention time; **RSI^b**: Reversed search index on TG-5MS capillary column, **RA^c%**: Relative area (peak area relative to the total peak area).

Table 7: List of Shortlisted Terpenes and Terpenoids

Class	Bioactive compound Name	PCID	SMILES
Terpenes (23)	Cyclohexene, 4-methylene-1-(1-methylethyl)-	66841	<chem>CC(C)C1=CCC(=C)CC1</chem>
	o-Cymene	10703	<chem>CC1=CC=CC=C1C(C)C</chem>
	2,6-Octadienal, 3,7-dimethyl-, (E)-	8843	<chem>CC(=CCCC(=CC=O)C)C</chem>
	α-Pinene	6654	<chem>CC1=CCC2CC1C2(C)C</chem>
	Caryophyllene	5281515	<chem>CC1=CCCC(=C)C2CC(C2CC1)(C)C</chem>
	Humulene	5281520	<chem>CC1=CCC(C=CCC(=CCC1)C)(C)C</chem>
	Germacrene D	5317570	<chem>CC1=CCCC(=C)C=CC(CC1)C(C)C</chem>
	Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)-	10887971	<chem>CC(C)C12CCC(=C)C1C2</chem>
	Linalool	6549	<chem>CC(=CCCC(C)(C=O)C</chem>
	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	11463	<chem>CC1=CCC(=C(C)C)CC1</chem>
	Linalyl acetate	8294	<chem>CC(=CCCC(C)(C=O)OC(=O)C)C</chem>
	ζ-Terpinene	7461	<chem>CC1=CCC(=CC1)C(C)C</chem>
	α-Ocimene	5320249	<chem>CC(=C)CCC=C(C)C=C</chem>
	2,4,6-Octatriene, 2,6-dimethyl-, (E,E)-	5368821	<chem>CC=C(C)C=CC=C(C)C</chem>
	Bicyclo[3.1.0]hex-2-ene, 4-methyl-1-(1-methylethyl)-	520384	<chem>CC1C=CC2(C1C2)C(C)C</chem>
	α-Terpineol	17100	<chem>CC1=CCC(CC1)C(C)(C)O</chem>
	Camphene	6616	<chem>CC1(C2CCC(C2)C1=C)C</chem>
	Tricyclo[2.2.1.0(2,6)]heptane, 1,7,7-trimethyl-	79035	<chem>CC1(C2CC3C1(C3C2)C)C</chem>
	Geraniol	637566	<chem>CC(=CCCC(=CCO)C)C</chem>
	Isoneral	20837773	<chem>CC(=CCC=C(C)CC=O)C</chem>
	cis-Calamenene	6429077	<chem>CC1CCC(C2=C1C=CC(=C2)C)C(C)C</chem>
	endo-Borneol	6552009	<chem>CC1(C2CCC1(C(C2)O)C)C</chem>
	α-Bisabolene	24798703	<chem>CC1=CCC(CC1)C(=CCC=C(C)C)C</chem>
Terpenoids (8)	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)-	5325830	<chem>CC1=CCC(CC1)(C(C)C)O</chem>
	Photocitral A	102684	<chem>CC1CCC(C1C=O)C(=C)C</chem>
	photocitral B	296248	<chem>CC1(C2CCC1(C2C=O)C)C</chem>
	2,6-Dimethyl-1,3,6-heptatriene	5368331	<chem>CC(=C)CC=CC(=C)C</chem>
	α-Bourbonene	530816	<chem>CC1=CCC2C1C3C2(CCC3C(C)C)C</chem>
	Geranyl acetate	1549026	<chem>CC(=CCCC(=CCOC(=O)C)C)C</chem>
	α-Cubebene	442359	<chem>CC1CCC(C2C13C2C(=CC3)C)C(C)C</chem>
	Bicyclo[3.1.0]hexane, 6-isopropylidene-	556529	<chem>CC(=C1C2C1CCC2)C</chem>

Table 8: The Top 10 Bioactive Ingredients Ranked Based on their Degree values

Sl. No	CID	Compound	Class	Degree
1	1549026	Geranyl acetate	Terpenoids	13
2	637566	Geraniol	Terpenes	12
3	6552009	endo-Borneol	Terpenes	11
4	5325830	3-Cyclohexen-1-ol,4-methyl-1-(1-methylethyl)-,(R)-	Terpenoids	11
5	6549	Linalool	Terpenes	10
6	8843	2,6-Octadienal, 3,7-dimethyl-,(E)-	Terpenes	9
7	20837773	Isoneral	Terpenes	8
8	8294	Linalyl acetate	Terpenes	7
9	24798703	α -Bisabolene	Terpenes	5
10	296248	Photocitral B	Terpenoids	5

