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Original Article

Effects of Biochemical, Antimicrobial, Green Synthesis Characterizations on Aqueous Extract of *Murraya koenigii* Leaf and its Influence on Hypertension using Molecular Docking Approach

Margaret Oladunni Oseni [1], Beauty Oladipupo [2], Funmilayo Adewumi [3], Andrie Mpetcha [4], Olatunde Abass Oseni *[5]

[1]Department of Chemistry, Faculty of Science, Federal University, Oye-Ekiti, Ekiti State, Nigeria.
[2]Department of Science Laboratory Technology, Faculty of Science, Ekiti State University, Ado-Ekiti, Nigeria.
[3]Department of Medical Laboratory Science, Faculty of Basic Medical Sciences, College of Medicine, Ekiti State University, Ado-Ekiti, Nigeria.
[4]Department of Anatomy, Faculty of Basic Medical Sciences, College of Medicine, Ekiti State University, Ado-Ekiti, Nigeria.
[5]Department of Medical Biochemistry, Faculty of Basic Medical Sciences, College of Medicine, Ekiti State University, Ado-Ekiti, Nigeria.

*Correspondence should be addressed to Olatunde Abass Oseni; *olatunde.oseni@eksu.edu.ng*

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Abstract

Background & Objective: Plants have been tremendously utilized as a source of medicine, therefore this study aimed at investigating the biochemical composition, antimicrobial properties and green synthesis characterization of *Murraya koenigi (Curry leaf)* using its aqueous extract. ***Method:*** Standard methods were used to analyse the various parameters of nutritional, antinutrients, phytochemicals, antioxidants, antimicrobial green synthesis and molecular docking. ***Results & Conclusion:*** The results of proximate composition revealed a nutrient-dense profile, it also contained nutritionally valuable minerals while anti-nutrient assessment showed minimal content within the daily recommended allowance. The phytochemical screening of the aqueous and ethanol extracts showed the presence of some bioactive compounds like flavonoids, alkaloids, tannins, and phenol. The antioxidant evaluation demonstrated remarkable free radical scavenging abilities, high content of some antioxidant compounds. Antimicrobial evaluation of the aqueous extract and its synthesized nanoparticles of silver (AgNP), copper (CuNP) and zinc (ZnNP) against a range of bacterial and fungal pathogens showed remarkable inhibitory zones. FTIR analysis of the aqueous extract also revealed the presence of some functional groups such as phenolics, carboxylic acids, and amines while UV/Visible spectrophotometric scanning displayed intensive absorption of light by the inherent chemical substances of the aqueous and synthesised nanoparticle solutions. Bioinformatics approaches identified potential molecular targets for the bioactive compounds. Docking simulations revealed strong binding affinities between key phytochemicals, such as citral, β-myrcene, and geraniol, and the 1Y9R (PDB ID MCR) receptor, demonstrating their potentials as therapeutic agents. Molecular interaction studies further illustrated the compatibility of these compounds with active site residues, reinforcing their drug-likeness properties. Clustering analysis of the major phytochemicals provided insights into their synergistic bioactivity, enhancing the overall therapeutic potentials of the extract.

Keywords: ***Murraya koenigii, Medicinal potentials, biochemical characterizations, green synthesis, molecular docking.***

Introduction

Murraya koenigii, commonly known as curry leaf, belongs to the *Rutaceae* family, within the genus *Murraya*, and its species name is *koenigii*. This aromatic shrub is native to the Indian subcontinent but has spread across Southeast Asia and other tropical regions [1,2]. The plant's taxonomic classification places it firmly in the *Rutaceae* family, which is known for its fragrant, oil-rich plants. Morphologically, the curry leaf tree is a small to medium-sized shrub or tree, typically growing up to 6 meters in height [2]. The leaves are pinnately compound, consisting of 11-21 small, elliptical leaflets arranged in a symmetrical pattern on a central stalk, which gives the leaves a finely textured, feathery appearance. The leaflets are glossy, dark green on the upper side, with a distinct aroma when crushed, and lighter green on the underside [1,2]. These leaves are not only valued for their culinary uses but also for their medicinal properties,

which are attributed to various bioactive compounds such as alkaloids, flavonoids, and terpenoids [2].

Curry leaf (*Murraya koenigii*) has long been utilized in traditional medicine systems such as Ayurveda and Unani to treat various ailments. The leaf is rich in essential oils, alkaloids, and flavonoids, which have demonstrated notable pharmacological properties, including anti-diabetic, anti-inflammatory, and anti-cancer activities [3].

Traditional healers have also used curry leaves to manage digestive disorders, infections, and high blood pressure. Given its extensive use, the scientific community is increasingly exploring the biochemical and therapeutic roles of curry leaves, particularly in addressing chronic diseases such as hypertension. This global health challenge affects over one billion people worldwide, significantly contributing to morbidity and mortality due to cardiovascular complications. Despite the availability of antihypertensive drugs, treatment outcomes are often limited by adverse effects and drug resistance, underscoring the need for alternative therapeutic agents [4]. Curry leaves, with their bioactive components, offer a promising natural solution that could complement existing hypertension therapies. Modern drug discovery is also leveraging advanced computational techniques, such as molecular docking, to evaluate the interactions between potential drug candidates and target proteins. Molecular docking is an essential tool in herbal research, as it provides insights into the mechanisms through which plant-derived compounds exert their therapeutic effects. This approach accelerates the identification of bioactive compounds, streamlines the drug development process, and bridges the gap between traditional knowledge and modern scientific innovation. In the context of curry leaves, molecular docking studies have revealed significant potential in targeting enzymes and receptors associated with hypertension and related disorders [5]. This synergy between traditional medicine and cutting-edge technology holds immense promise for the development of safer, more effective treatments, making it an area of great relevance in contemporary herbal research.

Materials and Methods

The collection and preparation of *curry leaf* (*Murraya koenigii*) involve a series of steps to ensure the integrity and efficacy of the aqueous extract. Proper collection and preparation are crucial for the consistency and reproducibility of results in biochemical, antioxidant, antimicrobial, and nanoparticle synthesis studies.

The plant material (leaves) was collected from Ikorodu, Lagos State, Nigeria in September 19, 2024. They were harvested directly from the stalk. This was done in the early morning to avoid moisture loss and maximize phytochemical content. The plant sample specimen was authenticated and deposited at the herbarium of the Department of Plant Science, Faculty of Science, Ekiti State University, Ado Ekiti, Nigeria. It was identified and confirmed by Mr. Omotayo, the Chief Technologist.

The leaves of (*Murraya koenigii*) were carefully removed from the plant and rinsed under running tap water to remove any surface dust or contaminants. The cleaned leaves were then air-dried for several days. Once adequately dried, the leaves were ground into a fine powder. A measured amount of 20 grams of this powdered leaf material was mixed with 100 mL of distilled water. This mixture was then agitated continuously overnight to facilitate thorough extraction of the leaf compounds

Aqueous Extraction

The aqueous extraction of *Murraya* koenigi leaves adhered to WHO guidelines, using a 20:100 (w/v) ratio of powdered leaves to distilled water, the mixture was shacking continuously overnight on mechanical shaker till properly extracted, the mixture was filtered and the filtrate was stored at 4°C for stability and further use.

Phytochemical Analysis of the sample.

Chemical tests were carried out on the aqueous and ethanol extracts of the leaves of the *Murraya* koenigi to screen for phytochemical constituents of flavonoids, alkaloids, saponin, phenolic compounds and steroidal nucleus as described by [6-8].

Some In-vitro Antioxidant Analyses of the Leaf Sample

Determination of DPPH Free Radical Scavenging Ability

The ability of the extract to neutralize 1,1-diphenyl-2-picrylhydrazyl (DPPH) free radicals was evaluated using a method adapted from [9]. Briefly, 1.0 mL of the extract at various concentrations (20, 40, and 80 mg/mL) was added to separate test tubes. To each tube, 1.0 mL of a 0.1 mM methanolic solution of DPPH was added. The samples were then mixed and left to incubate in the dark at room temperature for 30 minutes. Following incubation, the absorbance of the solutions was measured at 516 nm. A decrease in absorbance indicated the extract's scavenging activity against DPPH free radicals.

Determination of Ferric Reducing Antioxidant Power

The ferric reducing antioxidant power (FRAP) of the extract was evaluated using a modified method [10]. A lower absorbance indicated higher ferric reducing power, reflecting the sample's antioxidant capacity.

