INFORMATICS JOURNALS

Research Article

Journal of Natural Remedies
DOI: 10.18311/jnr/2026/55231

eISSN: 2320-3358 | Vol 26(6), 2026 | pp. 1655-1674

Valorisation of Mango Seed Kernels: Unlocking an Underutilised Agro Waste for Bioactive Ingredient Development

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Abstract

Background: Mango (*Mangifera indica* L.), widely known as the 'King of Fruits', belongs to the family *Anacardiaceae*. Mango seed kernels, a major byproduct of the fruit processing industry, are often discarded as agro-industrial waste despite being rich in valuable phytochemicals, including polyphenols, proteins and carbohydrates. **Aim:** This study investigates the phytochemical composition, antioxidant and anti-tyrosinase activities, and molecular docking interactions of mango seed kernel extracts derived from the Bellare variety. **Methods:** Phytochemical screening was performed using standard quantitative methods, and active compounds were characterised through Liquid Chromatography-Mass Spectroscopy (LC-MS). The antioxidant potential was assessed using DPPH radical-scavenging, reducing power, and phosphomolybdenum assays. Anti-tyrosinase activity was evaluated using Levodopa (L-DOPA) as a substrate and mushroom tyrosinase enzyme. Molecular docking studies were conducted using Autodock 4.2.6, and the mango seed kernels were further utilised in a kernel body butter formulation with virgin coconut oil. **Results:** The phytochemical analysis confirmed the presence of phenolic compounds, flavonoids, tannins, carbohydrates and proteins. The ethanolic extract exhibited strong antioxidant capacity and significant tyrosinase inhibition comparable to the standard, Kojic acid. LC-MS analysis identified three major bioactive compounds: Ethyl gallate, Gallic acid, and Syringic acid. Among these, molecular docking revealed that ethyl gallate showed the highest binding affinity toward mushroom tyrosinase, followed by gallic acid and syringic acid. These compounds find applications in the treatment of skin hyperpigmentation and scars, where the tyrosinase activity is higher. **Conclusion:** Overall, the mango seed kernel extract demonstrates promising potential as a natural antioxidant and skin-whitening agent with sustainable utilisation prospects for agro-industrial waste.

Major Findings: LC-MS analysis identified key bioactive compounds in mango seed kernels, including ethyl gallate, gallic acid and syringic acid. Molecular docking studies further revealed that these compounds exhibit significant binding affinity toward tyrosinase, suggesting their potential role in anti-tyrosinase activity.

Keywords: Ethyl Gallate, Gallic Acid, Molecular Docking, Mushroom Tyrosinase, Phenolics, Syringic Acid, Tyrosinase Inhibition

(Article Chronicle: Article Received on: 06.03.2026; Revised on: 11.05.2026; Accepted on: 23.05.2026)

1. Introduction

Mango (*Mangifera indica* L.), also referred to as the 'King of fruits', belongs to the family *Anacardiaceae*, thrive in tropical and subtropical regions, and its various parts are frequently utilised in traditional medicine to create a diverse array of remedies[1]. The mango is native to the Indian subcontinent, Southeast Asia, and Africa. Mango trees can reach up to heights of 35-40m, with their branches extending up to 10m in diameter[2]. In 2019, mango production worldwide reached approximately 56.5 Million Tons (MT),

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making it one of the most widely grown fruits across many countries[3]. The mango tree is an evergreen tree and is a tetraploid species with 40 chromosomes. India is the leading country in mango cultivation, responsible for 40% of the world's total mango production. With an annual production of 21,822.3 thousand MT and an area of 2,258.1 thousand ha, India is the largest global producer of mangoes. The country also boasts a productivity rate of 9.7 MT/ha and is a major contributor to the collection of mango germplasm accessions[4]. Mango fruits contain a variety of nutrients such as protein, fat, carbohydrates, minerals, and vitamins A, B, and C. They also produce a resin that contains mangiferin, mangiferolic acid, resinol, mangiferol and other compounds. The mango leaves have been found to contain saponins, glycosides, unsaturated sterols, polyphenols, euxanthin acid, mangiferin, and tannins, and its extracts have also been used as antiseptics for the treatment of burns, wounds, scalds, sores, abscesses, and infections in humans and animals, as reported in numerous ethnobotanical studies[5]. Due to their seasonal nature, approximately 20% of mangoes are processed into goods like puree, nectar, leather, chutney, juices, ice cream, canned slices, fruit bars, and pies. During the preparation of ripe mangoes, the peel and seed produce waste, which accounts for about 40-50% of the total fruit weight. Depending on the cultivar, the mango seed is of a single flat oblong shape and may have a fibrous or hairy surface. The kernel inside the seed accounts for 45 to 75% of the seed and around 20% of the entire fruit[6]. The potential of mango wastes, including the seed kernel and peel, is high both in terms of functionality and nutrition. Currently, over one MT of mango seeds are generated as waste every year, with no commercial use for them. The mango seed, which is considered a bio-waste, contains beneficial compounds such as phenolic compounds, vitamin C, carotenoids and dietary fibre that can promote human health. It is rich in carbohydrates (58-80%), essential amino acids, protein (6-13%), and lipids (6-16%) such as oleic acid and stearic acids[7].

Mango seed kernels contain various types of polyphenols, such as flavanols, xanthones, and gallotannins, which act as natural antioxidants. They have been found to have anti-tyrosinase, anti-alpha-glucosidase, anti-inflammatory, hepatoprotective, and antimicrobial properties. Chinese mango seed kernels were found to contain five gallotannins, namely penta-o-galloyl-glucoside, hexa-o-galloyl-glucoside, hepta-o-galloyl-glucoside, octa-o-galloyl-glucoside, and nona-o-galloyl-glucoside, while Hiesy mango seed kernels contained tri-o-galloyl-glucoside, tetra-o-galloyl-glucoside, penta-o-galloyl-glucoside, hexa-o-galloyl-glucoside, hepta-o-galloyl-glucoside, and octa-o-galloyl-glucoside. Tommy Atkins mango seed kernels were found to contain 21 gallotannins[8].

