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(Research Article)

Characterization, profiling, and molecular docking analysis of phytochemicals derived from *Daucus carota* for evaluating their potential role in cardiovascular disease (CVD) assessment

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Abstract

Cardiovascular disease (CVD) remains a significant global health challenge, prompting this research manuscript's investigation into the potential contributions of phytochemicals extracted from *Daucus carota,* commonly known as carrots, in assessing CVD. The study employed a comprehensive approach, including spectral characterization through ^{1}H and ^{13}C NMR, and quantitative profiling using HPTLC, to identify and quantify phytochemical markers, namely, p-hydroxybenzoic acid, caffeic acid, and chlorogenic acid. Spectral characterization using NMR confirmed the presence of saturated and unsaturated moieties within these markers. Subsequently, these phytoconstituents, three in number found in carrot roots, underwent *In-silico* screening using the protein structure (PDB ID: 5JAD). The results of the molecular docking simulations revealed that these phytoconstituents exhibited higher docking scores and lower glide energies compared to standard drugs like Felodipine. The methodology and key research sections encompassed the collection, identification, and preparation of carrot samples, as and-performance thin-layer chromatographic TLC and (HPTLC) profiling, NMR spectroscopy, and molecular docking studies. The result findings offer valuable insights into the potential health benefits of carrot phytochemicals, encourage further exploration of varietal differences, suggest optimization of extraction techniques, and advocate for the assessment of synergistic effects. Importantly, the promising cardioprotective properties of these phytochemicals highlight their role in preventing and managing cardiovascular disease (CVD). The phytoconstituents derived from *Daucus carota*, as evidenced by HPTLC and *In-silico* studies, demonstrate substantial anti-cardiac potential. This positions them as valuable phytochemicals for the development of innovative anti-CVD/anti-CHF medications, offering promising avenues for the treatment of diverse cardiac diseases and disorders in the future.

Keywords: CVD; Felodipine; HPTLC; *In-silico*; NMR; Phytochemicals

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1. Introduction

Fruits and vegetables are abundant sources of nutrients containing phytochemicals, also known as bioactive compounds, which are renowned for their nutraceutical properties and positive impacts on health [1]. Among these, the cultivated carrot, scientifically known as *Daucus carota* L., shown in Figure No. 1 holds a prominent position in the world of vegetables due to its exceptional yield potential and its versatility as both a fresh and processed product. Carrots, along with turnips, collectively contribute to an annual global production exceeding 428 million tons, cultivated across approximately 11.5 million hectares of land [2]. This places carrots firmly within the top 10 vegetable crops worldwide [3]. Their significance in human nutrition is underscored by their high nutritional value and impressive storage characteristics [4, 5]. Carrots derive their nutritional value from various phytochemicals, primarily falling into four categories: phenolic compounds, carotenoids, polyacetylenes, and ascorbic acid.

Figure 1 *Daucus carota*

1.1. The Carrot Plant

The edible carrot, scientifically known as *Daucus carota*, holds a paramount position as a globally cultivated root vegetable plant, belonging to the Apiaceae family [6]. The carrot can be primarily divided into two main parts: the stem and the root. The majority of the root is comprised of three layers, including the outer peel (periderm), a fleshy outer cortex (phloem), and an inner core (xylem). A visual representation of the carrot root's structure is depicted in Figure No. 2. Cultivated carrots exhibit a spectrum of colors, ranging from orange and reddish to purple, black, or yellow. While various parts of the carrot plant, including the stems and leaves, are edible, this review predominantly focuses on the root unless specified otherwise. Carrots hold great nutritional significance due to their rich content of nutrients and phytochemicals, resulting in nutraceutical effects and substantial health benefits. Carrots are renowned for their substantial contribution to human nutrition, driven by their high dietary value and remarkable storability. Furthermore, carrots exhibit a diverse array of phytochemicals, encompassing phenolic compounds, carotenoids, polyacetylenes, and ascorbic acid. This diversity hints at the potential for a wide range of health-promoting effects associated with carrot consumption.

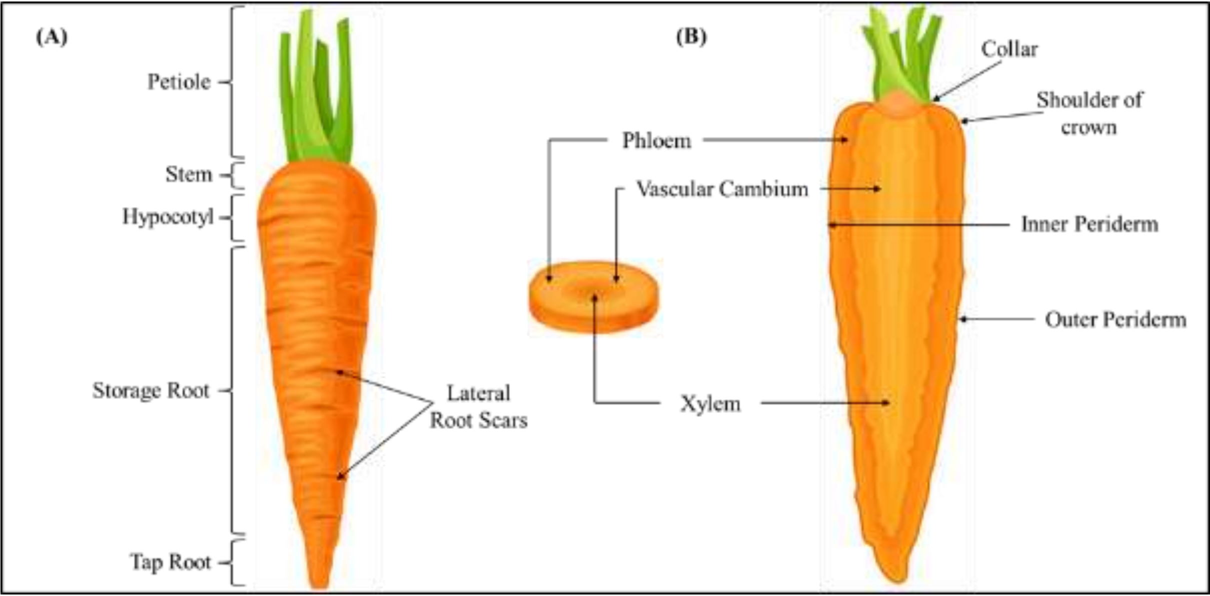
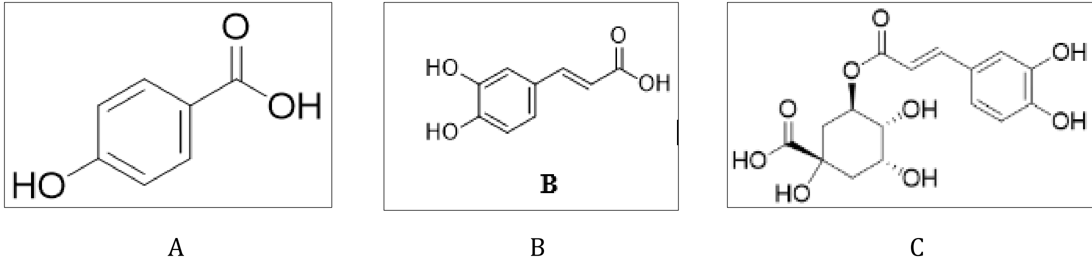