Estimation of Vitamin C

Estimation of vitamin C content was determined using method of [11]. Absorbance was measured at 520 nm, and ascorbic acid concentration was determined using a standard calibration curve and expressed as mg/g of the sample.

Green Synthesis and Characterization of the Synthesized Silver, Copper and Zinc Nanoparticles

The biosynthesis of the AgNPs, CuNPs and ZnNPs in the solutions were monitored and characterized by measuring the UV–visible and Fourier transform infrared (FTIR) spectra of the solutions of the reaction mixture(24). UV– visible spectra were recorded on double beam spectrophotometer (Shimazdu, model UV-1800, Kyoto, Japan) from 200 to 900 nm at a resolution of 1 nm while FTIR were recorded from 415 to 3800 cm^{-1} to detect the organic functional groups present in the leaf extract and AgNPs, CuNPs and ZnNPs [13-15].

Anti-microbial Analysis

The antimicrobial analysis was performed by the method of Gumgumjee and Hajar [16], this procedure was used in the determination of antibacterial and antifungal activities in the *Murraya koenigii* aqueous extract and its nanoparticles.

In silico ADME, and Molecular Docking Studies

The methodology outlines a multi-step in silico approach to study the phytochemical compounds of *Murraya koenigii*. First, the major phytochemicals were identified from literature, and their structures were obtained in SMILES format from the NCBI PubChem database. ADME (absorption, distribution, metabolism, excretion) screening was performed using the Swiss ADME server to assess the pharmacokinetics of the compounds. Clustering of the compounds based on physicochemical properties was done using the Chemmine R webserver. Target prediction for the phytochemicals was carried out using the Swiss Target Prediction and SEA Search servers, selecting Homo sapiens as the target organism. Protein-protein interactions (PPI) between the predicted targets were analysed using the STRING webserver. The target gene IDs were then subjected to network analysis, including transcription factor, PPI network, and kinase enrichment analysis using the eXpression2Kinases webserver. Finally, molecular docking studies were conducted using Auto-Dock Tools and Auto-Dock Vina to explore the interactions between the ligands and target proteins, with results visualized using PyMol and ezLigplot software. This comprehensive in silico approach integrates various tools to analyse the pharmacokinetics, target interactions, and docking of phytochemicals [17,18].

Results and Discussion

The results of the proximate composition of *Murraya koenigii*'s substantiate its value as a source of nutrients, bioactive compounds, and potential therapeutic agents. From Table 1.0, the observed moisture content contributes to the leaf's freshness and potential shelf life. The ash content reflects a diverse mineral profile, highlighting the presence of essential elements.

While the crude fat, carbohydrate and crude protein content was found to be slightly higher than some previous findings, which still indicates a moderate energy source and reinforce the nutritional significance of *M. koenigii* leaf as well as tissue growth and repair especially in regions with limited animal protein. As seen in this study, *Murraya koenigii*'s possesses a slightly rich nutritional profile while its ash content suggests significant mineral presence which are vital for various biochemical functions [19,20].

Table 1.0: proximate composition of Curry leaf (*Murrayakoenigii*)

Parameters	Values (%)
Moisture Content	15.49±0.01
Ash content	5.00±0.00
Crude Fat	7.31±0.00
Crude Fibre	4.61±0.01
Crude Protein	13.63±0.17

The crude fibre content of the leaf is beneficial for digestive health [21]. In general, these qualities can influence the suitability of the leaf of *Murraya koenigii*'s for nutritional and therapeutic applications, supporting its traditional use in herbal medicine [22].

Table 2.0 showed the presence of some antinutrients which is potentially a concern at high doses, though this is within acceptable ranges and may even offer health benefits.

Table 2.0: Antinutrient composition of Curry leaf (*Murrayakoenigii*)

Parameters	Values (%)
Tannin mg/L	35.75±0.05
Alkaloids	6.28±0.01
Saponin	5.30±0.01

The *Murraya koenigii*'s leaf contains antinutrients such as tannins, alkaloids and saponin, the high tannin may inhibit protein and mineral absorption while saponin is a toxic plant-derived secondary metabolite which also play numerous biological activities. Alkaloids have medicinal properties despite potential toxicity [23]. The proper processing methods like cooking and fermentation are recommended to mitigate the negative effects of these antinutrient compounds to enhance safety and benefits.

In Table 3.0 of the mineral composition of the *Murraya koenigii*'s leaf, it was revealed that phosphorus, potassium calcium and sodium were the most abundant elements, known for their crucial roles for various physiological functions. The sodium-potassium ratio is also important for blood pressure regulation. Phosphorus, calcium, and magnesium have been found to contribute to bone health and other vital processes in the body. The presence of trace elements like iron, copper, zinc, manganese, and cobalt further enhances the nutritional value of this plant. The detection of lead, albeit at low levels, raises concerns about potential environmental contamination and necessitates further monitoring. Many researchers [24-26] have reported the importance of minerals and toxicity of some heavy metals to biological systems as observed in this study.

Table 3.0: Mineral composition of Curry leaf (*Murraya koenigii*)

Parameters	Values (%)
K	3.72±0.01
Na	2.90±0.01
P	5.53±0.00
Ca	3.17±0.01
Cu	0.80±0.00
Mg	1.84±0.01
Fe	0.32±0.00
Mn	0.11±0.00
Pb	0.57±0.50
Zn	1.43±0.00
Co	0.03±000

The presence of some phytochemical compounds as seen in Table 4.0 confirmed the presence of key bioactive compounds, including saponins, phenols, tannins, flavonoids, alkaloids, and steroids.

Table 4.0: Phytochemical screening of Curry leaf (*Murrayakoenigii*)

Parameters	Values
Saponin	+
Phenol	+
Tannin	+
Flavonoid	+
Alkaloid	+
Terpenoids	_
Steroids	+
Glycoside	_
Phylobatannin	_

These compounds are known for their diverse biological activities, including antioxidant, antimicrobial, and anti-inflammatory effects. The absence of terpenoids and glycosides in this study, while reported in some *M. koenigii* varieties, could be due to variations in geographical location, extraction methods, or the specific cultivar studied.

Tables 5.0 and 6.0 displayed some antioxidant compounds and some radical scavenging antioxidant abilities respectively. The significant antioxidant activity observed across various assays (DPPH, TBARS, FRAP, NO, Fe^{2+}) highlights the potential of *M. koenigii* as a natural antioxidant source.

Table 5.0: Some Antioxidant compounds of Curry leaf (*Murrayakoenigii*)

Parameters	Values
Flavonoid (%)	3.10±0.01
Vitamin C (mg/100g)	27.80±0.02
Phenolic Compounds (mg GAE/g)	23.78±0.22

This activity is likely attributed to the synergistic action of the identified phenolic compounds and flavonoids.

Table 6.0: Free radicals scavenging abilities of Curry leaf (*Murrayakoenigii*)

Parameters	Values
DPPH %	52.05±0.13
TBARS (mg MDA/g)	59.42±0.69
FRAP (mg (Vit. C)/g)	32.02±0.54
NO %	42.49±0.01
FE2+ %	26.15±1.25

The *Murraya koenigii* plant demonstrates strong antioxidant potential, effective in combating free radicals and preventing chronic diseases. This observation has been reported previously on different plants by various researchers among which are [27,28].

The antimicrobial assays in Tables 7.0 and 8.0 revealed varying degrees of efficacy against tested bacterial and fungal strains. The superior performance of copper nanoparticles, particularly against several tested pathogens, is noteworthy. This enhanced activity could be attributed to the unique mechanisms of action of copper nanoparticles, including disruption of cell walls and interference with essential cellular processes. The differential activity observed among the nanoparticles (AgNP, CuNP, ZnNP) may be related to their distinct physicochemical properties.

The antibacterial potential of *Murraya koenigii* aqueous leaf extract and its studied nanoparticles showed high zone inhibition against Pseudomonas aeruginosa in comparison to all other organisms. Notably, the CuNP exhibited the highest activity, particularly against Pseudomonas aeruginosa followed by moderate activity against other strains. Other samples, including the leaf extract, AgNP and ZnNP, demonstrated relative minimal antibacterial effects than the CuNP.