Melanin acts as a protective pigment that helps shield the skin from Ultra-Violet (UV) damage, serving as a crucial defence mechanism against harmful factors. Tyrosinase is an enzyme that plays a crucial role in the initial stages of melanin production. It converts L-tyrosine into DOPA (3,4-dihydroxyphenylalanine) through hydroxylation and further oxidises DOPA into dopaquinone. Increased melanin production and buildup are observed in various skin conditions such as solar melanosis, ephelides (freckles), melasma, senile lentigos (age spots), and post-inflammatory hyperpigmentation. Inhibiting the activity of tyrosinase can be helpful in treating conditions characterised by excess pigmentation. However, existing tyrosinase inhibitors have limitations in terms of safety and effectiveness. Therefore, there is ongoing research to find new and improved inhibitors, particularly from natural sources, which are expected to have fewer adverse effects[9]. The extract of Thai mango seed kernel, specifically the '*Fahlun*' cultivar, contained high levels of pentagalloylglucoyranose (PGG) at 61.28%, along with smaller amounts of Methyl Gallate (MG) at 0.68% and Gallic Acid (GA) at 0.44%. They also observed that the extract and its isolated compounds displayed strong abilities to eliminate free radicals, act as antioxidants, reduce inflammation, and protect against liver damage caused by carbon tetrachloride in rats. The Thai mango seed kernel extract, derived from the '*Fahlun*' cultivar, has powerful and effective anti-tyrosinase activity that varies depending on the dosage and is specifically related to L-DOPA. The phenolic compound PGG exhibited greater anti-tyrosinase activity compared to MG and GA, which are also phenolic compounds[1].

Cosmetic applications often require tyrosinase inhibitors for their skin-whitening effects, as many individuals desire a lighter complexion. Due to their ability to enhance food quality, prevent pigmentation disorders, and address melanin-related health issues

in humans, tyrosinase inhibitors are now recognised as valuable and reliable options that are both safe and effective[10].

The main source of blood glucose comes from starches found in dietary carbohydrates, which are broken down by pancreatic alpha-amylase and absorbed by the small intestine with the help of alpha-glucosidases. The alpha-glucosidase plays a crucial role in the last stage of glucose absorption in the small intestine when digesting carbohydrates. Inhibiting α-glucosidase enzyme slows down the absorption of dietary carbohydrates and reduces postprandial hyperglycemia, potentially preventing the progression of Diabetes mellitus. The alpha-glucosidase inhibitory activity of fraction 3 of Mango Seed Kernel Extract (MSKE) from two different cultivars (Kaew and Choke-Anan) obtained by Sephadex LH-20 column chromatography showed significantly higher activity. However, acarbose, which is used as a reference standard, exhibited even greater activity than all crude extracts and fractions of MSKE[8].

Mango kernels contain approximately 15% of oils, which have been utilised in the cosmetics industry due to their abundance of phenolic compounds. These oils also contain beneficial microelements such as selenium, copper, and zinc. Mango kernel oil is primarily composed of oleic acid, making up about 45% of its fatty acid content, and stearic acid, which makes up about 38%. Oleic acid is a monounsaturated fatty acid that is important for human nutrition and has been shown to have various health benefits, including improving lipid levels and reducing the risk of heart disease. Additionally, the presence of oleic acid contributes to the increased stability of mango kernel oil, preventing it from oxidising easily. Stearic acid, on the other hand, is a saturated fatty acid that has been found to have binding and plasticising properties in proteins, specifically in human serum albumin and certain biomolecules[11].

This study characterises ethanolic and aqueous mango seed kernel extracts via qualitative and quantitative phytochemical analyses, determines kernel fat content, evaluates the antioxidant, anti-tyrosinase and antibacterial activities of mango seed kernel extracts and formulates and assesses a mango seed kernel-based body butter.

2. Materials and Methods

2.1 Collection of Sample

The *Mangifera indica* L. seeds of the *Bellare* variety were collected from Mangalore, Dakshina Kannada, Karnataka, India, in the month of June, 2023. The studied seed specimen was identified under the guidance of Dr Rama Bhat, Head of Post Graduate Biotechnology, Alva's College, Moodbidri, based on the morphological appearance and fragrance of mango (Figure 1A-D).

2.2 Chemicals and Instruments

2.2.1 Chemicals

Mushroom Tyrosinase, L-DOPA, Kojic acid, 50mM Phosphate buffer (pH 6.5), Gallic acid, Sodium carbonate, Folin-Ciocalteu reagent, Tannic acid, Folin-Denis reagent, Sodium tungstate, Phosphomolybdic acid, Sodium hydroxide, Sodium nitrate, Rutin, Yeast alpha glucosidase, Acarbose, Bovine serum albumin, Phenol, Concentrated Sulfuric acid, Sodium sulphite, Potassium sodium tartarate, Mayer's reagent, Wagner's reagent, DPPH, Ferric chloride, Trichloroacetic acid, 0.1M phosphate buffer (pH 6.9), Potassium ferrocyanide, Acetic anhydride, Ammonium molybdate, Orthophosphoric acid, Petroleum ether, chloroform, Potassium hydroxide, Phenolphthalein indicator.

2.2.2 Instruments

UV-visible Spectrophotometer (Systronics PC based double beamed spectrophotometer 2202), Water bath, Incubator, Hot air oven, Vortex mixer, pH meter.

2.2.3 Media

Nutrient Agar was used for the antibacterial activity of mango seed kernel extracts.

2.3 Preparation of Mango Seed Kernel Extracts

2.3.1 Preparation of the Mango Seed Kernel Powder

Mango seeds were cleaned and allowed to dry in the shade for two weeks. The kernels were removed from the seed coat manually with a stainless-steel knife and dried in a hot air oven at 50° C for 4 h. The dried seed kernels were powdered using a mortar and pestle. The

powdered kernels were stored in air-tight containers for further use[6].

2.3.2 Preparation of Ethanolic Mango Seed Kernel Extract

20g of mango seed kernel powder was mixed with 200mL of 95% ethanol in a blender for 5 min and was shaken in a rotary water bath for 5 h at 55°C. The obtained mixture was filtered through Whatman No.1 filter paper, and the filtrate was evaporated at 60°C in a water bath. The collected ethanolic extract was used for further analysis[10].

2.3.3 Preparation of Aqueous Mango Seed Kernel Extract

20g of powdered seed kernel sample was added to 200mL of distilled water and was shaken in a rotary water bath for 5 h at 55°C. Whatman No.1 filter paper was used to filter the mixture, and the filtrate was then evaporated in a water bath at 80°C. The aqueous extract was obtained and used for more investigation[12].

2.3.4 Extraction Yield

The extraction yield of prepared ethanolic and aqueous extracts was determined by using the formula:

$$Extraction\ yield\,(\%) = \frac{W_1}{W_2} \times 100$$

where W_1 is the mass of the crude dry extract, and W_2 is the mass of the sample used for extraction.

2.4 Qualitative Phytochemical Analysis

To determine the presence of various phytoconstituents, qualitative phytochemical tests were carried out for ethanolic and aqueous extracts[5,13].