Figure 2 Carrot Root anatomy: (A) Longitudinal View; (B) Cross-Section Displaying the Periderm, Phloem, and Xylem Layers [7]

1.2. Phenolic Compounds

Phenolic compounds are among the most widespread groups of plant metabolites and are present in both human and animal diets. Their role in preventing degenerative diseases like cancer, cardiovascular diseases, and neurodegenerative disorders has been documented. Over the past two decades, there has been a significant increase in interest in food phenolics due to their antioxidant capabilities and their ability to protect against oxidative stress caused by excessive reactive oxygen species [7]. These phenolic compounds are secondary metabolites in plants, primarily characterized by an aromatic ring containing one or more hydroxyl groups. They play a vital role in mitigating various forms of stress, such as exposure to ultraviolet radiation, encounters with pathogens, parasites, and herbivores, while also contributing to the sensory qualities of plants and plant-derived foods [8][9][10][11]. Phenolic compounds can be categorized into various subgroups, including phenolic acids, flavonoids, tannins, lignans, stilbenoids, and curcuminoids. Carrots have been reported to be rich in phenolic acids like p-hydroxybenzoic, caffeic, and chlorogenic acids, as well as anthocyanins, which belong to the flavonoid class (Figure 3) [12].



A B C

Figure 3 Chemical structures of phenolic acids present in the roots of *Daucus carota*: (A) p-hydroxybenzoic acid; (B) caffeic acid; (C) chlorogenic acid

- Phenolic Compounds in Carrots: The presence of phenolic compounds, such as p-hydroxybenzoic, caffeic, and chlorogenic acids, as well as anthocyanins in root of carrots, is highlighted Figure 3. These compounds are known for their antioxidant properties and have been associated with potential health benefits, including protection against degenerative diseases like cancer, cardiovascular diseases, and neurodegenerative disorders.
- Bitter Compounds as Quality Markers: Isocoumarins and phenolic acids are the potentially bitter compounds found in carrot peels. Czepa and Hofmann [13] reported that the bitter taste in carrots is caused by terpenoids and water-soluble phenolics. Therefore, their presences can be used as biological markers to assess the quality of fruits and vegetables during postharvest operations [14].

1.3. Potential Novel Research Directions:

- Exploring Health Benefits: Future research could delve deeper into the specific health benefits of different phytochemicals found in carrots. This could involve in-depth studies on their mechanisms of action in preventing degenerative diseases and their potential synergistic effects when consumed together.
- Varietal Differences: Investigating varietal differences in phytochemical composition among carrot cultivars could be intriguing. Some varieties might contain higher levels of certain beneficial compounds, potentially leading to the development of carrot varieties tailored for specific health outcomes.
- Extraction and Utilization: Optimizing extraction methods for phytochemicals from carrots and exploring their applications in functional foods or nutraceuticals could be an area of interest. This could involve developing novel food products fortified with carrot-derived phytochemicals.
- Bitter Compounds and Quality Assessment: Further research could focus on developing rapid and non-destructive techniques for assessing the bitterness of carrot peels. This would benefit the food industry by ensuring consistent product quality.
- Synergistic Effects: Investigating the potential synergistic effects of phytochemicals within carrots and their interactions with other food components could provide valuable insights into their overall health-promoting properties.

For this research manuscript a SOP is prepared to access *Daucus carota* for evaluating its phytochemicals identification, screening, Profiling and docking to evaluate its potential role against CVD.

2. Material and methods

2.1. Collection and identification of Plant

Plant known as Edible carrot, *Daucus carota* mentioned were procured from the local vendor of Jhansi, Uttar Pradesh. They were identified by the Dravyaguna and Botany experts at Bundelkhand Govt. Ayurvedic College Hospital, Jhansi. The Plant were authenticated by the Department of Pharmacognosy of Bundelkhand Govt. Ayurvedic College Hospital, Jhansi.