Table 7.0: Antibacterial potential properties of curry leaf (*Murraya koenigii*) aqueous leaf extract and its nanoparticles (zone inhibition in mm)

Samples	*Xanthomonas azonopodis*	*Salmonella typhi*	*Pseudomonas aeruginosa*	*Erwinia carotovora*	*Streptococcus mutant*
Murraya koenigi) Leaf extract	1.5	1.5	11.0	2.0	5.0
Murraya koenigii AgNP	3.0	1.0	12.0	8.0	8.0
Murraya koenigii CuNP	6.0	4.0	15.0	5.0	5.0
Murraya koenigii ZnNP	5.0	1.5	10.0	6.0	3.0
Standard (Streptomycin Sulphate)	30	30	35	38	30

The antifungal potential of *Murraya koenigii* aqueous leaf extract and its nanoparticle, CuNP produced highest percentage mycelia growth inhibition against Aspergillus flavus, Fusarium oxysporium and Phythophthora infestant respectively. The *Murraya koenigii* ZnNP exhibited lowest antifungal potential against all the three fungi in the study.

Table 8.0: Antifungal potential properties of curry leaf (*Murraya koenigii*) aqueous leaf extract and its nanoparticles

	Mycelial growth inhibition (%)		
Samples	***Fusarium oxysporium***	***Phythophthora infestant***	***Aspergillus flavus***
Murraya koenigii Leaf extract	28.57	32.22	68.56
Murraya koenigii AgNP	11.91	24.44	32.58
Murraya koenigii CuNP	66.67	66.67	58.43
(*Murraya koenigii)* ZnNP	14.29	22.22	25.17
Standard (Ketoconazole tablet)	98	98	98

UV-Visible spectroscopy in Figure 4.0 corroborated the presence of phenolic compounds and flavonoids. The identified phytochemicals, including fatty acids, esters, terpenes, and glycosides, further contribute to the diverse pharmacological potential of *M. koenigii*.

The UV-Visible performed using a UV-1800 Series spectrophotometer characterization of *M. koenigii* leaf aqueous extract and *M. koenigii* CuNP showed similar absorption while the AgNP and ZnNP displayed distinctive different absorptions. The absorbance peaks were observed at 280.00 nm (1.700 absorbance) and 318.00 nm (1.333 absorbance). The spectrum indicates significant absorbance in the UV region, highlighting the potential presence of bioactive compounds. The UV-Visible characterization of nanoparticles synthesized from the aqueous extract of *M. koenigii* indicates the successful synthesis of AgNPs, CuNPs, and ZnNPs, with significant absorption observed in the UV-Vis region.

Wave length Measurement Properties

Wavelength Range (nm.):	200.00 to 900.00
Sampling Interval:	0.5
Scan Mode:	Single
Instrument Type:	UV-1800Series
Measuring Mode:	Absorbance
Slit Width:	1.0nm
Light Source Change Wavelength:	350

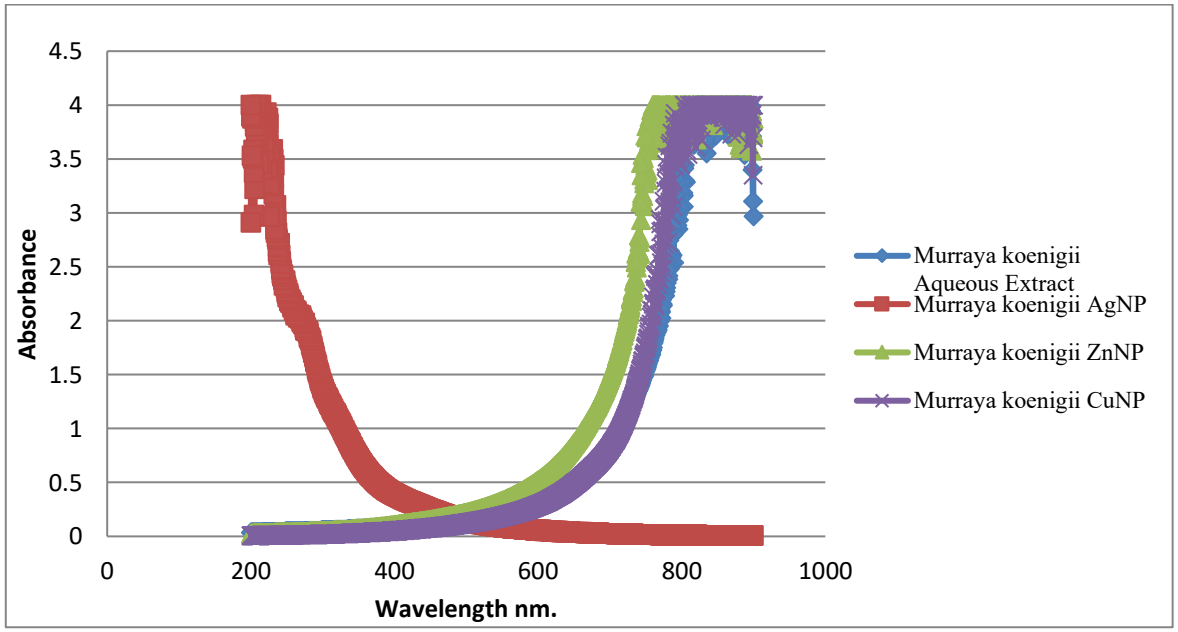


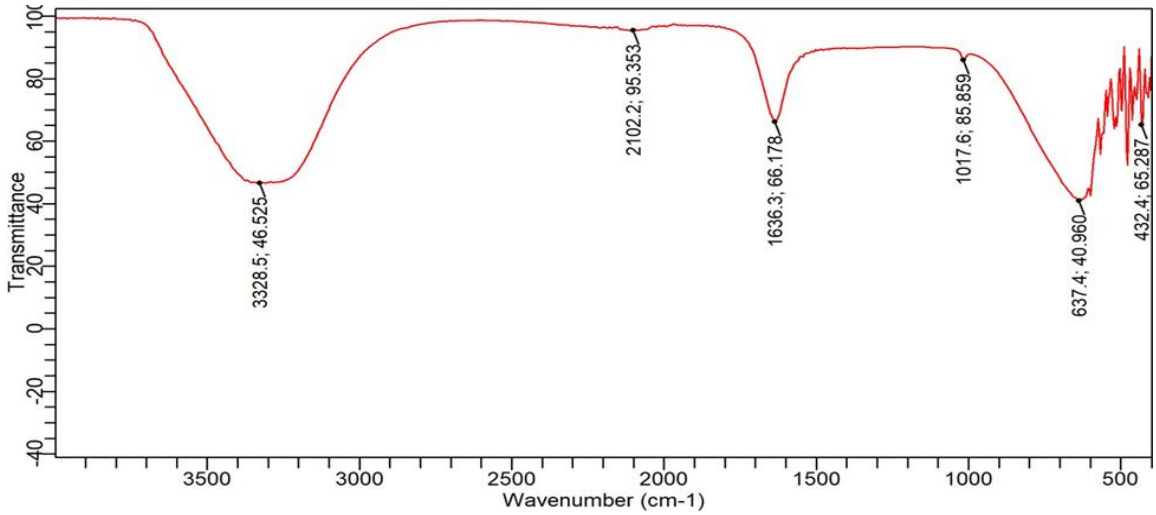
Figure 4.0: The UV-Visible Characterization of Curry Leaf (*Murraya koenigii*) of leaf aqueous extract

The FTIR spectra measured for the extract and the nanoparticles exhibit varied absorption peaks at 432 to 3329 cm^{-1}, 483 to 3899 cm^{-1}, 477 to 3297 cm^{-1} and 417 to 3313 cm^{-1} for the extracts and its nanoparticles respectively to show the presence of carboxylic acid C=O and/or O-H groups, alcohol, aromatic and phenol groups, alkynes which are identified by the presence of the C-C-H:C-H group, which is observed at a wavelength of 1774 cm^{-1}. The O-H technique, representing a carboxylic group, results in an absorption peak at 1606 cm^{-1} and 1540 cm^{-1}.

The presence of the band at 3330 cm^{-1} and 2356 cm^{-1} in samples indicates the presence of C-O and/or O-H functional groups, which denote phenol and alcohol groups, respectively. The presence of the C-C-H:C-H group at 1473 cm^{-1} and 1250 cm^{-1} is indicative of alkynes. The band at 1378 cm^{-1} is attributed to the presence of the carboxylic group, denoted as O-H. However, whether this band appears at 1200 cm^{-1} depends on other factors such as the presence of signalling overtones from the C-C and/or C-H groups, the nature of the aromatic compounds (saturated or unsaturated), whether it is dimerized, or if it has internal hydrogen bonding as seen from Figures 4.1a to 4.1d.