2.5 Proximate Analysis

The proximate analysis of *M. indica* seed included moisture and ash content, which were analysed[2].

2.5.1 Moisture Content Determination

This procedure measures the amount of moisture that is lost when *M. indica* seed is dried at a temperature of 105°C. 2g of the powdered seed kernel was carefully weighed into a crucible that had been previously weighed. After that, the crucible was kept in a drying oven for three hours at 105°C. The crucible was then taken out of the oven, let to cool in a desiccator, and weighed once more. The weight loss that occurred due to the removal of moisture was calculated using the formula:

$$Moisture\,content\,(\%) = \frac{W_1 - W_2}{W_2 - W_0} \times 100$$

where, W_o= Weight of the empty crucible (g), W_1= Weight of the kernel powder + empty crucible (g) and W_2= Weight of dried powder sample + empty crucible (g).

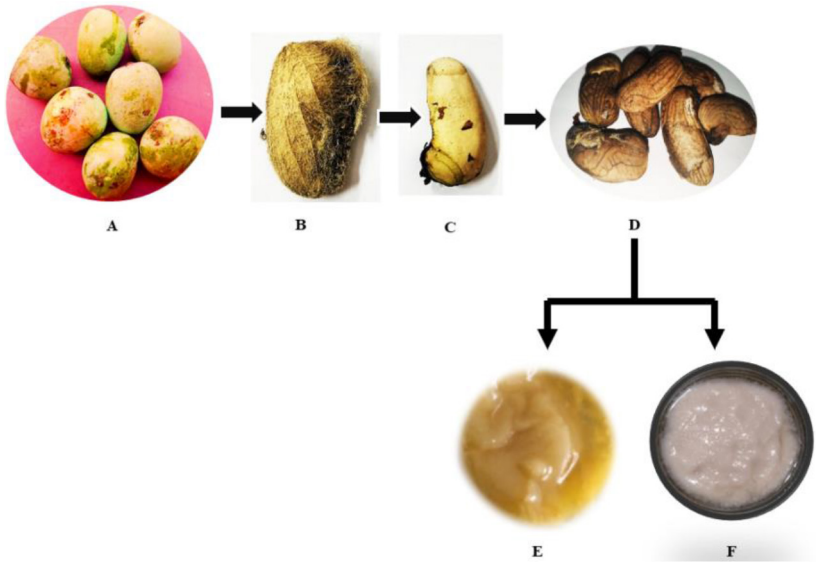


Figure 1. Processing of *Bellare* mango seed kernels **(A).** *Bellare* cultivar of Mango; **(B).** Mango seed; **(C).** Mango seed kernel; **(D).** Dried mango seed kernels; **(E).** Fat extracted from mango seed kernels; **(F).** Mango seed kernel body butter.

2.5.2 Ash Content Determination

After cleaning and drying in a hot air oven for half an hour, the crucible was cooled in a desiccator for another half an hour. After weighing the crucible and adding 2g of the sample, the weight of the crucible was noted. Next, the sample was heated with a Bunsen flame to remove any carbon and turn it into white ash. The crucible with the ash was then transferred to a muffle furnace, which was set at a temperature of 500°C, and left there for one hour to ensure complete decarbonisation. After the crucible and ash were cooled down, their weight was recorded. Ash content is obtained by dividing the weight of ash by the original weight of the sample and is expressed as a percentage. The ash content was estimated by using the formula:

$$Ash\,content\,(\%) = \frac{W_1 - W_2}{W_2 - W_0} \times 100$$

Where, W_o= Weight of the empty crucible (g), W_1= Weight of the kernel powder + empty crucible (g) and W_2= Weight of white ash + empty crucible (g).

2.6 Quantitative Estimation of Phytochemical Constituents

2.6.1 Estimation of Total Carbohydrate Content

Determination of carbohydrates for ethanol and aqueous extract was done by the phenol-sulfuric acid method[14,15]. Ethanolic solution and aqueous solution of the extract in a concentration of 1mg/mL were used in the analysis. Glucose of 1mg/mL was used as a standard stock solution. Different concentrations, viz., 200, 400, 600, 800 and 1000 mg/mL were taken as standard and were made up to 1mL by using distilled water. To this 1mL of solution, 1mL of 0.5% phenol and 5mL of 96% Sulphuric acid were added. After 10 min, the mixture was stirred using a vortex mixer and was incubated for 30 min. The absorbance was read at 490nm using a colourimeter.

2.6.2 Estimation of Total Reducing Sugar

Analysis of total reducing sugar content in the ethanolic and aqueous extracts was done by the 3,5-dinitrosalicylic acid (DNS) method[16]. The concentration of ethanolic and aqueous extracts used was 25mg/mL. Glucose was used as a standard for this assay. Different concentrations such as 100, 200, 300, 400 and 500µg/mL were taken as standards and were made up to 1mL by using distilled water. 2mL of the DNS reagent was added to this, and it was incubated for 10 min in a boiling water bath. After incubation, add 1mL of Rochelle's salt solution (40% Potassium sodium tartarate solution) and allowed to stand for 20 min. Blank was composed of all reagents except the standard glucose. When the reducing sugar is heated with DNS reagent under alkaline conditions, in the presence of tartarate reagent gives a red colour which can be read colourimetrically at 520nm.

2.6.2.1 Preparation of DNS (3,5-dinitrosalicylic acid) Reagent

0.2g of crystalline phenol and 0.05g of sodium sulphite in 100mL of 1% NaOH, and store the reagent at 4°C.

2.6.3 Estimation of Total Protein Content

Evaluation of protein content for ethanolic and aqueous extract was carried out[17]. An ethanolic solution and aqueous solution of the extract in a concentration of 25mg/mL were used for the estimation. Bovine Serum Albumin (BSA) was utilised as the standard stock solution. Different concentrations, viz., 100, 200, 300, 400 and 500µg/mL were taken as standard and were made up to 1mL by using distilled water. After adding 5mL of alkaline copper tartarate to this 1mL, it was left to stand at room temperature for 10 min. After the incubation period, 0.5mL of Folin-Ciocalteu Reagent (FCR) was mixed in. The absorbance was measured at 660nm using a colourimeter.

2.6.3.1 Preparation of Alkaline Copper Tartarate

Combine 48mL of 2% sodium carbonate (Na_2CO_3) dissolved in 0.1N sodium hydroxide (NaOH) with 1mL of a solution containing 1% sodium potassium tartrate dissolved in distilled water. Finally, add 1mL of a solution containing 0.5% copper sulphate pentahydrate ($CuSO_4.5H_2O$) to get the final solution.