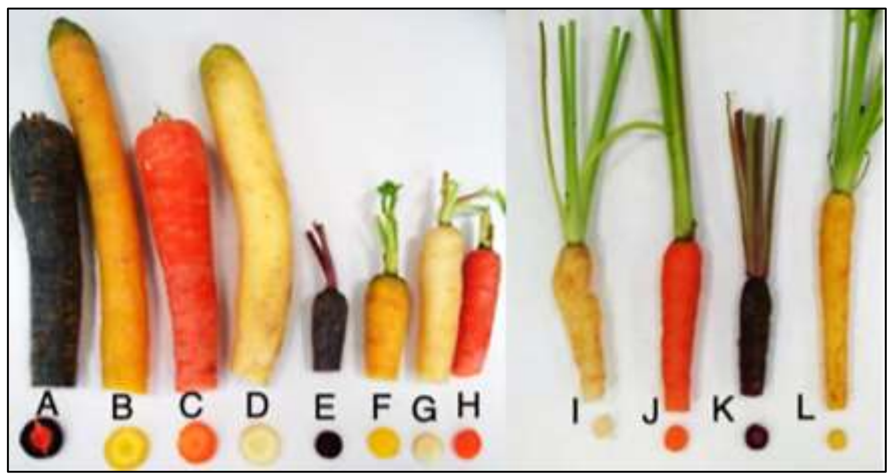


Figure 4 Different species of carrots evaluated for their Pomology characters {A—normal purple carrot (NPC), B—normal yellow carrot (NYC), C—normal orange carrot (NOC), D—normal white carrot (NWC), E—mini purple carrot (MiPC), F—mini yellow carrot (MiYC), G—mini white carrot (MiWC), H—mini orange carrot (MiOC), I—micro white carrot (MWC), J—micro orange carrot (MOC), K—micro purple carrot (MPC), L—micro yellow carrot (MYC)}

2.2. Standard operating procedure (SOP) of preparation of *Daucus carota*

Carrots, which were identified and acquired from vendors in the city of Jhansi, located in Uttar Pradesh, were subjected to a series of quality control assessments as part of our laboratory investigations. These assessments were conducted at different stages: immediately after harvesting, following storage in a cold room at temperatures between (4–5 °C), and after one month of freezing at (−18 °C). To determine the moisture content of the carrots, we employed a gravimetric method, and we also assessed the color content in the carrots using the procedure outlined in the phytochemical parameters.

- Extraction Conditions: The carrot roots were sliced into pieces measuring 2 mm in width and 1 cm in length. To extract carotenes, we conducted experiments at various temperatures (20 °C, 40 °C, and 60 °C) using a mixture of 96% ethanol and 2-propanol. Initially, 25 grams of sliced carrot samples were combined with 100 grams of 96% ethanol. These carrot slices underwent extraction in a water bath at the specified temperatures. We shook the samples every 10 minutes, and after each hour of extraction, we collected 5 ml samples, which were then mixed with 20 ml of petroleum ether. Water was introduced to facilitate phase separation. After separation, the petroleum-ether-carotenoid phase was adjusted to a total volume of 50 ml.
- Carotene Determination: The content of β-carotene in the petroleum-ether extract was assessed through spectrophotometry. We measured absorbance at a wavelength of 450 nm using a spectrophotometer.
- The concentration of carotenes, expressed as β-carotene (g/100 ml), was calculated using the following formula: β-carotene = A × d × V / (E1% × w × 1cm), where A represents absorbance, d is dilution, V is volume (ml), E1% is the coefficient of absorbance (2592 for petroleum-ether), w is the weight of the sample (g), and 1cm denotes a 1 cm path length.
- Preparation of Fine *Daucus carota* powder: *Daucus carota* samples of pharmacopoeial quality were acquired and subsequently identified by experts in Dravyaguna and Botany at Bundelkhand Govt. Ayurvedic College Hospital, Jhansi. The carrots were then meticulously cleaned, washed, and dried. We powdered the *Daucus carota* using a pulverizer equipped with an 80-mesh screen. The resulting material was further sifted through a vibro sifter with an 80-mesh sieve to obtain a fine powder. We ensured the integrity of the sieve before and after sifting. Residue from the *Daucus carota* was collected, weighed, and combined with fresh material, followed by recording the weight.
- Blending of Fine Powder: The accurately weighed *Daucus carota* powder was mixed to create a homogeneous blend of markers as specified in the formulation composition. Subsequently, we added 2% Gum Acacia solution, 5% starch solution, and 2% silicon dioxide as binding agents to the blend. After thorough mixing, we processed the mixture into granules by passing it through a granulator with a No. 10 sieve size. These granules were then evenly distributed in suitable test tubes and subjected to sonication at 60 °C for 15 minutes.

2.3. Chromatographic Analysis: Thin-layer chromatography (TLC)

- Sample Preparation: Precisely measured 1.5 g samples of *Daucus carota* and its markers were individually dissolved in 15 ml of methanol. These solutions were then refluxed on a water bath at a temperature between 90-100 °C for 15 minutes. Afterward, they underwent filtration and were evaporated down to 5 ml in a porcelain dish, which was subsequently used for TLC profiling.
- Solvent System: The solvent system used for p-hydroxybenzoic acid, caffeic acid, and chlorogenic acid markers was a mixture of Toluene, Ethyl Acetate, and Formic Acid in a ratio of 7:2:1 (v/v). Through a trial and error process, the optimal solvent system was determined to be Toluene, Ethyl Acetate, and Formic Acid in a ratio of 5:4:1 (v/v) for achieving the best separation. This system was employed to develop the TLC plates.
- Development: The methanolic extracts were applied onto Silica Gel 60 F254 plates with a thickness of 0.2 mm, and the development process took place in the previously mentioned solvent system.
- Visualization: The developed TLC plates were first examined under ultraviolet light at wavelengths of 254 nm and 366 nm. Subsequently, the plates were subjected to derivatization using anisaldehyde-sulphuric acid reagent and heated to 110 °C until colored spots developed, which were then observed in daylight. The color and Rf (retention factor) values of the resolved spots were recorded for *Daucus carota* markers such as p-hydroxybenzoic acid, caffeic acid, and chlorogenic acid.