Sample ID: Curry (*Murraya koenigii*) leaf aqueous extract

Sample Scans: 32	Background Scans: 32
Resolution: 8	Range: 4000-400

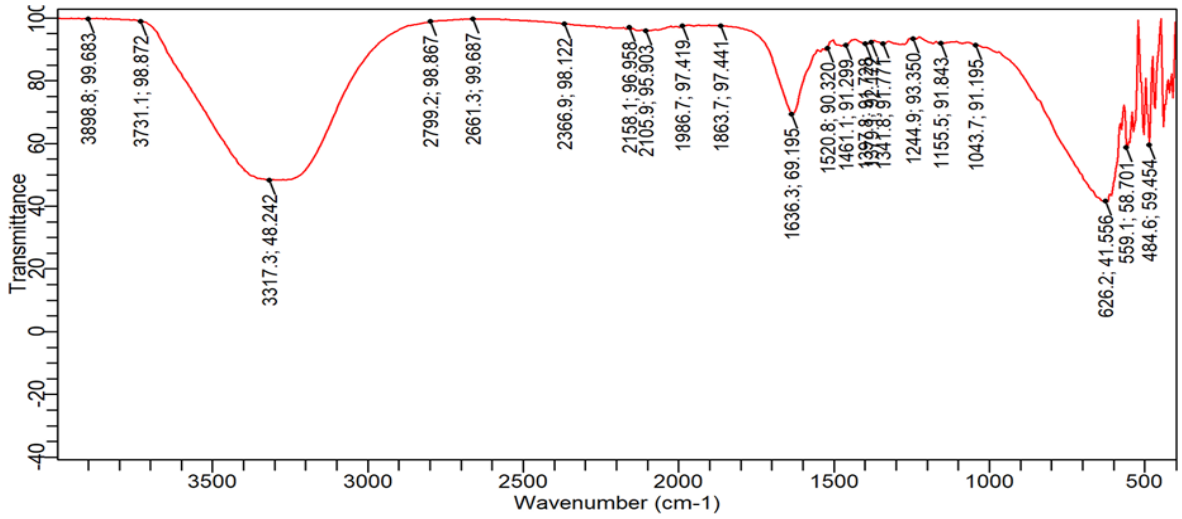


PeakNumber	Wavenumber (cm^{-1})	Intensity
1	432.37119	65.28720
2	637.37477	40.96002
3	1017.56323	85.85922
4	1636.30131	66.17834
5	2102.21854	95.35344
6	3328.51269	46.52547

Figure 4.1a: FTIR Characterization of Curry Leaf (*Murraya koenigii*) of leaf aqueous extract

Sample ID: Curry leaf (*Murraya koenigii*) AgNP

Sample Scans: 32 Background Scans: 32
Resolution: 8 Range: 4000 – 400

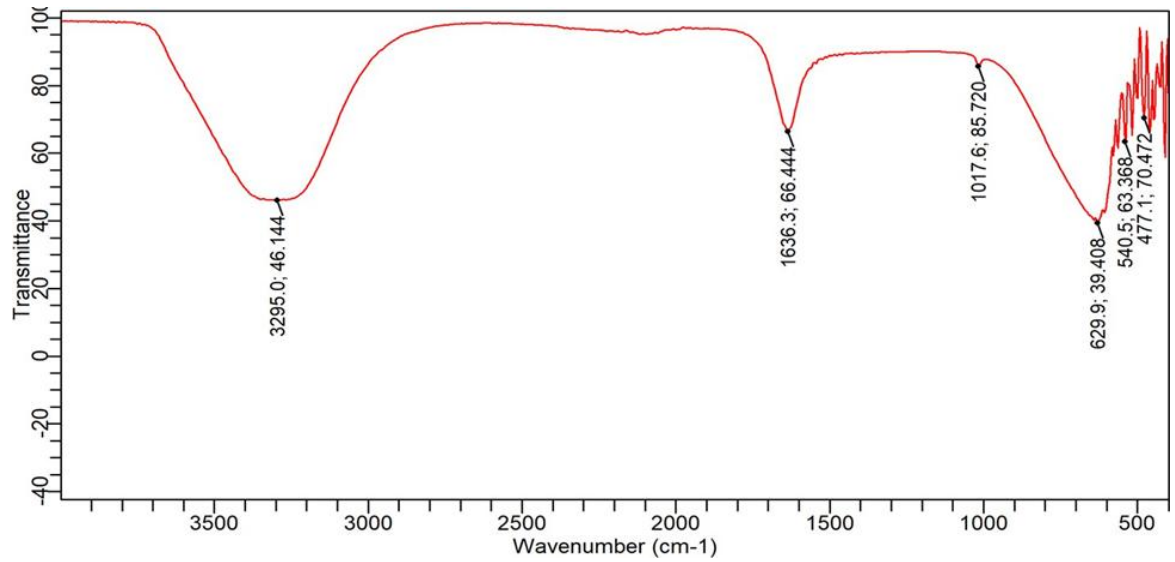


Peak Number	Wavenumber (cm^{-1})	Intensity
1	484.55392	59.45420
2	559.10068	58.70096
3	626.19276	41.55573
4	1043.65459	91.19522
5	1155.47473	91.84322
6	1244.93084	93.35021
7	1341.84162	91.77125
8	1379.11500	92.17151
9	1397.75169	91.72783
10	1461.11643	91.29933
11	1520.75384	90.32037
12	1636.30131	69.19469
13	1863.66892	97.44112
14	1986.67107	97.41863
15	2105.94588	95.90293
16	2158.12861	96.95828
17	2366.85953	98.12210
18	2661.31922	99.68749
19	2799.23072	98.86670
20	3317.33068	48.24175
21	3731.06518	98.87220
22	3898.79538	99.68322

Figure 4.1b: FTIR Characterization of Curry Leaf (*Murraya koenigii*) silver nanoparticle (AgNP)

Sample ID: Curry leaf (*Murraya koenigii*) CuNP

SampleScans: 32 BackgroundScans: 32
Resolution: 8 Range: 4000– 400



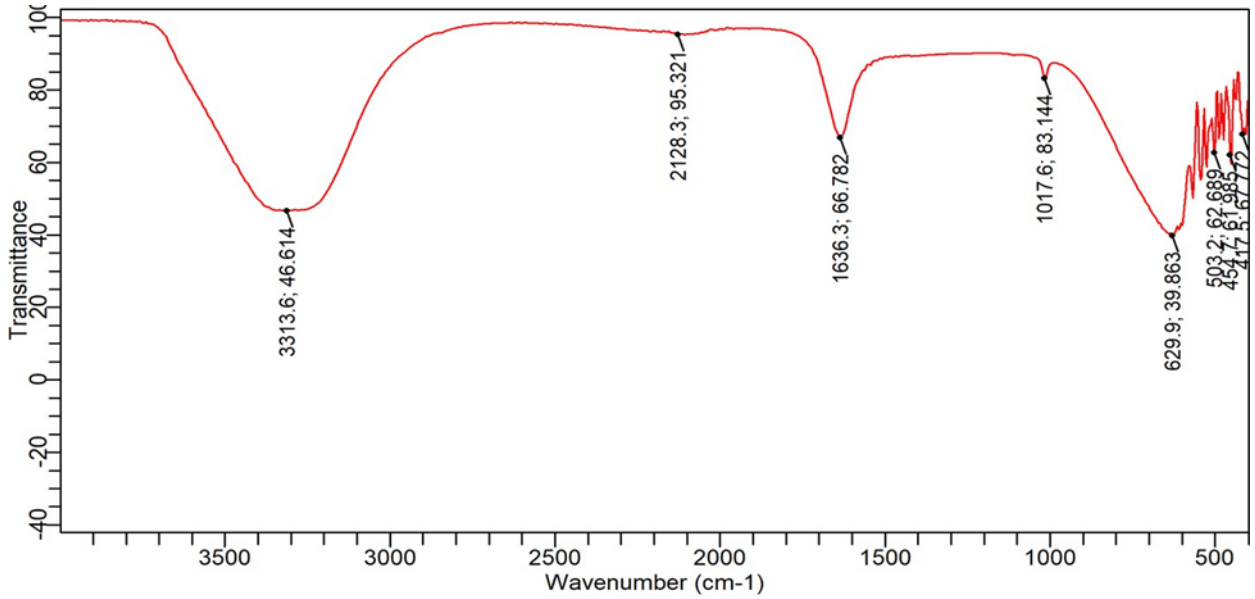
PeakNumber	Wavenumber(cm^{-1})	Intensity
1	477.09924	70.47169
2	540.46399	63.36820
3	629.92009	39.40830
4	1017.56323	85.71999
5	1636.30131	66.44373
6	3294.96665	46.14384

Figure 4.1c: FTIR Characterization of Curry Leaf *Murraya* oenigii) copper nanoparticle (CuNP)

Sample ID: Curry leaf (*Murraya koenigii*) ZnNP

SampleScans: 32 BackgroundScans:32

Resolution: 8 Range: 4000– 400



PeakNumber	Wavenumber(cm^{-1})	Intensity
1	417.46184	67.77162
2	454.73522	61.98532
3	503.19061	62.68923
4	629.92009	39.86308
5	1017.56323	83.14383
6	1636.30131	66.78247
7	2128.30991	95.32063
8	3313.60334	46.61379

Figure 4.1d: FTIR Characterization of Curry Leaf (*Murraya koenigii*) Zinc nanoparticle (ZnNP)

The results of in silico analysis of the *Murraya koenigii* extract from Tables 9.0 to 11. 0 and Figures 4.2 to 4.7e were displayed. The predicted binding affinities and interactions with specific enzymes suggest potential therapeutic applications in various disease conditions.