2.6.4 Estimation of Total Phenolic Content

Total Phenolic Content (TPC) in the ethanolic and aqueous extracts was assessed by the Folin–Ciocalteu colourimetric method[18,19]. Gallic acid was used as a standard, which was prepared by adding 10mg of it in 100mL of ethanol (100µg/mL). Several concentrations of gallic acid solution in ethanol (20, 40, 60, 80 and

100 µg/mL) were prepared from the standard solution. An ethanolic solution and aqueous solution of the extract in a concentration of 25mg/mL were used for the estimation. To each tube, 0.5mL of 10% FCR and 2mL of 5% sodium carbonate were added. The resultant blue coloured mixture was vortexed well and incubated in the dark for 60 min at room temperature. The absorbance was measured at 760nm against a blank using a spectrophotometer. Total phenolic content of the extracts was expressed as mg Gallic Acid Equivalents (GAE) per gram of seed extract (mg/g). The total phenolic content in both the extracts was calculated by using the formula:

$$P = C(V/E)$$

where, P=Total phenolic content mg GAE/g dry extract, C = concentration of gallic acid obtained from calibration curve in µg/mL, V = volume of extract in mL, and E = mass of extract in grams.

2.6.5 Estimation of Total Flavonoid Content

The Aluminum chloride colourimetric assay was used to assess the total flavonoid content of ethanolic and aqueous extracts[20]. Rutin was used as a standard, and different concentrations of standard solution, viz., 100, 200, 300, 400, 500µg/ml, were used for analysis. For the estimation, 1mL aliquot of an ethanolic and aqueous extract solution with a concentration of 1 mg/mL was utilised. 0.3 mL of 5% sodium nitrite solution was added to each tube, followed by 0.3 mL of 10% aluminum chloride after 5 minutes, and 2mL of 1M sodium hydroxide at the end of 6 minutes. The absorbance was measured at 510nm using a UV-visible spectrophotometer. The Total Flavonoid Content (TFC) was expressed as mg Rutin Equivalents (RE) per gram of the seed extract (mg/g) based on the calibration curve.

2.6.6 Estimation of Total Tannin Content

Analysis of tannins of aqueous and ethanolic extracts was performed[21]. In an alkaline solution, tannins convert phosphotungstomolybdic acid to create a bright blue solution whose intensity is directly correlated with the tannin content. Tannic acid was used as a standard. Different concentrations of the extract as well as standard were used, viz., 20, 40, 60, 80 and 100µg/mL. To 1mL of the extract, 0.5mL of Folin-Denis reagent and 1mL of 35% Na_2CO_3 were added and allowed to stand for about 30 min, and the intensity of blue colour was read at 760nm using a spectrophotometer. The total tannin content was exhibited as mg tannic acid equivalents per gram of the plant extract (mg/g) based on the standard graph.

2.6.6.1 Preparation of Folin Denis Reagent

20g of phosphomolybdic acid and 100g of sodium tungstate were added to 750 mL of distilled water, and later, 50mL phosphoric acid was added to the solution. The mixture was refluxed for 2 hours, and the final volume was adjusted to one litre with distilled water.

2.7 Determination of Anti-tyrosinase Activity

Determination of tyrosinase inhibition by the ethanolic and aqueous extracts was done by the mushroom tyrosinase inhibition assay[9,22]. The anti-tyrosinase assay used L-DOPA as substrate. The reaction mixture (1640µL) contained 700µL of phosphate buffer (50mM, pH 6.5), 40µL of mushroom tyrosinase enzyme (160 Units/mL), 200µL of seed kernel extract and 200µL of 2.5mM L-DOPA. After incubation for 24 h at 37°C, the absorbance was measured at 492nm for dopachrome formation in the reaction mixture. Kojic acid was employed as a standard. The concentration range of extract and standard Kojic acid used for the mushroom tyrosinase inhibition assay was 100, 200, 300, 400, 500µg/mL. Each measurement was made in triplicate. The control contained all the reagents except the seed kernel extract. The phosphate buffer was used as a blank. The IC_{50} value, a concentration giving 50% inhibition of tyrosinase activity, was determined. The percentage of tyrosinase inhibition was calculated by using the formula:

$$\% \text{ Tyrosinase inhibition activity} = [(Abs_{control} - Abs_{sample})/Abs_{control}] \times 100$$

2.8 Determination of Antioxidant Activity

2.8.1 DPPH (2,2-diphenyl-1-picrylhydrazyl) Free Radical Scavenging Assay

The DPPH radical scavenging activity of ethanolic and aqueous extracts was evaluated[7]. 0.1mM DPPH solution was prepared by dissolving 3.94mg of DPPH in 100mL ethanol. Ascorbic acid was used as a

standard. Different concentrations of the extract and the standard (20, 40, 60, 80, 100 µg/mL) were prepared. Then, 500µL of extract from each concentration was mixed with 3mL of DPPH solution. Control was prepared by adding 500µL of ethanol or distilled water to 3mL of DPPH solution. The mixture was shaken thoroughly and allowed to stand in the dark for 30 min. The absorbance of the resultant mixture was then determined spectrophotometrically at 517nm. The scavenging activity of each extract on DPPH radical was assessed using the following formula:

$$\% \text{ Radical Scavenging activity (RSA)} = [(Abs_{control} - Abs_{sample})/Abs_{control}] \times 100$$

2.8.2 Reducing Power Assay

The reducing power of the ethanolic and aqueous extracts was investigated according to standard procedures[7,18,23]. Ascorbic acid was used as a standard. Different dilutions of the extract and the standard (20, 40, 60, 80, 100 µg/mL) were prepared. To 1ml of extract, 2mL of 1% potassium ferricyanide solution and 2mL of phosphate buffer (0.05M, pH 6.6) were added. This mixture was incubated in a water bath at 50˚C for 20 min and was quickly cooled. To stop the reaction, 2ml of (10%) trichloroacetic acid solution was added to each sample. The reaction mixture (2.5 ml) was diluted with 2.5ml of distilled water. To this mixture, 0.5mL of 0.1% $FeCl_3$ was added, and the tubes were allowed to stand for 20 min. The absorbance was measured at 700nm in a spectrophotometer as the reducing power. The higher absorbance of the reaction mixture depicts the increased reducing power.