2.4. High-Performance Thin-Layer Chromatography (HPTLC) Analysis

To conduct HPTLC profiling of *Daucus carota* markers, including (A) p-hydroxybenzoic acid, (B) caffeic acid, and (C) chlorogenic acid, the following steps were carried out:

- Preparation of Test Solutions: Methanolic solutions of *Daucus carota* markers were prepared at a concentration of 100 mg/ml. To create these methanolic solutions, 100 mg of the sample was dissolved in 1 ml of methanol and then sonicated for 10 minutes at 25 °C.
- Standard Solution: Standard solutions of *Daucus carota*, as well as reference solutions for compounds like p-hydroxybenzoic acid, caffeic acid, and chlorogenic acid (both E and Z isomers), were prepared in methanol. These standard solutions had a concentration of 1 mg/ml.
- Quality Control for *Daucus carota* Markers: Quality control parameters, including organoleptic, microscopic, and macroscopic assessments, as well as physico-chemical parameters such as loss on drying, pH (at 10%), total ash, acid insoluble ash, and values for water extractability and ethanol extractability, were not performed. The focus was solely on profiling for quantification and identification of these markers. Additional quality

control parameters were conducted for the formulation, as mentioned in API standards [16, 17, 18, and 15], to ensure the proper identification and quantification of *Daucus carota* markers.

Stationary Phase: Pre-coated aluminum plates measuring 10x10 cm with a thickness of 0.2 mm, containing Silica Gel 60F254, were prewashed with methanol and activated at 60°C for 5 minutes before chromatography.

- Sample Preparation: Methanolic extracts were diluted with methanol to achieve a concentration of 1 mg/ml and were then filtered using 0.45 Millipore filters.
- Application of Sample: An auto-sampler system, CAMAG Linomat 5, was used to apply 2 ml of each marker sample with a width of 8 mm.
- Development: HPTLC plates were developed in a CAMAG glass twin-through chamber (20x10 cm) that had been previously saturated with the solvent for 60 minutes. The chamber was maintained at 60°C and 40% relative humidity (RH), with a development distance of 9 cm. The mobile phase used was a mixture of Toluene, Ethyl Acetate, and Formic Acid in a ratio of 5:4:1 (v/v).
- Visualization: The developed HPTLC plates were visualized both before and after spraying with an anisaldehyde-sulfuric acid reagent at wavelengths of 254 nm, 366 nm, and 540 nm.
- Instrumentation and Method: For the HPTLC profiling of *Daucus carota* markers, such as p-hydroxybenzoic acid, caffeic acid, and chlorogenic acid, a CAMAG HPTLC instrument, a 100 ml syringe, and a glass twin-trough chamber were employed. Methanolic extracts of ingredients (10 ml), three markers of *Daucus carota* (10 ml each), and standard solutions (5 ml) were applied to an aluminum plate pre-coated with 0.2 mm thick silica gel 60 F254 (Merck, India) using a CAMAG Linomat-5 applicator and visionCats software. The plate was developed in a glass twin-through chamber that had been presaturated for 15 minutes with a mobile phase consisting of chloroform, ethyl acetate, formic acid, and acetic acid (in a ratio of 7.5:2.25:0.5:0.5 v/v/v/v). The developed plate was visualized at 254 nm and 366 nm using a CAMAG visualizer. Subsequently, the plate was derivatized with an anisaldehyde-sulfuric acid reagent and heated to 105 °C until visible spots appeared. The derivatized plate was also visualized using a CAMAG visualizer. The visible spots on the derivatized plate were scanned at 514 nm using a CAMAG Scanner-4. Rf values and densitograms were recorded using the CAMAG visionCats software, and the final report is presented in the figures.

After profiling and identifying the markers in the HPTLC analysis of *Daucus carota* markers at 254nm, 366nm and 514nm, such as p-hydroxybenzoic acid (1), caffeic acid (2), and chlorogenic acid (3), (as shown in Figures 11), these markers were further subjected to spectral characterization, specifically NMR (^{1}H NMR and ^{13}C NMR).

2.5. Nuclear Magnetic Resonance (NMR) Spectroscopy

NMR spectroscopy is the preferred method for determining the structures of natural products, and it has gained prominence in plant metabolomics. Metabolomics aims to qualitatively and quantitatively analyze the maximum number of metabolites with high throughput. While most metabolomics labs utilize various spectroscopic techniques, NMR spectroscopy offers several advantages as an initial screening method compared to other analytical platforms. NMR spectroscopy simplifies sample preparation compared to alternative methods, allowing for high sample throughput with minimal instrument drift. Unlike certain mass spectrometry methods that rely on metabolite derivatization or ionization capability, NMR is non-discriminatory. Metabolite screening requires maximum sensitivity and broad compound coverage, often focusing on the most sensitive and commonly occurring magnetic nucleus, such as ^{1}H. However, additional insights into metabolite flux can be gained by observing other nuclei, particularly ^{13}C and ^{15}N.In this research article, we emphasize the progress made in profiling *Daucus carota* markers, including p-hydroxybenzoic acid, caffeic acid, and chlorogenic acid, using ^{1}H-NMR and ^{13}C-NMR spectroscopy. This method enables the identification of nodes such as OH, CH, C, and H, each with distinct shift values, facilitated by software like CHEM DRAW ULTRA. The results are presented in Figures 5, 6, 7, 8, 9, 10, and Table 1.

2.6. Molecular docking study:

For virtual derivative screening, the structures of *Daucus carota* markers such as *p*-hydroxybenzoic acid; caffeic acid; chlorogenic acid were sketched using ChemDraw 19.1. For molecular docking, Schrodinger suite v 13.1 was employed.

2.6.1. Protein preparation

For the molecular docking research of a chosen data set of *Daucus carota* markers such as *p*-hydroxybenzoic acid; caffeic acid; chlorogenic acid, transcriptional regulation (PDB Id: 5JAD) was picked from the Protein Data Bank as shown in Figure 12. The typical structure file downloaded from the PDB is not suitable for immediate use in calculations for molecular modelling. Among other things, a typical PDB structure file includes co-crystallized ligands, water molecules,

metal ions, and cofactors. The protein preparation wizard preprocessed, optimised, and reduced protein before creating it. A refined, hydrogenated ligand and ligand-receptor complex structure is the end product, which can be applied to various Schrodinger modules [19].