Table 9.0 Ligand Preparation Identification of major phytochemical constituents of Curry Leaf (*Murraya koenigii*)

S/N	Compound Name	PubChem CID No.	Canonical Smiles
1.	Propane, 1,1,3-triethoxy-	24624	CCOCCC(OCC)OCC
2.	1,2-Ethanediol, monoacetate	10960	CC(=O)OCCO
3.	1-Methyl-pyrrolidine-2-carboxylic acid	557	CN1CCCC1C(=O)O
4.	ethyl beta-D-glucopyranoside	121667	CCO[C@H]1[C@@H]([C@H]([C@@H]([C@H](O1)CO)O)O)O
5.	Methyl 14-methylpentadecanoate	21205	CC(C)CCCCCCCCCCCCC(=O)OC
6.	n-Hexadecanoic acid	985	CCCCCCCCCCCCCCCC(=O)O
7.	Hexadecanoic acid, ethyl ester	12366	CCCCCCCCCCCCCCCC(=O)OCC
8.	Oleic acid, methyl ester	5364509	CCCCCCCC/C=C\CCCCCCCC(=O)OC
9.	Phytol	5280435	C[C@@H](CCC[C@@H](C)CCC/C(=C/CO)/C)CCCC(C)C
10.	9,12-Octadecadienoic acid (Z,Z)-	5280450	CCCCC/C=C\C/C=C\CCCCCCCC(=O)O
11.	alpha-Himachalene	520909	CC1=CC2C(CC1)C(=C)CCCC2(C)C
12.	1,2-Benzenedicarboxylic acid, and diisooctyl ester	33934	CC(C)CCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCC(C)C
13.	Isolongifolene, 4,5-dehydro-	583154	CC1(CCC=C2C13CC(C2(C)C)C=C3)C

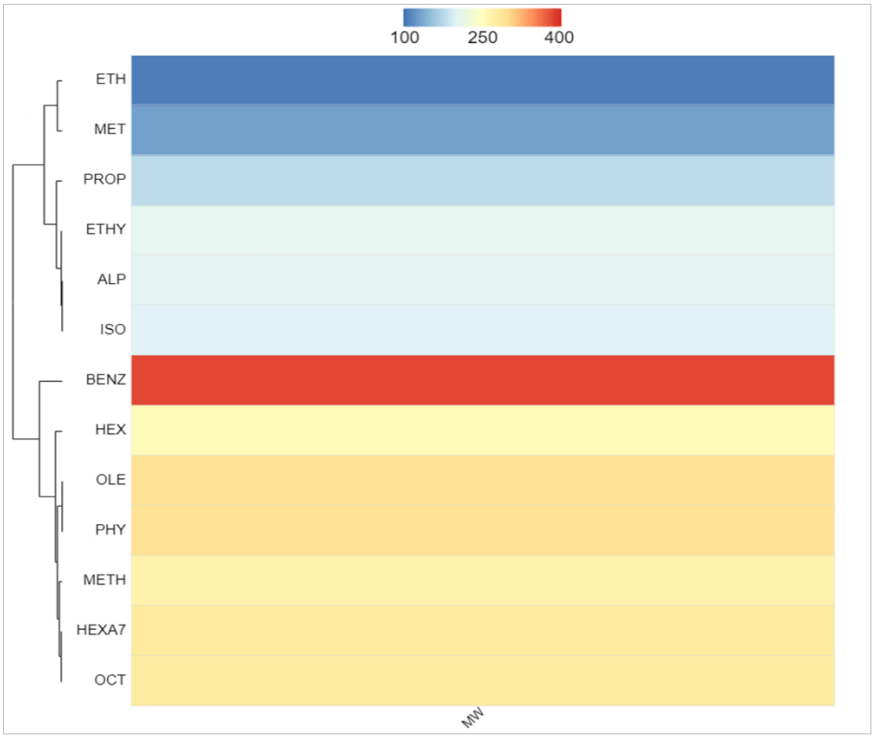


Figure 4.2 Clustering Analysis

Table 10.0 IN SILICO TARGET PREDICTION

The in silico ADME (absorption, distribution, metabolism, and excretion) screening of the compounds

Compound name	Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability	Known actives (3D/2D)
Methyl 14-methylpentadecanoate	Carbonic anhydrase II	CA2	P00918	CHEMBL205	Lyase	0.504893512	377 / 4Â Â Â Â Â
Methyl 14-methylpentadecanoate	Carbonic anhydrase I	CA1	P00915	CHEMBL261	Lyase	0.504893512	310 / 6Â Â Â Â Â
n-Hexadecanoic acid	Fatty acid binding protein adipocyte	FABP4	P15090	CHEMBL2083	Fatty acid binding protein family	0.935895337	20 / 3Â Â Â Â Â
n-Hexadecanoic acid	Peroxisome proliferator-activated receptor alpha	PPARA	Q07869	CHEMBL239	Nuclear receptor	0.935895337	160 / 9Â Â Â Â Â

n-Hexadecanoic acid	Fatty acid binding protein muscle	FABP3	P05413	CHEMBL3344	Fatty acid binding protein family	0.935895337	9 / 5Â Â Â Â Â
n-Hexadecanoic acid	Fatty acid binding protein epidermal	FABP5	Q01469	CHEMBL3674	Fatty acid binding protein family	0.935895337	3 / 2Â Â Â Â Â
n-Hexadecanoic acid	Peroxisome proliferator-activated receptor delta	PPARD	Q03181	CHEMBL3979	Nuclear receptor	0.935895337	148 / 7Â Â Â Â Â
n-Hexadecanoic acid	Fatty acid binding protein intestinal	FABP2	P12104	CHEMBL4879	Fatty acid binding protein family	0.935895337	1 / 1Â Â Â Â Â
n-Hexadecanoic acid	Free fatty acid receptor 1	FFAR1	O14842	CHEMBL4422	Family A G protein-coupled receptor	0.598213028	151 / 3Â Â Â Â Â
9,12-Octadecadienoic acid (Z,Z)-	Fatty acid binding protein adipocyte	FABP4	P15090	CHEMBL2083	Fatty acid binding protein family	1	26 / 4Â Â Â Â Â
9,12-Octadecadienoic acid (Z,Z)-	Peroxisome proliferator-activated receptor gamma	PPARG	P37231	CHEMBL235	Nuclear receptor	1	364 / 22Â Â Â Â Â
9,12-Octadecadienoic acid (Z,Z)-	Peroxisome proliferator-activated receptor alpha	PPARA	Q07869	CHEMBL239	Nuclear receptor	1	225 / 18Â Â Â Â Â
9,12-Octadecadienoic acid (Z,Z)-	Fatty acid binding protein muscle	FABP3	P05413	CHEMBL3344	Fatty acid binding protein family	1	15 / 5Â Â Â Â Â
9,12-Octadecadienoic acid (Z,Z)-	Cyclooxygenase-1	PTGS1	P23219	CHEMBL221	Oxidoreductase	0.794011839	4 / 2Â Â Â Â Â
9,12-Octadecadienoic acid (Z,Z)-	Free fatty acid receptor 1	FFAR1	O14842	CHEMBL4422	Family A G protein-coupled receptor	0.794011839	168 / 3Â Â Â Â Â
9,12-Octadecadienoic acid (Z,Z)-	Peroxisome proliferator-activated receptor delta	PPARD	Q03181	CHEMBL3979	Nuclear receptor	0.775875873	177 / 10Â Â Â Â Â