Table 9: Top 10 HUB genes ranked based on their degree

Rank	Gene symbol	Gene Name	Degree
1	ALB	Serum albumin	32
2	CASP3	Caspase-3	23
3	TP53	Cellular tumor antigen p53	21
4	MAPK14	Mitogen-activated protein kinase 14	19
5	ESR1	Estrogen receptor 1	19
6	MAPK1	Mitogen-activated protein kinase 1	18
7	APP	Amyloid-beta A4 protein	18
8	NOS3	Nitric-oxide synthase 3	18
9	MAPK8	Mitogen-activated protein kinase 8	16
10	PPARG	Peroxisome proliferator-activated receptor gamma	16

Table 10: Molecular Docking Results

Compounds	Targets	Binding Energy (kcal/mol)	Van der Waals interactions	Alkyl and Pi interactions
24798703 - α -Bisabolene	ALB	-7.3	VAL-116, PRO-118, MET-123, GLU-141, ILE-142	LEU-115(3), ARG-117, LYS-137, TYR-138(2) , TYR-161(2) , LEU-182(2), LEU-185, ARG-186(2)
	ESR1	-7.7	THR-347, LEU-349 , GLU-353, TRP-383, ARG-394, MET-421, GLY-521	MET-343, LEU-346 , ALA-350(2) , LEU-384 , LEU-387 , LEU-391 , PHE-404(2) , ILE-424 , HIS-524(2), LEU-525(2)
	MAPK1	-7.4	PRO-58 , THR-68, GLU-71 , ASP-167	TYR-36(2) , LYS-54 , ILE-56(3) , TYR-64(2) , ARG-67(2)
	NOS3	-8.7	GLY-186, GLN-189, SER-226, SER-354, ALA-227, GLY-355	TRP-178(5) , LEU-193(2) , ILE-228 , PHE-473, PHE-353(2) , TRP-356(2)
	MAPK8	-7.1	GLN-37, GLU-109, LEU-110, MET-111, ALA-113 , ASP-169	ILE-32(2) , VAL-40(2) , ALA-53(2) , LYS-55, ILE-86, MET-108(2) , VAL-158(2) , LEU-168(4)
	PPARG	-7	GLN-271, ARG-280, GLN-283, GLY-284 , GLN-286, SER-342	LEU-270(2), PHE-287(2), HIS-466
1549026 - Geranyl acetate	NOS3	-7.1	GLY-186, GLN-189, SER-226, SER-354, GLY-355	TRP-178(3) , CYS-184, LEU-193 , ILE-228 , PHE-473(2) , PHE-353(4), TRP-356

*Bolded amino acid residues are the residues that matched with active residues from the literature and PDB