2.8.3 Phosphomolybdenum Assay

Total Antioxidant Capacity (TAC) or Phosphomolybdenum assay of the ethanolic and aqueous extract[24]. The extract or fractions reduced Mo (vi) to Mo (v), resulting in the formation of a green phosphomolybdate (v) complex at acidic pH. Different dilutions of the extract and the standard (100, 200, 300, 400, 500 µg/mL) were prepared. 100µL of the extract was mixed with 1mL of reagent (28mM sodium phosphate, 0.6M Sulphuric acid, and 4mM ammonium molybdate). The phosphomolybdate reagent was made by adding 50mL each of 28 mM sodium phosphate, 0.6M Sulphuric acid and 4mM ammonium molybdate. Ascorbic acid was utilised as the standard. After being sealed, the tubes were incubated for 90 minutes at 95°C in a boiling water bath. By using a spectrophotometer, absorbance was measured at 695nm against a blank once the samples had cooled to room temperature. The blank solution included 3mL of reagent solution and 100µL of the same solvent used for the sample. The antioxidant capacity was measured as the equivalent of ascorbic acid.

2.9 Determination of Fat Content

2.9.1 Extraction of Fat

The Fat content of *M. indica* L. seed kernels was extracted by Soxhlet extractor[2,11]. Mango seed kernels were powdered using a mortar and pestle. A 250mL round-bottom flask was cleaned, dried in an oven at 105°C for an hour, chilled in a desiccator, and then weighed. After being cleaned with the extraction solvent, the thimbles were oven-dried and desiccator-cooled. 20g of moisture-free samples were weighed, wrapped in muslin fabric, and put in a thimble with 200ml of petroleum spirit in a round-bottom flask. The extraction was done in a Soxhlet extractor for eight hours at 50°C. Following extraction, the solvent was evaporated, and the weight of the leftover fat was recorded and calculated as a percentage of the sample. The yield of fat was calculated.

2.9.2 Determination of Free Fatty Acids

The free fatty acid content of the extracted fat was evaluated[25]. The amount of Potassium Hydroxide (KOH) needed to neutralise the free fatty acids in one gram of the sample is known as the acid number. 1g of fat was combined with 50mL of neutral solvent. After adding a few drops of phenolphthalein indicator, the mixture was titrated against 0.1N potassium hydroxide until a light pink colour was attained. The free fatty acid content was determined by the formula:

$$\text{Acid value (mg KOH/g)} = \text{Titre value} \times \text{Normality of KOH} \times 56.1/\text{Weight of sample (g)}$$

2.10 Determination of Antibacterial Activity

2.10.1 Antibacterial Activity

The antimicrobial activity of ethanolic and aqueous extracts was tested by the agar well diffusion method[26].

The nutrient agar (Table.1) plates were prepared. Gram positive *Staphylococcus aureus*, Gram negative *Escherichia coli* and *Klebsiella pneumoniae* bacteria were employed as test microorganisms. Plates containing nutrient agar were spread with 0.1mL of all the test microbes using a glass spreader and then, 8 mm wells were punched by using a cork-borer. 0.1mL of seed extracts was added to these wells. The plates that were inoculated with various isolates were incubated for 24 h at 37°C. The diameter of the inhibition zones was measured to determine the antibacterial property following incubation.

2.11 Preparation of Mango Seed Kernel Butter Formulation

The dried seed kernels were made into pieces by using a mortar and pestle. The virgin coconut oil was collected from the coconut oil mill, Karwar, Karnataka. 30g of seed kernel sample was added to 250mL of coconut oil. The mixture was heated for 20 min at 80°C, cooled and stored in a glass container at -20°C for further use[27].

2.11.1 Antimicrobial Activity of Kernel Butter

The antimicrobial activity of kernel butter was tested by the agar well diffusion method[26]. The nutrient agar (Table 1) plates were prepared. Gram negative bacteria like *E. coli* and *K. pneumoniae,* and Gram positive bacteria like *S. aureus* were employed as test microorganisms for this assay. Plates containing nutrient agar were spread with 0.1ml of all the test microbes using a glass spreader and then, with a cork-borer, making 8mm wells in the agar. 80 and 100µL of kernel Butter was inoculated in the 8mm wells in nutrient agar plates and were incubated at 37°C for 24h. After the incubation, results were obtained by measuring the diameter of the zone of inhibition.

Table 1. The composition of the nutrient agar for 250mL

Components	Quantity
Peptone	1.25g
Yeast Extract	0.375g
Sodium Chloride	1.25g
Agar, Type 1	4g
Distilled Water	250mL

2.12 LC-MS (Liquid Chromatography-Mass Spectrometer) Analysis

LC-MS analysis of the ethanolic extract of *M. indica* seed kernel was carried out at Transdiscipline Research Foundation, Dr P.S. Babu Health Centre, Shivamogga, Karnataka. LC–MS analysis was performed using a HPLC model Waters 2965 (Conquer Scientific, USA) furnished with two solvent delivery modules, a thermoautosampler, a column oven, a diode array detector, and a degasser. UV-visible spectra were captured between 200 and 800nm in wavelength. The components were separated using a 4.6 ID×100mm, 3µm, Inertsil ODS-3 column. The injection volume was 10µL. The flow rate was 1mL/min. Mobile phase A included a 0.1% formic acid solution in water, whereas mobile phase B had 0.1% formic acid in acetonitrile. The LC system was connected to Waters Micromass ZQ, and the software used was Mass Lynx. With the following settings, the mass spectrometer is run in electrospray ionisation mode: Source temperature: 140°C, capillary voltage: 3 kV°C, 400°C for dissolution, and 800L/h for gas flow. The mass spectrometer is configured to scan the mass range between 100 and 1000 m/z. Individual components were identified by their retention times and m/z ratios.

2.13 Molecular Docking

2.13.1 Protein Preparation

The crystal structure of the protein Mushroom Tyrosinase enzyme (PDB ID: 2Y9W) was downloaded from the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB) (http://www.rcsb.org/). It is a hetero-2-mer, X-ray crystallographic structure with a sequence length of 391 amino acids. All water molecules and heteroatoms were removed, polar hydrogens and Kollman charges were added, and the structure was converted to Protein Data Bank Partial Charge and Atom Type (PDBQT) using AutoDock tools.

2.13.2 Ligand Preparation

The three-dimensional structure of the EGR (Ethyl gallate) (PubChem CID: 13250), gallic acid (PubChem CID: 370) and syringic acid (PubChem CID: 10742) were retrieved from the PubChem database. The ligand structures were retrieved in SDF format, energy-minimised, and converted to PDBQT files by assigning Gasteiger charges using AutoDock tools.

2.13.3 Determination of Active Site

Ligands can bind more efficiently to the active site of the protein. The active site of the protein was identified using CASTp. The PDB ID of the protein was submitted to this tool, and active site residues were noted[28].