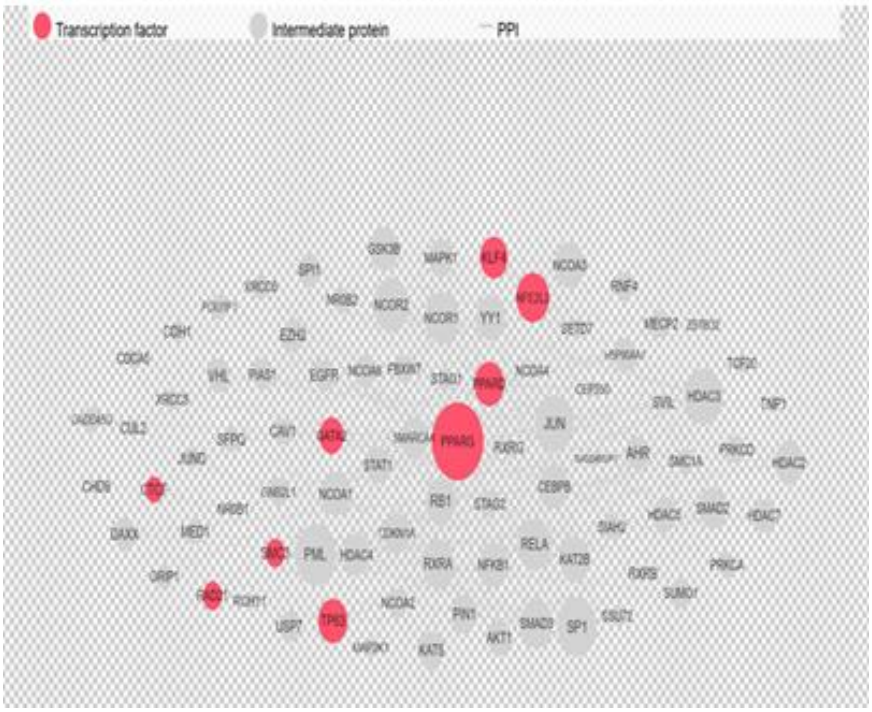


Figure 4.3 protein-protein interaction expansion

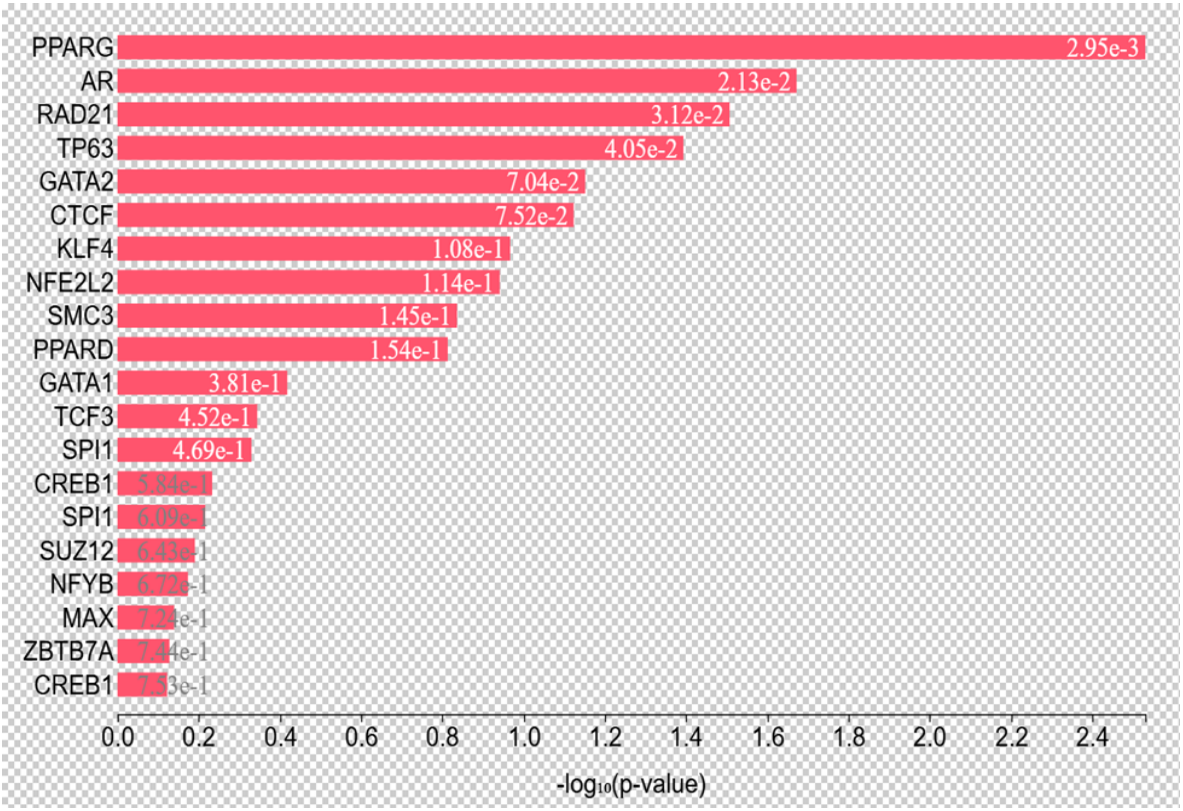


Figure 4.4: Transcription factor enrichment analysis (TFEA)

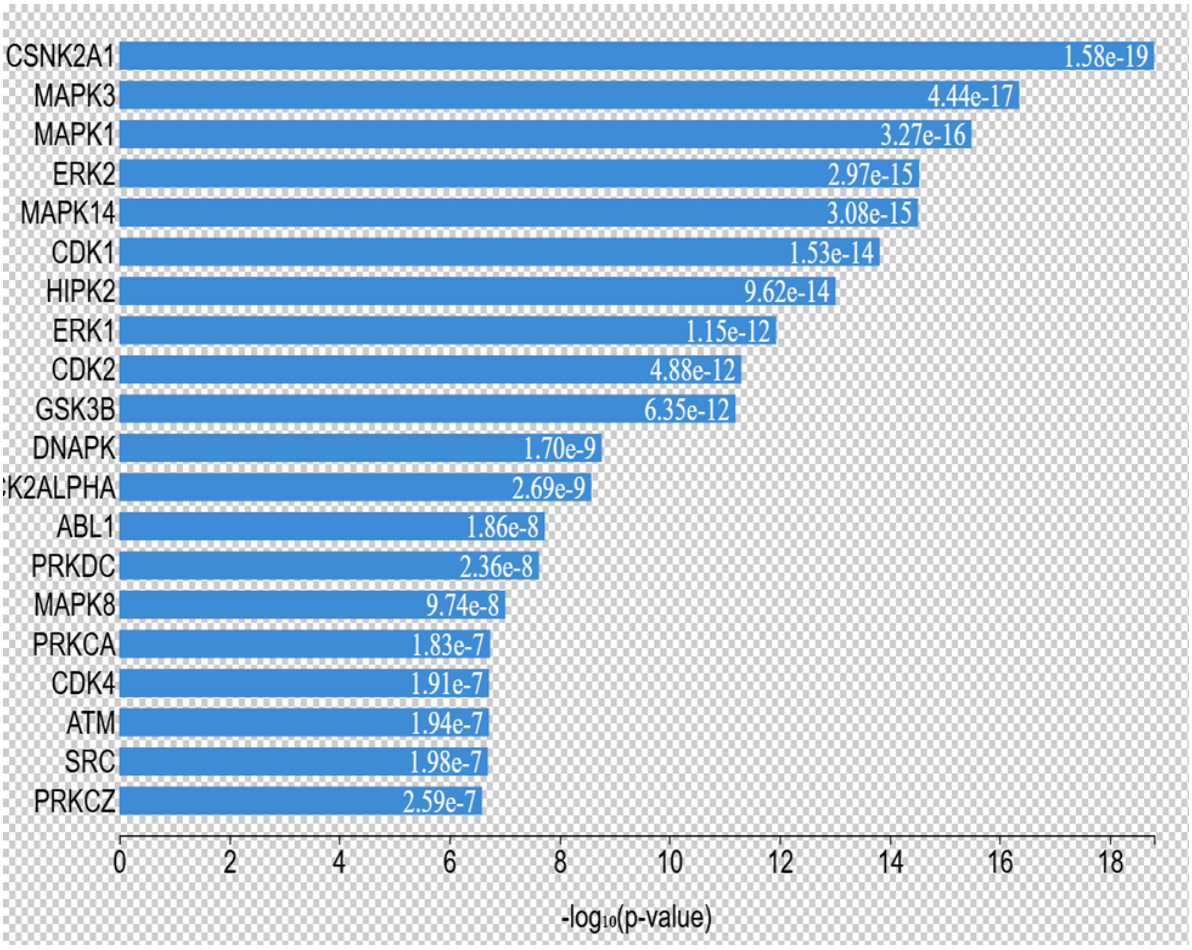


Figure 4.5 Kinase Enrichment Analysis (KEA)