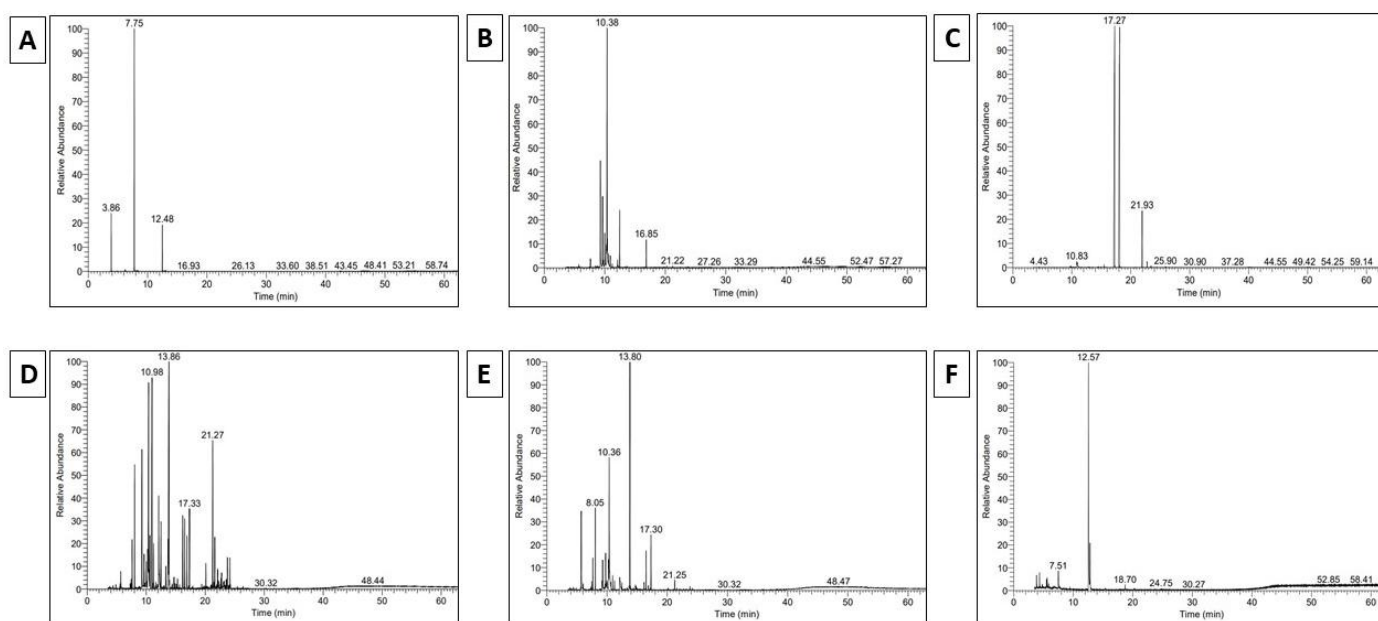


Figure 1. A) GCMS Chromatogram of *Allium odorum*. B) GCMS Chromatogram of *Xanthoxylum acanthopodium*. C) GCMS Chromatogram of *Elsholtzia griffithii*. D) GCMS Chromatogram of *Ocimum canum* (flower), E) GCMS Chromatogram of *Ocimum canum* (leaves), and F) GCMS Chromatogram of *Allium ascalonicum*.

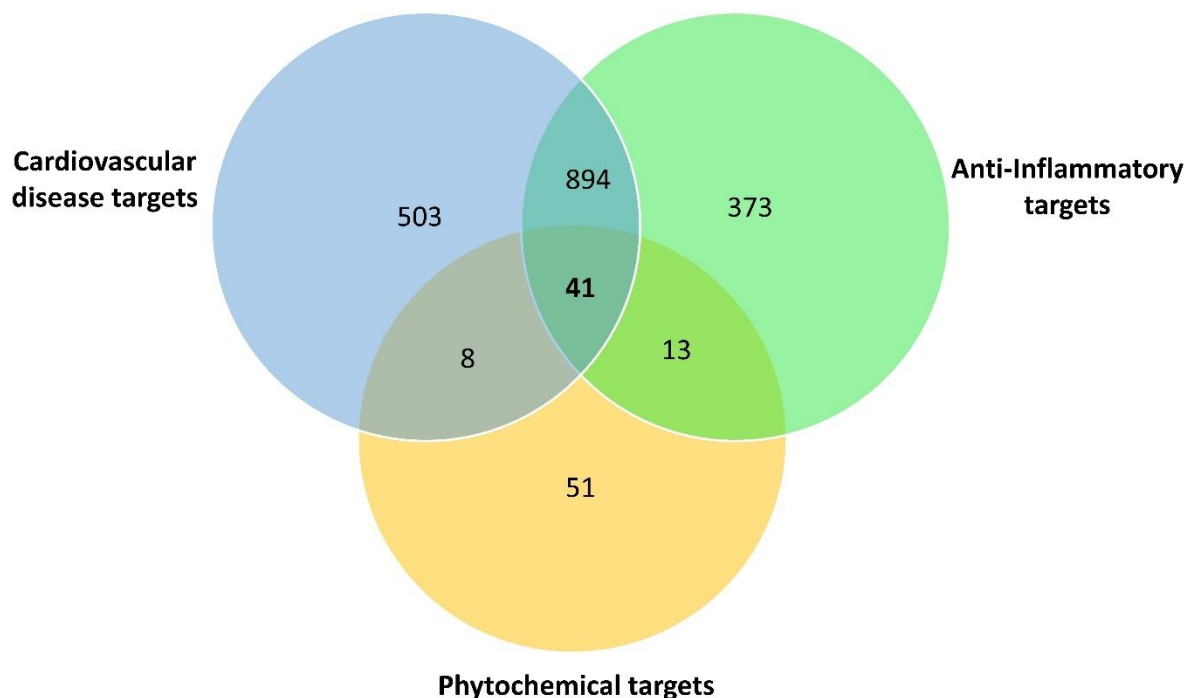


Figure 2. The Venn diagram illustrates the common gene targets among bioactive compounds, cardiovascular, and inflammatory diseases.