2.6.2. Ligand Preparation

The Maestro v 13.1 LigPrep module is used to prepare the ligands for the optimum docking outcomes. The docked structures need to be accurate representations of the real ligand structures as they would appear in a protein-ligand complex. The structures must therefore comply with the following Glide docking software criteria. Three dimensions are required. Glide solely modifies the ligand's internal torsional coordinates; hence, the other geometric parameters must be modified in advance. Each of them must consist of a single molecule, without any covalent receptor attachments or other pieces like counter ions or solvent molecules. They must be hydrogen-filled (valences). They need to be properly protonated for physiological pH levels, which are around 7 [20,21].

2.6.3. Grid generation

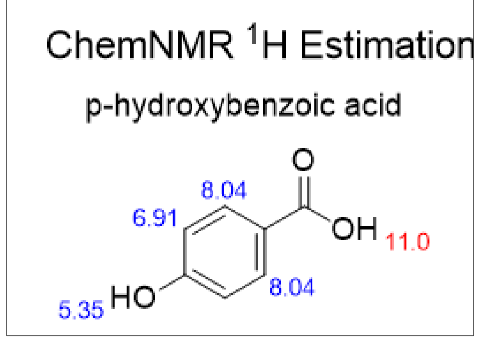
The grid is produced by Maestro version 13.1's receptor grid generation module. The co-crystallized ligand's binding site is surrounded by a grid that makes it possible for other molecules to bind there while keeping the co-crystallized ligand out [22].

2.6.4. Molecular docking

After creating the glide grid zip file and preparing the ligands, docking was carried out using the maestro v 13.1 ligand docking module. The XP module conducts more accurate molecular docking of certain *Daucus carota* markers, such as *p*-hydroxybenzoic acid; caffeic acid; chlorogenic acid. The size of the data gathering decreases as the level of precision increases. In Maestro v 13.1 [23,24], the XP parameters docking score, glide energy, and glide model value were estimated. *P-hydroxybenzoic* acid; caffeic acid; chlorogenic acid, three *Daucus carota* markers were subjected *to In-silico* screening. We next create a library of 4 chemical strcture including 3 phytochemicals present in roots of *Daucus carota* and 1 standard medication Felodipine. *Daucus carota* markers with the necessary parametric compounds, and select Felodipine as the standard medication, out of which we select our top three docked score markers of *Daucus carota* binding at receptor (5JAD) shown in Fig No. 12. When compared to standard anti-CVD drug like Felodipine, the top 3 markers of *Daucus carota* demonstrate higher docking scores and glide energies, respectively shown in Table No. 2 and Fig. 13,14,15,16 depict a 2D and 3D ligand-protein interaction. Also some research already done to assessed potential and viable efficacy of *In-silico* analysis to predict the medications obtained from medicinal plants to treat various diseases and disorders such as Monkeypox [26], epilepsy [27] and *In silico* for some conventional drugs such as *In-silico* design of a novel silver metal ciprofloxacin compound [28]. Even the foundation of our study is computational molecular docking, it's critical that the scientific tool Maestro 12.8 employed for molecular docking research proves its validity.

3. Results and discussion

3.1. NMR results of phytochemicals present in *Daucus carota* at ^{1}H and ^{13}C



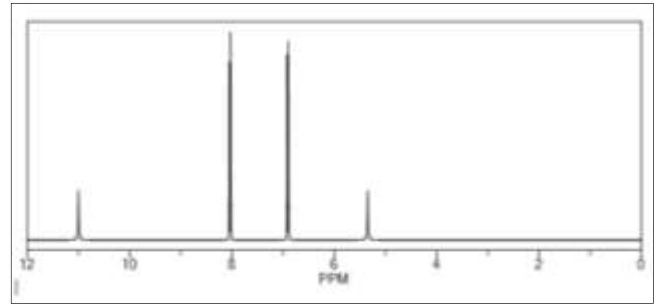


Figure 5 ^{1}H NMR IDENTIFCATION OF P-hydroxybenzoic acid via. CHEM DRAW ULTRA

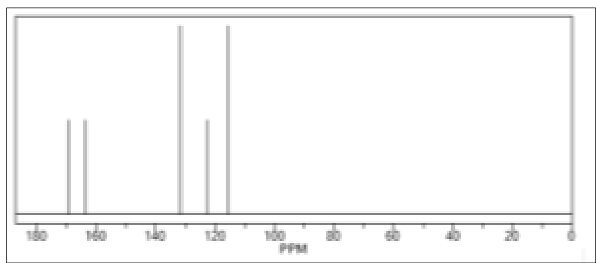
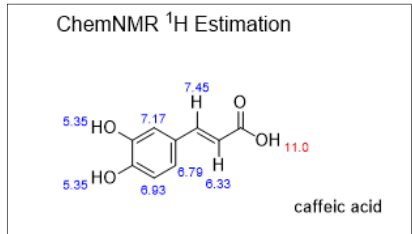


Figure 6 ^{13}C NMR IDENTIFCATION OF P-hydroxybenzoic acid via. CHEM DRAW ULTRA



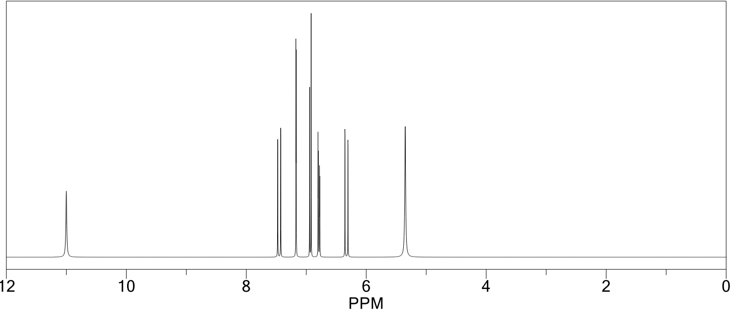
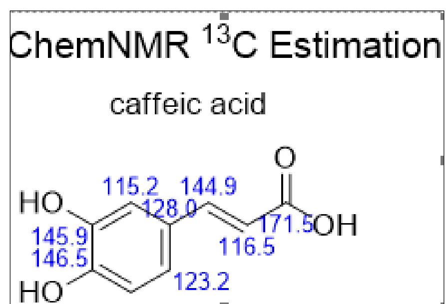