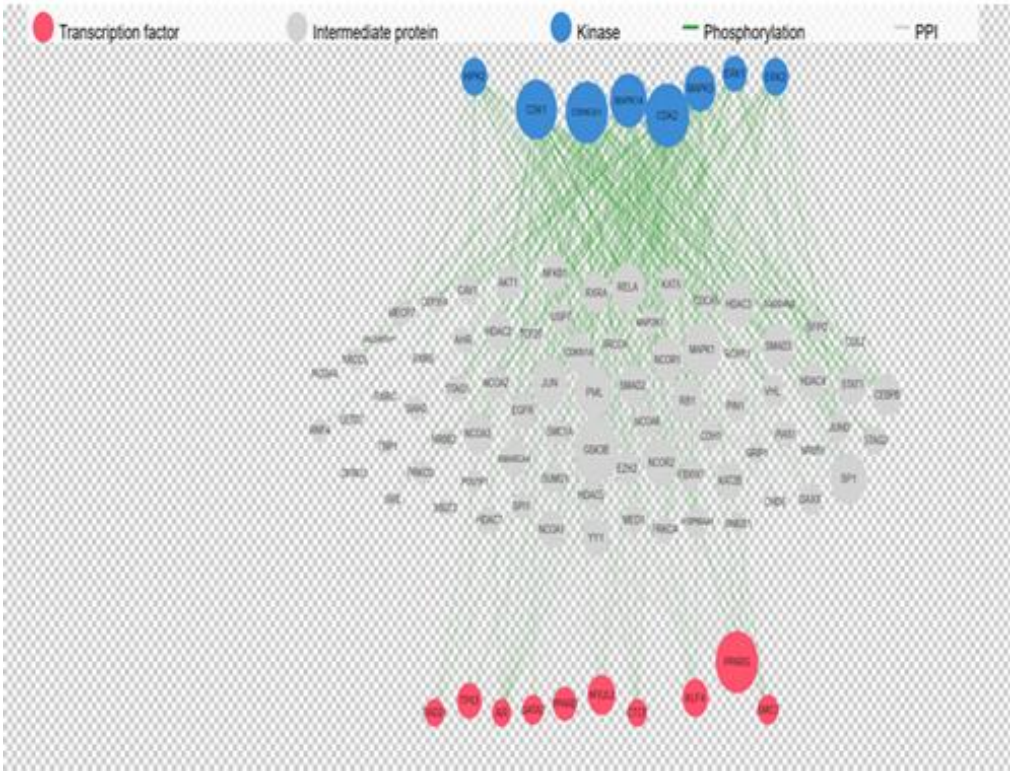


Figure 4.6: eXpression2Kinases Network

Table 11.0: Docking Score for 1Y9R (PDB ID MCR)

Compound name	Docking Score
Propane, 1,1,3-triethoxy-	-4.2
1,2-Ethanediol, monoacetate	-3.8
1-Methyl-pyrrolidine-2-carboxylic acid	-5
ethyl beta-D-glucopyranoside	-5.9
Methyl 14-methylpentadecanoate	-5.4
n-Hexadecanoic acid	-5
Hexadecanoic acid, ethyl ester	-
Oleic acid, methyl ester	-
Phytol	-5.3
9,12-Octadecadienoic acid (Z,Z)-	-5.8
alpha-Himachalene	-
1,2-Benzenedicarboxylic acid, and diisooctyl ester	-
Isolongifolene, 4,5-dehydro-	-6.1

2D structure of (1Y9R PDB ID MCR)

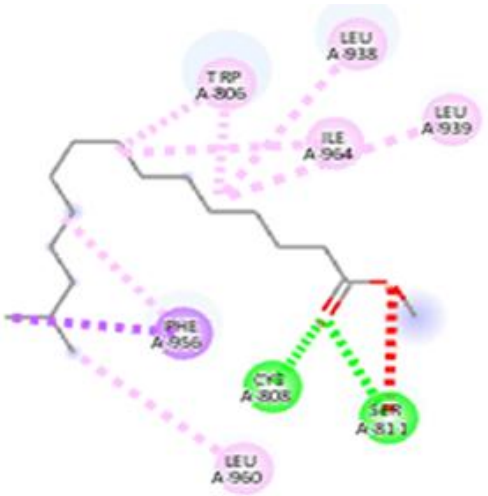


Figure 4.7 a: MCR docked against Methyl 14-methylpentadecanoate

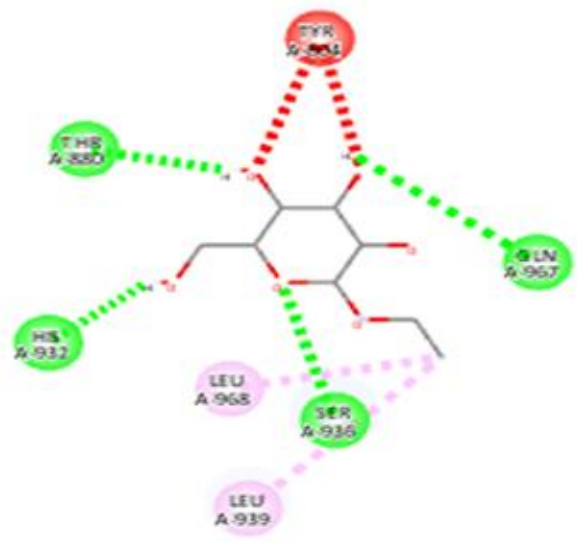


Figure 4.7b: MCR docked against ethyl beta-D-glucopyranoside

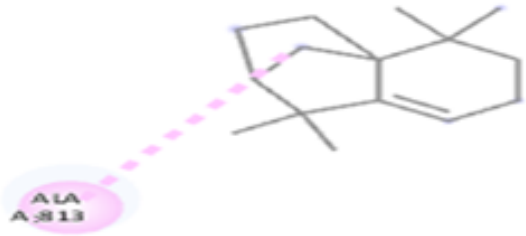


Figure 4.7c: MCR docked against Isolongifolene, 4,5-dehydro-

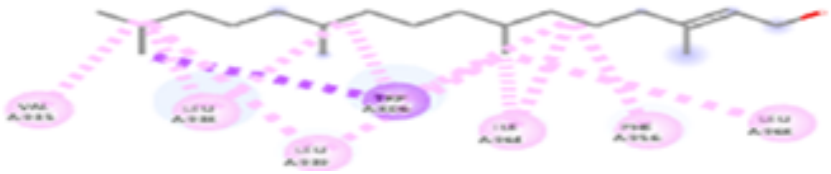


Figure 4.7d: MCR docked against phytol

Figure 4.7e: MCR docked against 9,12-Octadecadienoic acid (Z,Z)-

The clustering analysis, TFEA, PPI, KEA, and X2K analyses further elucidated the complex interplay of these compounds and their potential biological effects, highlighting potential regulatory roles and pathways involved. The docking studies with MCR provided insights into the binding affinities and interactions of various compounds with this enzyme, suggesting its potential role in catalysing diverse substrates.

While this study provides valuable information, certain limitations exist. The number of tested bacterial and fungal strains was limited. Further research would explore the activity against a broader range of pathogens, including drug-resistant strains. Furthermore, in vivo studies are needed to confirm the observed in vitro and in silico findings.

Future research should focus on elucidating the specific mechanisms of action of the identified compounds, particularly their antimicrobial and antioxidant effects. In vivo studies are crucial to assess the safety and efficacy of *M. koenigii* extracts and nanoparticles. Clinical trials may be warranted to explore their potential therapeutic applications. Investigating synergistic effects with existing drugs could also be a fruitful area of research [29-31].

In conclusion, this study provides compelling evidences for the nutritional and therapeutic potential of *Murraya koenigii* leaves. The rich composition of bioactive compounds, coupled with significant antioxidant and antimicrobial activities, positions *M. koenigii* as a promising functional food and a source of potential therapeutic agents. Further research is encouraged to fully realize the potential of this valuable natural resource.