2.13.4 Docking

Molecular docking was carried out using AutoDock 4.2.6. The binding site was defined by placing a grid box around the active-site residues identified from CASTp. The grid box was centred at coordinates x = 9.733, y = 37.104, and z = 67.537. Grid dimensions of 80 × 78 × 94 points along the x, y, and z axes, respectively, were selected. A total of 100 docking poses were generated for each ligand by running AutoGrid and AutoDock with the specified parameters. Upon successful completion, a .dlg file was generated, containing the binding energy values for each run. The results were analysed, and the final protein–ligand complexes were saved in PDBQT format[29].

2.13.5 Visualisation

PyMOL 2.3 (The PyMOL molecular graphics system, Version 2.3 Schrödinger, LLC) and Discovery Studio 3.5. were used to visualise and study the two-dimensional and three-dimensional structure of the protein-ligand complexes.

2.14 Statistical Analysis

All experiments were conducted in triplicate (n=3). The data were recorded, analysed, and presented as mean ± standard deviation. Statistical analysis was performed using a two-way Analysis of Variance (ANOVA) and a post-hoc test (Fischer's Least Significant Difference test), wherever applicable. A p-value of <0.05 was judged statistically significant. Statistical analysis was performed using GRAPES software[30].

3. Results and Discussions

3.1 Extraction Yield

The current research on the seed kernel of *M. indica* indicates that the aqueous extract achieved a higher extraction yield of 13.3%, while the ethanolic extract yielded a lower extraction rate of 12.1% (Table 2). Previous studies reported that the colour of sun-dried Mango seed kernel ethanolic and aqueous extracts was darker than that of oven-dried mango seed kernel extracts, and ethanolic and aqueous extracts of oven-dried seed kernels showed higher extraction yield of 3.19% and 3.83%, respectively, compared to sun-dried mango seed kernel extracts. The colour of sun-dried and oven-dried mango seed kernel ethanolic and aqueous extracts was yellow and dark brown, respectively. The colour and extraction yield of extracts varied depending on the drying conditions and extraction solvent[10]. Extraction of yield of seed kernels of three Sri Lankan varieties, Willard, Karuthacolomban and Vellaicolomban was 6.83%, 4.98% and 4.34% respectively[18]. The extraction yield of fractions of Thai Kaew and Choke-Anan mango cultivars seed kernel extracts obtained from Sephadex LH-20 column chromatography ranged from 6.41–17.11 and 9.49–27.90%, respectively[8]. The extraction yield of the seed kernel of the Kent cultivar of mango was found to be 12.72%[31]. The extraction yield of alcohol and aqueous extracts was found to be 18% and 21% respectively[32].

3.2 Phytochemical Analysis

In the present study, the ethanolic extract of *M. indica* L. seed kernel showed the presence of flavonoids, cardiac glycosides, alkaloids, carbohydrates, phenolics, proteins, quinones, resins, tannins, and terpenoids, and aqueous extract showed the presence of carbohydrates, cardiac glycosides, flavonoids, phenols, proteins, quinones, tannins and terpenoids (Table 3). Earlier studies have reported that the ethanolic extract of seed kernels revealed the presence of phytosterols, alkaloids, carbohydrates, saponins, fixed oils and fats, resins, phenols, tannins, flavonoids, proteins and amino acids[5]. The ethanolic extract of the *M. indica* seed kernel shows the presence of flavonoids, saponins, tannins, lignin, glycosides, cardiac glycosides, proteins, amino acids and phenolic compounds. The aqueous extract shows the presence of alkaloids, flavonoids, saponins, lignin,

Table 2. Extraction yield and colour of the ethanolic and aqueous extracts of *M. indica* seed kernel

Extracts	Extraction Yield (%)	Colour and Texture
Ethanolic extract	12.1	Mustard yellow semisolid
Aqueous extracts	13.3	Dark brown semisolid

glycosides, cardiac glycosides, proteins, carbohydrates, amino acids and phenolic compounds. The kernel powder revealed the presence of alkaloids, terpenoids, flavonoids, saponins, tannins, lignin, fat and oil, glycosides, cardiac glycosides, proteins, carbohydrates, amino acids, and phenolic compounds[32].

3.3 Proximate Analysis

In the present investigation, the moisture and ash content of *M. indica* seed kernel powder were found to be 6.66±0.94% and 7.16±1.8%, respectively. The low moisture content suggests that the seed kernel powder has good storage stability and a lower risk of microbial growth if stored for long periods. The ash content reflects that the total mineral content may contain a considerable amount of inorganic minerals, which contribute to its potential nutritional value. Prior research indicated that sun-dried mango seed kernel had a final moisture content of 9.81 ± 0.34% (dry weight basis). The moisture content of the sun-dried and oven-dried mango seed kernel extracts ranged from 4.13-4.23% and 3.11-3.15%[10]. Moisture content of 8.39% and ash content of 2.77% in *Mangifera haden* seeds[7]. The moisture content and ash content of 5.9% and 2.43% in *M. indica* seed kernels[2]. The seed kernels of four mango varieties (Apple, Ngowe, Kent and Sabine) had a moisture content which ranged from 5.70%-7.94% and ash content from 1.78%-2.89%[33]. The moisture content and ash content of mango seed kernel powder were found to be 4.32±0.10% and 2.59±0.35% respectively[34].

3.4 Quantitative Estimation of Phytochemical Constituents

The quantitative phytochemical analysis of *M. indica* L. seed kernel ethanolic and aqueous extracts for carbohydrates, reducing sugar, proteins, phenolics, flavonoids and tannins is given in Figure 2. The total carbohydrate content of ethanolic and aqueous seed kernel extracts was evaluated by using glucose as a standard. Among the extracts, the ethanolic extract showed the highest amount of carbohydrates with 680±1.15mg/g and the lowest amount was observed in the aqueous extract, which was 621±1.0 mg/g. Because of the increased amount of carbohydrates, mango seed kernels can be a good source of energy and nutrition. Earlier research has demonstrated that *M. indica* seed kernels contained 0.049mg/g of carbohydrates[32]. *Mangifera haden* seeds had the carbohydrate content of 625.5mg/g[7]. The seed kernels of four mango varieties (Apple, Ngowe, Kent and Sabine) had a carbohydrate content ranging from 728.6 to 759.2mg/g[33]. The *M. indica* seed kernels contained 761.4mg/g carbohydrate content[2]. The experimental values for carbohydrate content in the mango seed kernels showed a strong correlation and were comparable to those observed in the seed kernels of other cultivars, which indicates

Table 3. Phytochemical analysis of ethanolic and aqueous extracts of *M. indica* seed kernels

Phytochemicals	Qualitative Tests	Ethanolic Extract*	Aqueous Extract*
Alkaloids	Mayer's test	+	-
	Wagner's test	+	-
Carbohydrates	Molisch's test	+	+
	Benedict's test	+	+
Anthranal glycosides	Modified Bontrager's test	-	-
Cardiac glycosides	Keller-Killiani test	+	+
Flavonoids	Alkaline Reagent test	+	+
Phenol derivatives	Ferric chloride test	+	+
Phytosterols	Acetic anhydride test	-	-
Proteins	Xanthoproteic test	+	+
Quinones	Sulphuric acid test	+	+
Resins	Acetone-water test	+	-
Tannins	Lead acetate test	+	+
Terpenoids	Salkowski's test	+	+

*'+' indicates present and '-' indicates absent

that the carbohydrate composition and accumulation patterns in the kernels are relatively conserved across the tested mango cultivars, reflecting similar metabolic behaviour with respect to starch and /or soluble sugar deposition during seed development.