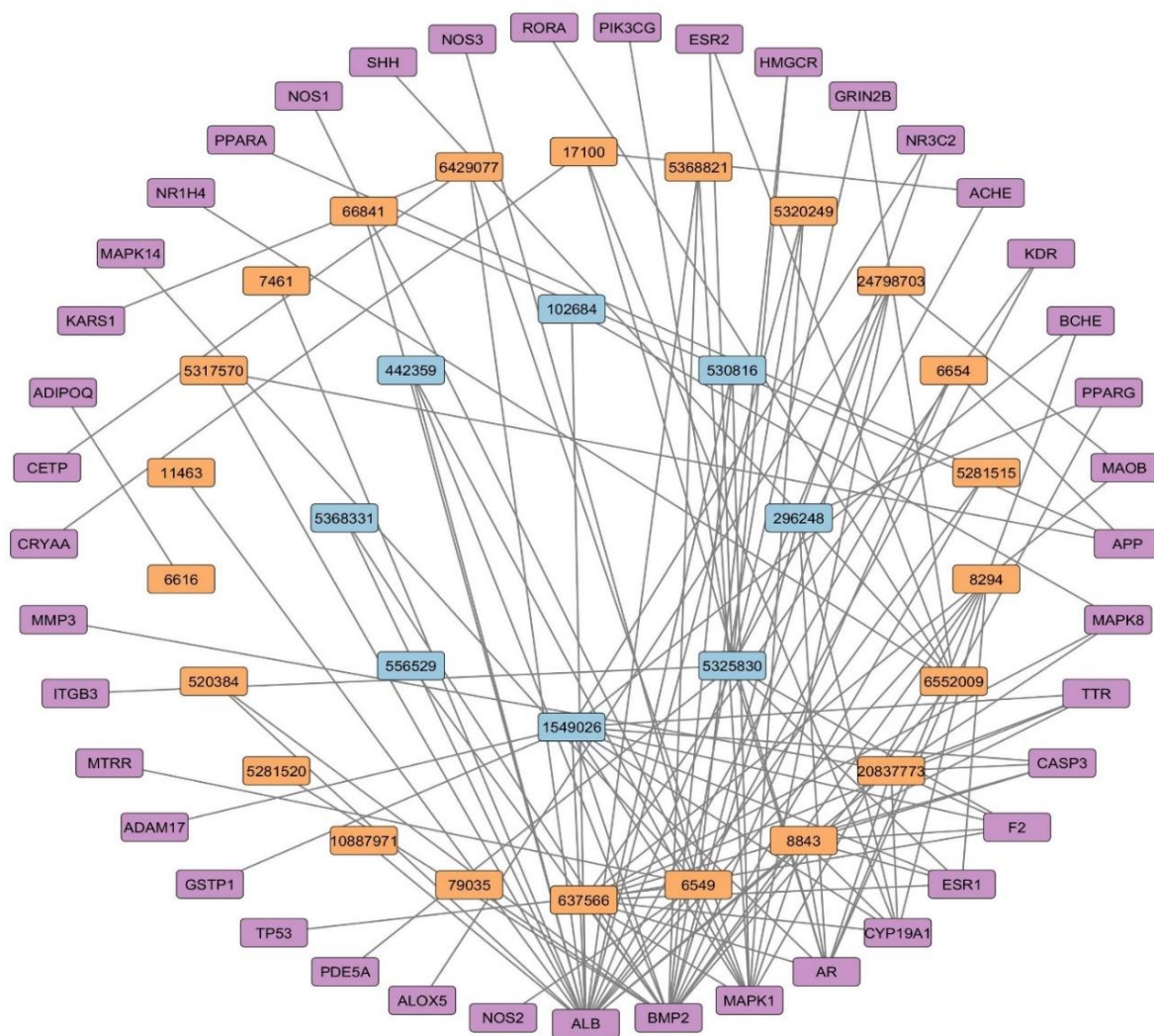


Figure 3. Compound-Target Network obtained through Cytoscape, purple are the gene targets, blue are the terpenoids and orange are the terpenes.