Declarations

Ethics approval and consent to participate

Not Applicable

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Data Availability

All data contributing to this article were derived exclusively from previously published studied that are accessible through PubMed (https://pubmed.ncbi.nlm.nih.gov) or discoverable on google scholar. The complete search for data and full biography of included studied are available in the 'References' section. The summarized data have been identified and have been submitted to the repository holding derived datasets, extraction sheets and analysis codes

Conflict of interest

The authors declare there is no conflict of interest among the authors concerning this paper.

Consent for publications

All the authors gave approval for the publication of the manuscript.

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Conceptualization: Oseni Olatunde and Oladipupo Beauty Data curation: All authors were involved in data curation.

Formal analyses: All authors were involved in analyses of the sample. Methodology: All Authors involved.

Supervision: Oseni Olatunde Writing–original draft: Oseni Olatunde A., Adewumi Funmilayo and Oladipupo Beauty. Writing–review & editing: All Authors.

References

[1] Franyoto YD, Nurrochmad A, Fakhrudin N. (2024) *Murraya koenigii* L. Spreng.: An updated review of chemical composition, pharmacological effects, and toxicity studies. *J Appl Pharm Sci*.; 14(06):011–027. DOI: 10.7324/JAPS.2024.169254

[2] Sangwan N, Kau, R, Pandey S. (2020). Phytochemical and pharmacological properties of curry leaf (*Murraya koenigii*): A comprehensive review. *International Journal of Herbal Medicine*, 8(1), 45-56.

[3] Mishra S, Awasthi S, Sharma V. (2022). Pharmacological significance of *Murraya koenigii*: A review of its medicinal properties and applications. *Journal of Ethnopharmacology,* 287, 115074.

[4] Whelton PK, Carey RM, Aronow WS, Casey DE, Collins KJ, Himmelfarb CD. (2018). Guidelines for the prevention, detection, evaluation, and management of high blood pressure in adults. *Journal of the American College of Cardiology*, 71(19), e127–e248.

[5] Sharma V, Gupta P, Kumar A (2021). Molecular docking studies of bioactive compounds from *Murraya koenigii* against hypertension-related enzymes. *Computational Biology and Chemistry*, 91, 107375.

[6] Sofowora A. (2006). Medicinal plant and traditional medicine in Africa Spectrum Book Limited Ibadan Nigeria. 289

[7] Trease GE, Evans WC. (1989). Pharmacognsy. 11th edn. Brailliar Tiridel Can. Macmillian publishers.

[8] Harborne JB. (1998). A Guide to Modern Technique of plant Analysis, 3rd ed. Chapman and Hall, London, 285.

[9] Chaves JO, De Souza MC, Da Silva LC, Lachos-Perez D, Torres-Mayanga PC, Machado APDF, Rostagno MA. Extraction of flavonoids from natural sources using modern techniques. *Frontiers in Chemistry*. 2020; 8:507887. DOI: 10.3389/fchem.2020.507887

[10] Pulido KDP, Dulcey AJC, Martínez JHI. New caffeic acid derivative from Tithonia diversifolia (Hemsl.) A. Gray butanolic extract and its antioxidant activity. *Food and Chemical Toxicology*. 2017; 109:1079-1085

[11] Wang H, Zhang H, Li J, Wei J, Zhai R, Peng B, Qian X. A new calibration curve calculation method for absolute quantification of drug metabolizing enzymes in human liver microsomes by stable isotope dilution mass spectrometry. *Analytical Methods* 2015; 7(14): 5934-5941.

[12] Salaudeen IO, Olajuwon MO, Ajala AB, Abdulkareem TO, Adeniyi SA, Jisu SA, Adeyemo GA. Green Synthesis, Characterization and In-vitro Antioxidant Property of Silver Nanoparticles Using the Aqueous Leaf Extract of Justicia carnea. *Asian Journal of Biochemistry, Genetics and Molecular Biology*. 2021; 7(3): 20-30.

[13] Abosede OO, Obiyenwa GK. Green synthesis of copper oxide nanoparticles using Justicia Carnea. *Int. J. Chem. Stud.* 2022; 10(2): 21-25.

[14] Bandeira M, Giovanela M, Roesch-Ely, M., Devine, D. M., & da Silva Crespo, J. (2020). Green synthesis of zinc oxide nanoparticles: A review of the synthesis methodology and mechanism of formation. *Sustainable Chemistry and Pharmacy*, 15, 10022

[15] Mourdikoudis S, Pallares RM, Thanh NT. Characterization techniques for nanoparticles: comparison and complementarity upon studying nanoparticle properties. *Nanoscale*, 2018; 10(27): 12871-12934.

[16] Gumgumjee NM, Hajar AS. Antimicrobial efficacy of *Casuarina equisetifolia* extracts against some pathogenic microorganisms. *Journal of Medicinal Plants Research*. 2012; 6(47):5819-25. DOI: 10.5897/JMPR12.741

[17] Mohan R, Patel H, Singh J. (2023). Molecular docking and clustering analysis of enzyme inhibitors: A case study on potential anticancer drugs. *Computational Biology and Chemistry*, 98, 107-115.

[18] Morris GM, Huey R, Lindstrom W, Sanner MF, Belew RK, Goodsell DS, Olson AJ. (2009). Auto Dock4 and Auto Dock Tools4: Automated docking with selective receptor flexibility. *Journal of Computational Chemistry*, 30(16), 2785–2791.

[19] Bell LN. Moisture effects on food's chemical stability. Water activity in foods: fundamentals and applications. 2020; 227-253. doi: 10.1002/9780470376454.ch7.

[20] Alamgir ANM. Therapeutic use of medicinal plants and their extracts: volume 1. Springer International Publishing AG. 2017; 1(2):30-39.

[21] He Y, Wang B, Wen L, Wang F, Yu H, Chen D, Zhang C. Effects of dietary fiber on human health. *Food Science and Human Wellness*. 2022; 11(1):1-10. https://doi.org/10.1016/j.fshw.2021.07.001.

[22] Adelakun SA, Ukwenya VO, Peter AB, Siyanbade AJ, Akinwumiju CO. Therapeutic effects of aqueous extract of bioactive active component of Ageratum conyzoides on the ovarian-uterine and hypophysis-gonadal axis in rat with polycystic ovary syndrome: Histo morphometric evaluation and biochemical assessment. *Metabolism Open*. 2022; 15:100201. https://doi.org/10.1016/j.metop.2022.100201.

[23] Adamski Z, Blythe LL, Milella L, Bufo SA. Biological activities of alkaloids: from toxicology to pharmacology. *Toxins*. 2020; 12(4):210. https://doi.org/10.3390/toxins12040210.

[24] Wang Y, Anesi J, Maier MC, Myers MA, Oqueli E, Sobey CG, Drummond GR, Denton KM. Sympathetic nervous system and atherosclerosis. *International Journal of Molecular Sciences*. 2023; 24(17):13132.

[25] Kumar A, Prasad MNV. Plant-lead interactions: transport, toxicity, tolerance, and detoxification mechanisms. *Ecotoxicology and Environmental Safety*. 2018; 166:401-418.

[26] Joseph DA, Oseni MO, Oseni OA. Biochemical investigations and green synthesis characterization using aqueous extract of Ageratum conyzoides L. leaf. *Journal of Biochemicals and Phytomedicine*. 2024; 3(2): 9-19. doi: 10.34172/jbp.2024.15.

[27] Oseni OA, Seyinde D, Abe TO, Igbe F. Chemical and Some Biochemical Assessments of Various Parts of Passion Fruit (Passiflora edulis Sims) *Plant. Asian J. Biol. Sci.* 2024; 17(1): 32-40. https://doi.org/10.3923/ajbs.2024.32.40

[28] Kaji N, Horiguchi K, Iino S, Nakayama S, Ohwada T, Otani Y, Hori M. Nitric oxide-induced oxidative stress impairs pacemaker function of murine interstitial cells of Cajal during inflammation. *Pharmacological Research*. 2016; 111:838-848.

[29] Zhang Q, Liu Y, Chen Z. Phytochemical profiling of Citrus indicum and its potential therapeutic effects. *Phytochemistry Reviews*, 2022; 21(4), 1231-1245.

[30] Zhang X, Perez-Sanchez H, Lightstone FC. A comprehensive docking and MM/GBSA rescoring study of ligand recognition upon binding antithrombin. *Current Topics in Medicinal Chemistry*, 2017; 17, 1631-1639.

[31] Zhao H, Zhang M, Liu J. Role of oxidative stress in hypertension and its modulation by antioxidants. *Oxidative Medicine and Cellular Longevity*, 2023; Article ID 7245627.