Total reducing sugar in ethanolic and aqueous extracts of *M. indica* seed kernels was estimated using glucose as a standard. Aqueous extract showed maximum concentration of reducing sugar, which was 49.8±0.72 mg/g and the minimum concentration was observed in ethanolic extract with 37.6±1.24 mg/g. The presence of a lower amount of reducing sugars, such as monosaccharides (glucose), than the total carbohydrates in mango seed kernel makes it ideal for maintaining an optimum blood sugar level.

Total protein contents in the ethanolic and aqueous extracts of *M. indica* seed kernels were estimated using Bovine Serum Albumin (BSA) as a standard. The highest amount of protein was observed in seed kernel ethanolic extract with 167±1.7 mg/g and the lowest in seed aqueous extract with 121.4±0.69 mg/g. The *M. indica* seed kernels contained 0.0336mg/g of protein[32]. The *M. haden* seeds had crude protein content of 48.2mg/g[7]. Both the extracts exhibited significantly higher protein content compared to other cultivars. This suggests that the mango seed kernels of this cultivar are rich in storage of proteins, which may enhance their nutritional quality for use in protein-rich food formulations.

The TPC in the ethanolic and aqueous extracts of *M. indica* L. seed kernels were estimated using gallic acid as a standard. Seed kernel ethanolic extract had the highest amount of phenolic content of 5.33±0.81mg GAE/g compared to aqueous extract, which was 4.21±0.0mg GAE/g. Previous findings suggested that the TPC of sun-dried mango seed kernel ethanolic and aqueous extracts were 89.92 ± 0.23 mg TAE/g and 68.1±0.13 mg TAE/g, respectively, and oven-dried mango seed kernel ethanolic and aqueous extracts were 53.7± 0.54 mg TAE/g and 44.5± 0.36 mg TAE/g and the results were expressed as tannic acid equivalents[10]. When compared to the phenolic content of the present study, the values were comparatively lower. The TPC of seed kernel of three mango cultivars: Willard, Vellaicolomban and Karuthacolomban had a phenolic content of 270.56±4.89mg GAE/g, 132.95±3.59mg GAE/g and 187.63±11.18 mg GAE/g respectively[18]. The total polyphenols of four mango fruit varieties (Apple, Kent, Ngowe and Sabine) seed kernel extracts ranged from 68.71 to 72.05 mg GAE/g[33]. Both mango seed kernel extracts exhibited lower phenolic content, which depicts that this cultivar accumulates fewer phenolic compounds, such as flavonoids and tannins, in its kernels, which is responsible for their antioxidant potential.

The TFC in the ethanolic and aqueous extracts of *M. indica* seed kernels were estimated using Rutin as a standard. The maximum flavonoid concentration was found in the seed kernel ethanolic extract (5.33±0.81 mg RE/g) compared to aqueous extract (85.3±1.4mg RE/g). The results were expressed in milligrams Rutin Equivalents per gram (mg RE/g). The TFC of seed kernel of three mango cultivars: Willard, Vellaicolomban and Karuthacolomban had a flavonoid content of 108.07±16.53 mg QE/g, 98.34±11.60 mg QE/g and 110.11±7.22 mg QE/g, respectively, and the results were expressed in Quercetin Equivalents per gram (QE/g)[18]. Previous study showed that the mango seed kernel had a flavonoid content of 0.00129 mg/g[32]. Both extracts showed lower flavonoid content compared to seed kernels of the other cultivars, reflecting reduced levels of flavonoids in this particular variety.

Total tannin contents in the ethanolic and aqueous extracts of *M. indica* L. seed kernels were estimated using tannic acid as a standard. Ethanolic extract had the highest amount of tannin content of 193±1.54mg/g compared to aqueous extract, which was 67.33±0.94mg/g. Prior research showed that seed kernels of mango cultivar *Chausa* and *Dusheri* had a tannin content of 1.9mg/g and 4.4mg/g respectively[35]. *M. indica* L. seed kernel had a tannin content of 0.00022mg/g [32]. The results indicate that both extracts contain appreciable levels of tannins. This reinforces the potential of mango seed kernel extracts as a good source of natural tannins for applications in food and nutraceutical systems. This suggests that ethanol is a more efficient solvent for extracting tannins from mango seed kernels, due to its better solubilising capacity of polyphenols and tannins present in mango seed kernels.

3.5 Determination of Anti-tyrosinase Activity

The tyrosinase inhibition activity of ethanolic and aqueous extracts of *M. indica* seed kernel was

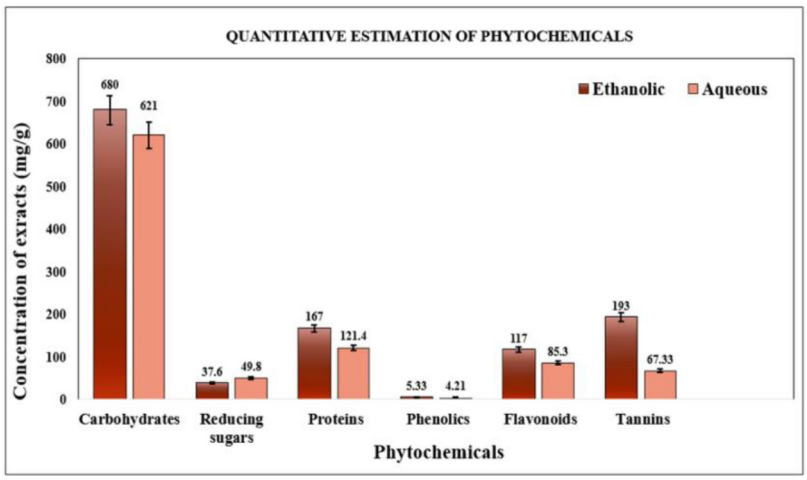


Figure 2. Quantitative estimation of phytochemicals in ethanolic and aqueous extracts.