Figure 7 ^{1}H NMR IDENTIFCATION OF caffeic acid via. CHEM DRAW ULTRA



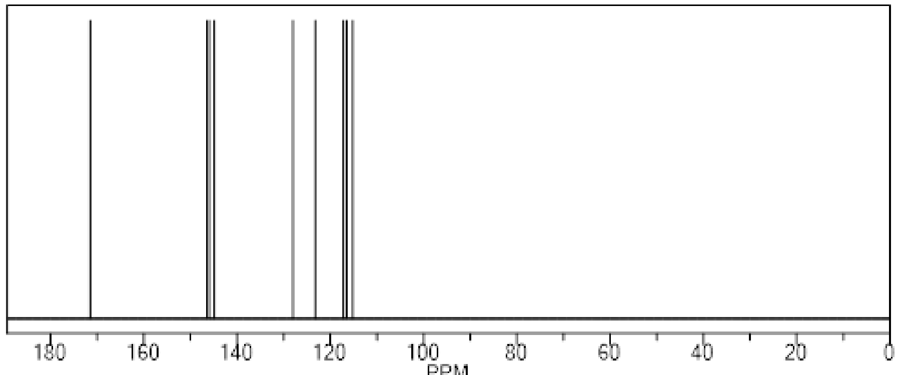
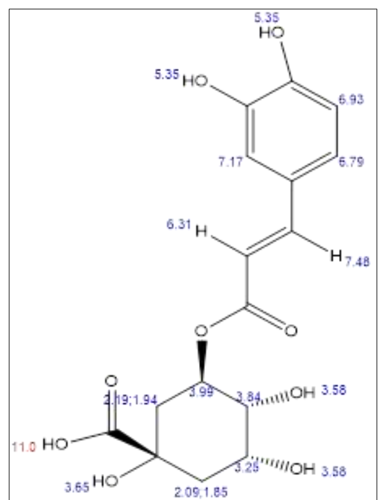


Figure 8 ^{13}C NMR IDENTIFCATION OF caffeic acid via. CHEM DRAW ULTRA



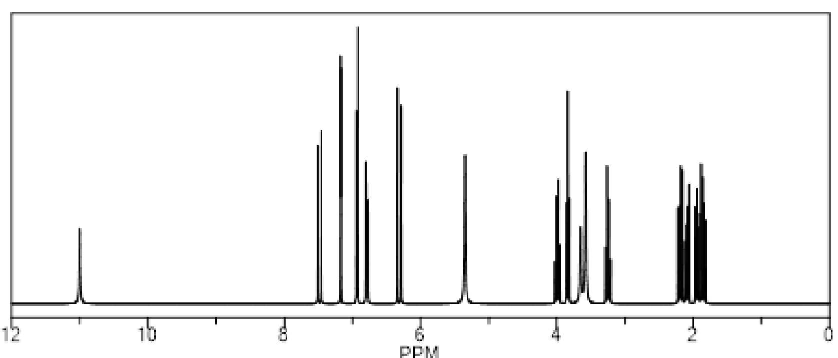
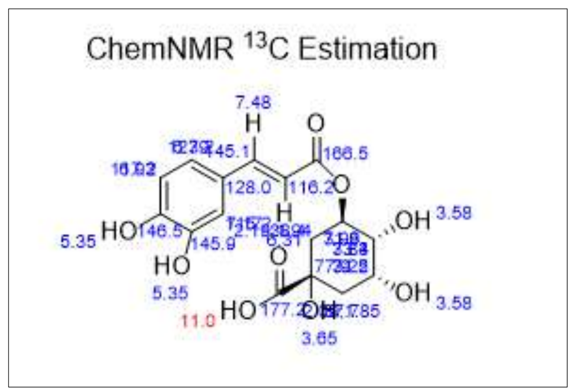


Figure 9 ^{1}H NMR IDENTIFCATION OF chlorogenic acid via. CHEM DRAW ULTRA



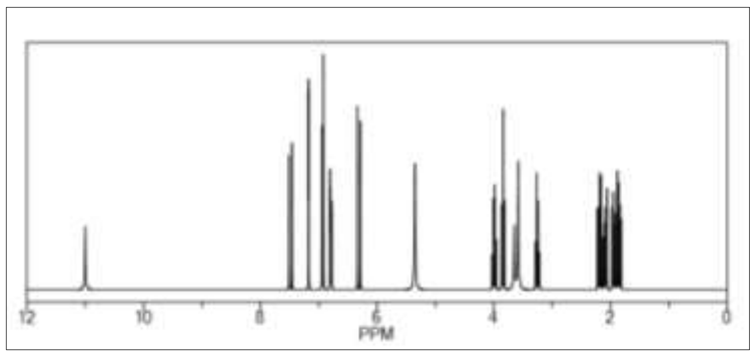


Figure 10 ^{13}C NMR IDENTIFCATION OF chlorogenic acid via. CHEM DRAW ULTRA

Table 1 Phenolic acids NMR Predicted results for ^{1}H & ^{13}C

S. No.	Structures of phenolic acids	Node	Shift	Base+Inc.	Results
1.	***P*-hydroxybenzoic acid**				
	^{1}H NMR Predicted results of ***p*-hydroxybenzoic acid**	OH	5.35	5.00 0.35	Aromatic C-OH
		OH CH	11.0 6.91	11.00 7.26 -0.53 0.21 -0.03	Carboxylic acid 1-benzene
		CH	8.04	7.26 -0.17 0.87 0.08	1-benzene
		CH	6.91	7.26 -0.53 0.21 -0.03	1-benzene
	^{13}C NMR Predicted results of ***p*-hydroxybenzoic acid**	C	163.7	128.5 28.8 5.2 1.2	1-benzene