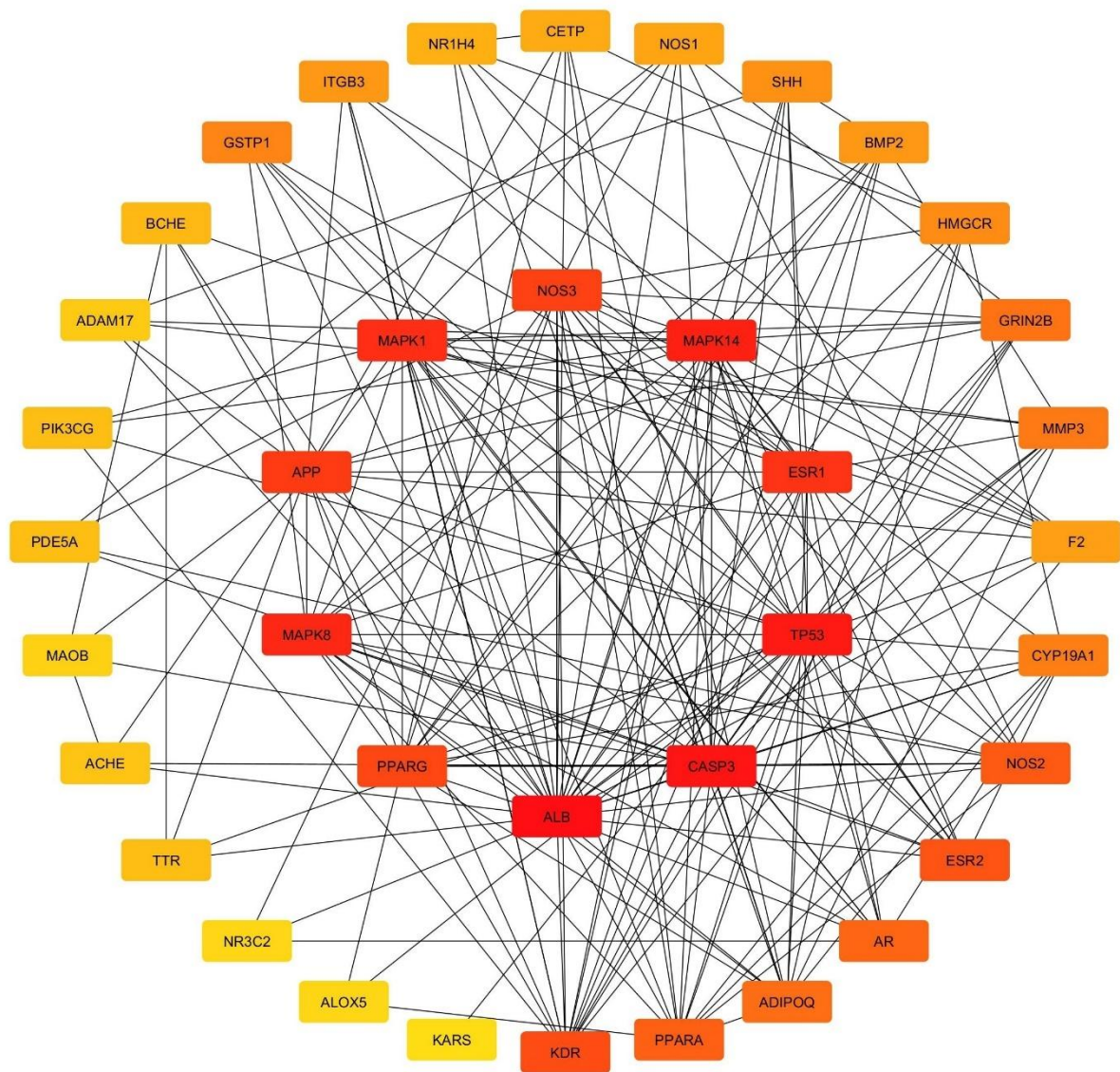


Figure 4. Protein-Protein Interaction network (PPI) of 41 common targets colored by their degree red (high) and yellow (low).