		CH	115.8	128.5 -12.8 -0.1 0.2	1-benzene
		CH	131.7	128.5 1.4 1.6 0.2	1-benzene
		C	169.3	166.0 6.0 -2.7 -0.4	1-carboxyl
2.	Caffeic acid				
	^{1}H NMR Predicted results of caffeic acid	OH	5.35	5.00 0.35 7.26 -0.53 0.21 -0.03	Aromatic C-OH
		OH	11.0	11.00	Carboxylic acid
		CH	7.17	7.26 -0.53 0.17 0.04 0.57	1-benzene
		H	7.45	5.25 1.38 0.98 -0.16	1-ethylene
	^{13}C NMR Predicted results of caffeic acid	C	145.9	128.5 28.8 -12.8 -0.1 1.5	1-benzene
		C	171.5	166.0 4.0 1.5	1-carboxyl
		CH	123.2	128.5 -7.4 1.4 -2.3 3.0	1-ethylene

		CH	144.9	123.3 12.5 9.8 -0.7	1-ethylene
3.	Chlorogenic acid				
	^{1}H NMR Predicted results of chlorogenic acid	OH	5.25	7.00 1.25 6.26 -0.18 0.30 -0.01	Aromatic C-OH
		OH	7.0	15.00	Carboxylic acid
		CH	7.17	7.26 -0.58 0.19 0.01 0.01	1-benzene
		H	7.45	5.25 1.29 0.78 -0.11	1-ethylene
	^{13}C NMR Predicted results of chlorogenic acid	C	150.6	181.5 70.8 -10.8 1.0 -1.5	1-benzene
		C	171.5	153.0 8.0 11.5	1-carboxyl
		CH	120.2	128.5 -11.4 1.0 -1.3 13.0	1-ethylene
		CH	168.5	113.3 11.0 9.6 -0.1	1-ethylene

3.2. HPTLC analysis result depicted *Daucus carota* markers in profiling

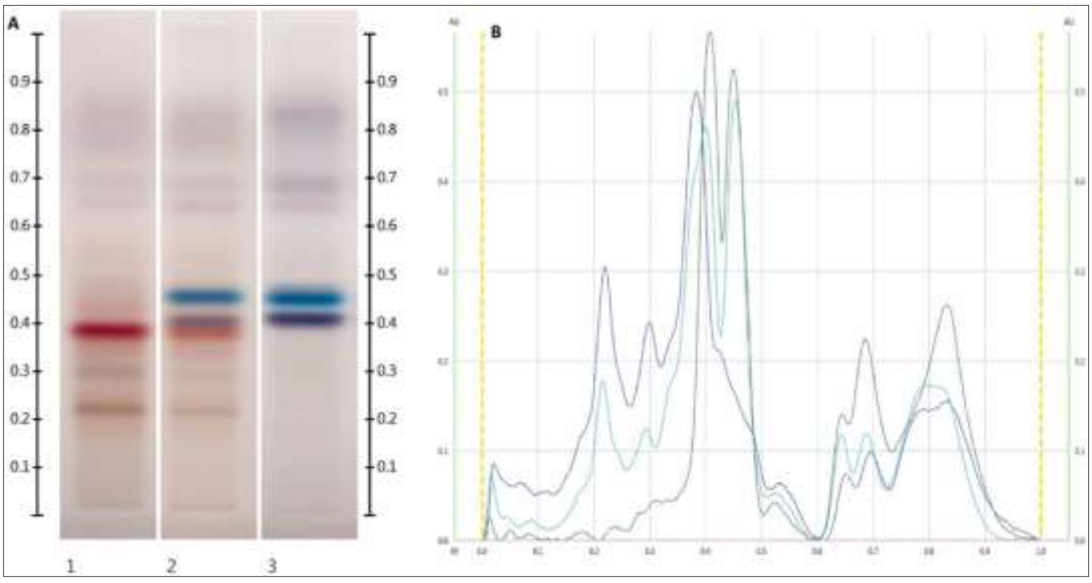


Figure 11 HPTLC analysis of p-hydroxybenzoic acid (1), caffeic acid (2), chlorogenic acid (3), at 254nm 366 nm and 514nm

5JAD: Compound binding to Human Lipoprotein-Associated Phospholipase A2 (Lp-PLA2) discovered through fragment screening [25].

- Classification: HYDROLASE
- Organism(s): Homo sapiens
- Expression System: Escherichia coli BL21(DE3)
- Mutation(s): No

Figure 12 3D- Structure of protein (5JAD)

Table 2 *Daucus carota* markers docking screening result in comparison to standard anticardiac medication

S.No	Name of Compounds	Chemical Structure	Docking score (PDB ID: 5JAD)	Glide energy	Molecular Weight	cLogP
1.	p-hydroxybenzoic acid		-4.641 kj/mol	-28.729	138.12	1.557
2.	Caffeic acid		-6.778 kj/mol	-23.581	180.16	0.975
3.	Chlorogenic acid		-3.675 kj/mol	-50.819	354.31	-1.879
4.	Felodipine (Standard drug)		-3.069 kj/mol	-33.182	384.25	5.296