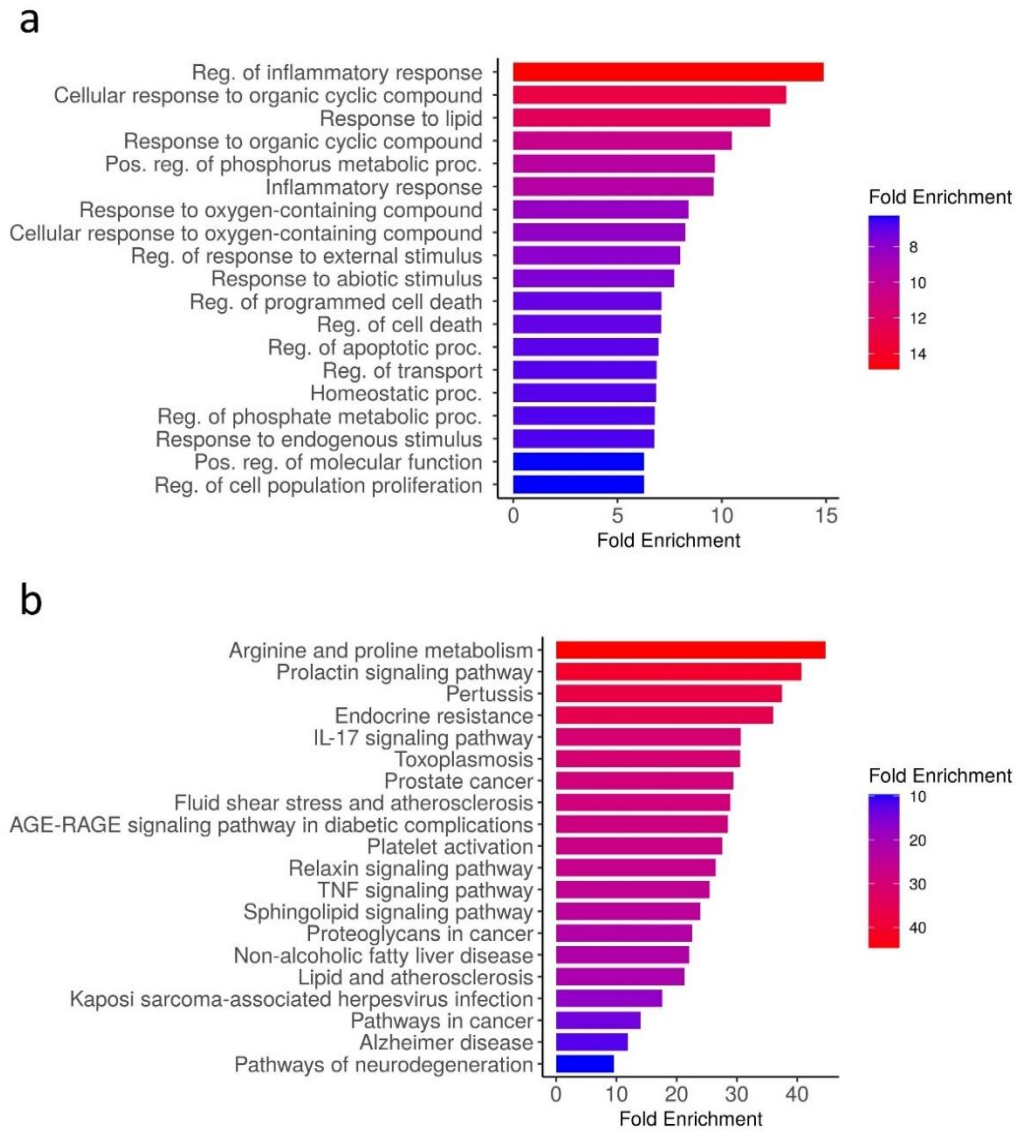
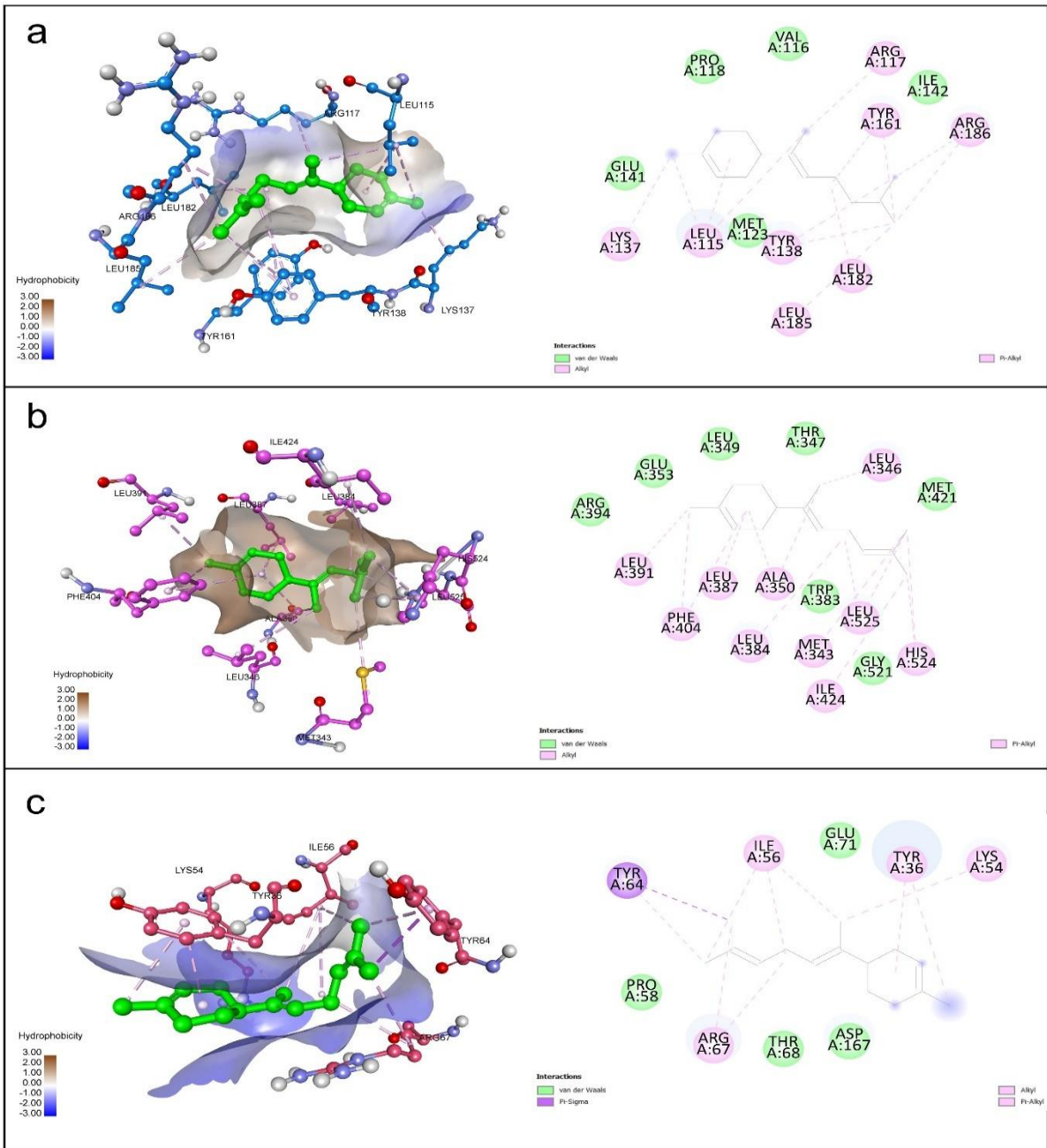
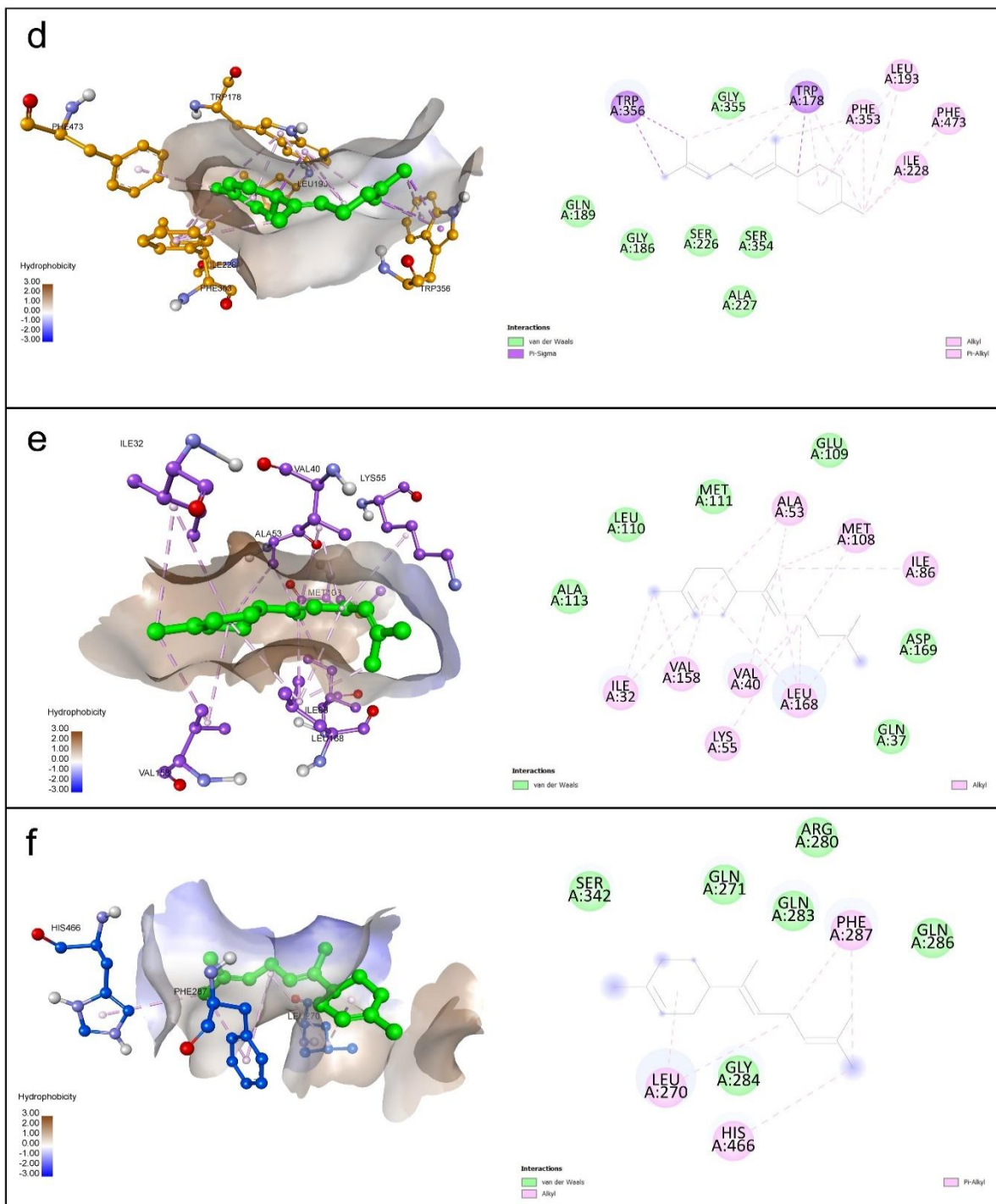