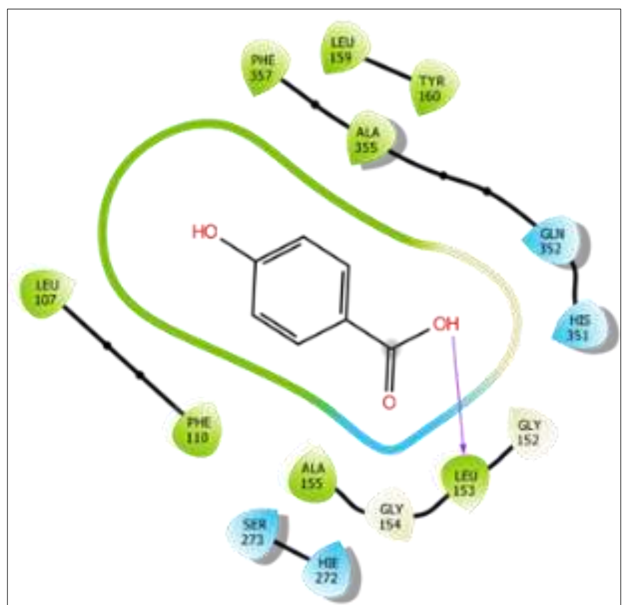


Figure 13 p-hydroxybenzoic acid 2D diagrams of docked conformation compound

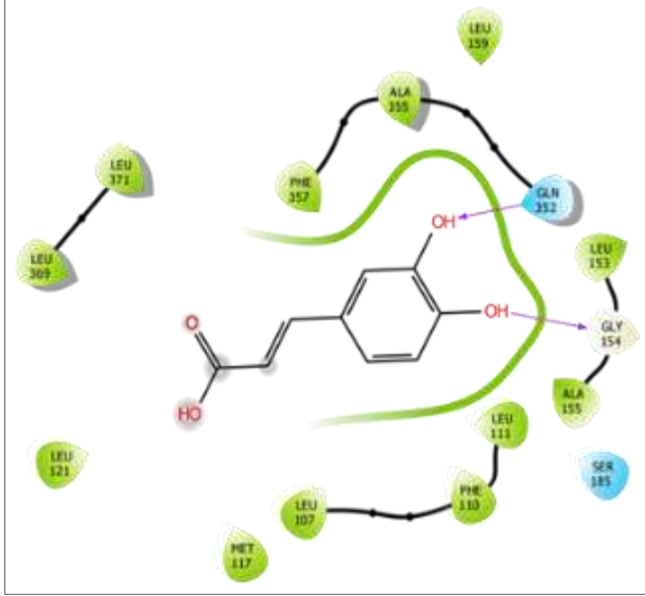


Figure 14 Caffeic acid 2D diagrams of docked conformation compound

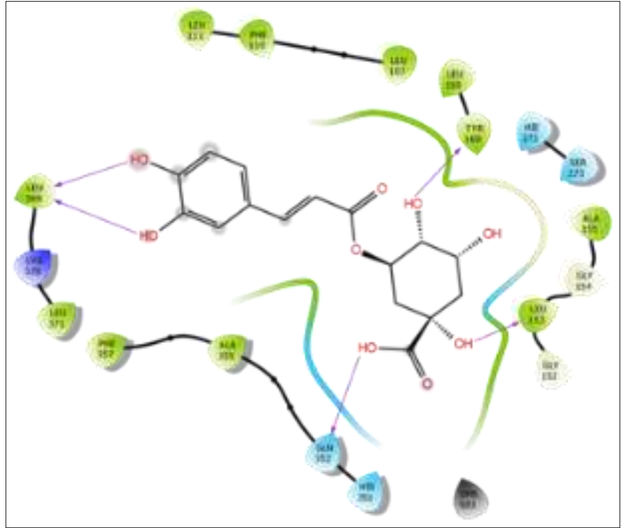


Figure 15 Chlorogenic acid 2D diagrams of docked conformation compound

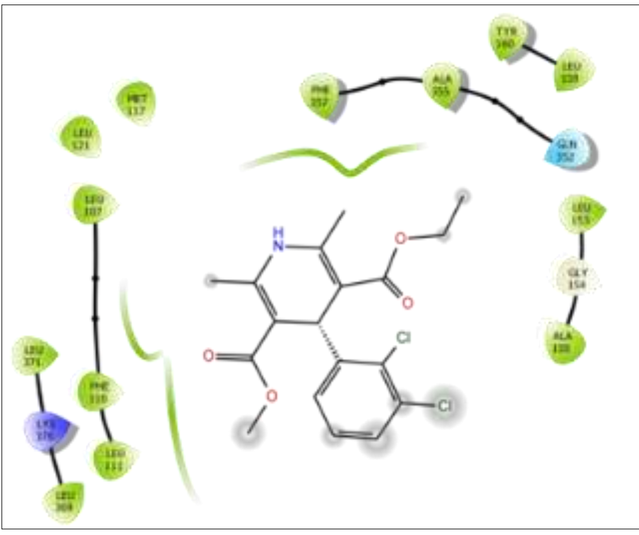


Figure 16 Felodipine 2D diagrams of docked conformation compound

4. Conclusion

Carrots, particularly their roots, are a valuable reservoir of phytochemicals, including phenolic compounds and anthocyanins, which hold promise for promoting health. Future research avenues should delve into elucidating the precise health advantages offered by these carrot phytochemicals, exploring potential differences among carrot varieties, optimizing extraction techniques, and assessing potential synergistic effects. The methodology employed in this research article encompassed a comprehensive approach, encompassing HPTLC profiling, which successfully identified three key phytochemicals in *Daucus carota*, namely p-hydroxybenzoic acid, caffeic acid, and chlorogenic acid. Additionally, NMR spectral characterization (^{1}H and ^{13}C) confirmed the presence of both saturated and unsaturated moieties within these markers. Furthermore, through *In-silico* screening using the protein structure (PDB ID: 5JAD), these three phytoconstituents, originating from the root of *Daucus carota*, exhibited notably superior docking scores and lower glide energies in comparison to standard drugs like Felodipine. Notably, caffeic acid displayed the highest docking score of 6.778 KJ/Mol among all the phytochemicals assessed. The findings from HPTLC and *In-silico* investigations highlight the substantial potential of these phytoconstituents from *Daucus carota*, particularly in terms of their anti-cardiac properties. These results position them as valuable candidates for the development of innovative anti-cardiovascular disease (CVD) and anti-congestive heart failure (CHF) medications, offering promising prospects for addressing a range of cardiac ailments and conditions in the future.

Compliance with ethical standards

Acknowledgments

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Disclosure of conflict of interest

The authors declare there is no conflict of interest in this study.

Statement of informed consent

Informed consent was obtained from all individual participants included in the study.

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