Figure 5. Bar plot representing Functional enrichment analysis of top 20 (a) Biological Processes and (b) KEGG pathways.

	ALB	CASP3	TP53	MAPK14	ESR1	MAPK1	APP	NOS3	MAPK8	PPARG
Native ligand	-7.66	-7.6	-9.06	-10.6	-10.7	-9.6	-5.8	-7.04	-8.2	-9.3
1549026	-6.3	-5.1	-6.4	-5.4	-6.4	-5.7	-4.2	-7.1	-5.5	-5.9
637566	-5.5	-4.6	-5.7	-5.1	-5.8	-5.3	-4.4	-5.8	-5.2	-5.6
6552009	-5.6	-4.4	-6.4	-5.5	-6	-5.5	-4.1	-5	-4.7	-5
5325830	-6	-5	-5.9	-5.7	-6	-5.9	-4.1	-6.5	-5.4	-5.8
6549	-5.4	-4.4	-5.6	-5.1	-5.4	-5.7	-4.1	-5.9	-4.7	-5.4
8843	-5.6	-4.7	-6.4	-5.3	-5.7	-5.1	-3.6	-6.2	-5	-5.5
20837773	-5.5	-4.8	-5.2	-4.9	-5.6	-5.4	-4	-6.1	-4.9	-5.3
8294	-6	-4.6	-6.1	-5.5	-6	-6.3	-4.1	-6.4	-5.4	-5.9
24798703	-7.3	-6.7	-6.4	-6.8	-7.7	-7.4	-5.3	-8.7	-7.1	-7
296248	-5.6	-3.9	-5.6	-5.8	-5.5	-5.4	-3.7	-4.7	-4.6	-5.2

Figure 6. Heat map representation of binding energies (in kcal/mol) obtained through molecular docking between Top 10 compounds and Top 10 hub genes.





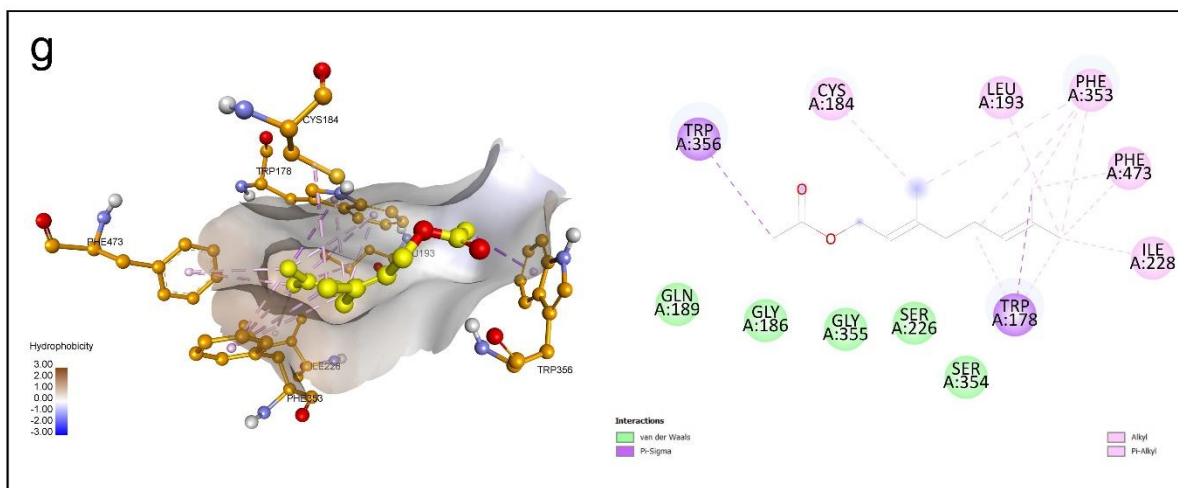


Figure 7. Molecular Docking results visualization between trans-alpha-bisabolene (α -Bisabolene) and a) ALB, b) ESR1, c) MAPK1, d) NOS3, e) MAPK8, f) PPARG and g) Molecular Docking results visualization between Geranyl acetate and NOS3.

Tables and figure titles and legend:

Table 1: Major Volatile Organic Compounds Present in the leaves of *Allium odorum*

RT^a: Retention time; **RSI^b:** Reversed search index on TG-5MS capillary column, **RA^c%:** Relative area (peak area relative to the total peak area).

Table 2: Major Volatile Organic Compounds Present in the leaves of *Xanthoxylum acanthopodium*.

RT^a: Retention time; **RSI^b:** Reversed search index on TG-5MS capillary column, **RA^c%:** Relative area (peak area relative to the total peak area).

Table 3: Major Volatile Organic Compounds Present in *Elsholtzia griffithii* inflorescence

RT^a: Retention time; **RSI^b:** Reversed search index on TG-5MS capillary column, **RA^c%:** Relative area (peak area relative to the total peak area).

Table 4: Major Volatile Organic Compounds Present in the fruits of *Ocimum canum*

RT^a: Retention time; **RSI^b:** Reversed search index on TG-5MS capillary column, **RA^c%:** Relative area (peak area relative to the total peak area).

Table 5: Major Volatile Organic Compounds Present in the leaves of *Ocimum canum*

RT^a: Retention time; **RSI^b:** Reversed search index on TG-5MS capillary column, **RA^c%:** Relative area (peak area relative to the total peak area).

Table 6: Major Volatile Organic Compounds Present in the leaves of *Allium ascalonicum*

RT^a: Retention time; **RSI^b:** Reversed search index on TG-5MS capillary column, **RA^c%:** Relative area (peak area relative to the total peak area).

Table 7: List of Shortlisted Terpenes and Terpenoids

Table 8: The top 10 bioactive ingredients ranked based on their degree values

Table 9: Top 10 HUB genes ranked based on their degree

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