determined by using Kojic acid as a standard, as shown in Figure 3(A). The ethanolic extract showed the highest inhibition of 53.32±0.41%, and the aqueous extract showed the lowest inhibition of 38.83±1.06% at the highest concentration (500µg/mL) of extracts. The IC_{50} values of ethanolic and aqueous extracts were 389.21±1.6µg/mL and 695.30±1.9µg/mL, respectively, and were comparatively higher than the IC_{50} of standard kojic acid, which was 330.7±1.4µg/mL. The ethanolic extract was less effective compared to Kojic acid, but its activity was close to the inhibitory activity of kojic acid. Earlier investigations reported that the IC_{50} of seed kernel ethanolic extract of Fahlun cultivar of mango in anti-tyrosinase activity was 98.63±1.62 µg/mL, and the phenolic principles of mango seed kernel extract: gallic acid, pentagalloylglucoyranose and methyl gallate exhibited IC_{50} of 644±14.0µg/mL,42.65±1.8µg/mL and 62.50±0.5µg/mL respectively[1]. The ethanolic extract of Kaew and Choke-Anan cultivar of *M. indica* prepared by ultrasonic-assisted extraction exhibited IC_{50} of 20.64±0.32µg/mL and 19.86±1.22µg/mL, and IC_{50} value of arbutin was 20.46±0.33µg/mL, which was used as a standard for the assay[36]. The fraction 3 of seed kernel extract of Kaew and Choke-Anan mango cultivar obtained by Sephadex column chromatography had an IC_{50} of 17.10±0.15µg/mL and 15.35±0.63µg/mL, respectively, and Arbutin was used as standard (20.64±0.75µg/mL)[8].

3.5.1 Dose Response Curve

A comparative dose-response analysis of tyrosinase inhibition between ethanolic and aqueous extracts and a standard reference, kojic acid, was done by plotting a semi-logarithmic scale (log_{10} on the x-axis) to linearise the sigmoidal relationship typical of biochemical assays, as shown in Figure 3(B). The tyrosinase inhibition was taken as the response, whereas both extracts and the standard were taken as the dose. While all three substances exhibit dose-dependent inhibitory activity, their kinetics differ significantly. The kojic acid standard shows a steep, high-potency response curve, reaching near-maximal inhibition at 500 µg/mL. In contrast, the ethanolic and aqueous extracts demonstrate a more gradual increase in activity, with the ethanolic extract outperforming the aqueous extract at higher concentrations, suggesting a higher concentration of bioactive phytochemicals in the organic solvent fraction

3.6 Determination of Antioxidant Activity

3.6.1 DPPH Free Radical Scavenging Assay

In the present study, the DPPH radical scavenging activity of ethanolic and aqueous extracts of *M. indica* seed kernels was evaluated by using ascorbic acid as a standard, as given in Figure 4A. As the concentration of extracts was increased, the percentage of radical scavenging activity also increased. Among the extracts, the highest scavenging activity was shown by the ethanolic extract of 95.6±0.1% with an IC_{50} of 8.80±0.6µg/mL and the lowest scavenging activity was shown by the aqueous extract with 74.4±0.32%, and its IC_{50} value was 64.72±0.08µg/mL at the highest concentration of extracts (100µg/mL). These values were compared with the standard ascorbic acid,

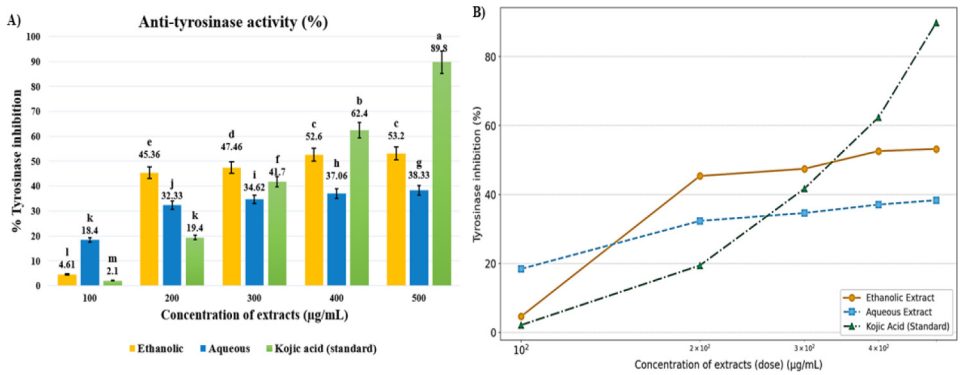


Figure 3. **(A).** Anti-tyrosinase activity in *M. indica* seed kernel extracts. Values are expressed as mean ± SD of the three replicates (n=3). Different letters above bars indicate statistically significant differences between treatment combinations determined via ANOVA followed by post-hoc Least Significant Difference (LSD) (p≤ 0.05). **(B).** Dose -response curve showing comparative tyrosinase inhibitory activity of ethanolic and aqueous extracts and kojic acid standard. Data points represent mean inhibition (%) across a concentration range of 100-500µg/mL. The x-axis is presented on a logarithmic scale to illustrate the dose-dependent kinetics.

which exhibited an IC_{50} of 2.94±1.8µg/mL, and both extracts showed less scavenging activity than the standard. DPPH radical scavenging activity increased with concentration for all samples, approaching a plateau at higher doses. Across all concentrations, the aqueous extract showed significantly lower scavenging activity than the ethanolic extract and ascorbic acid, as indicated by distinct letters ($p<0.05$). The ethanolic extract was comparable to ascorbic acid at lower concentrations (20-40µg/mL) and statistically indistinguishable from ascorbic acid at 100 µg/mL, where both reached approximately 95–97% scavenging activity. The ethyl acetate extract of the seed kernel of *Karuthacolomban*, *Vellaicolomban* and *Willard* mango cultivar exhibited scavenging activity (IC_{50}) of 7.73±0.26µg/mL,13.68±0.31µg/mL and 12.23±0.18µg/mL[18]. The mean percentage scavenging ability of mango kernel extracts of Apple, Sabine, Ngowe and Kent cultivar at the concentration of 20 mg/mL was 92.22%[33]. The crude ethanolic mango seed kernel extract of *Kaew* and *Choke-Anan* cultivar exhibited DPPH scavenging activity of 10.22±0.05µg/mL and 7.17±0.03µg/mL, respectively. The fraction 3 obtained by column chromatography showed DPPH antioxidant capacity of 6.63±0.08µg/mL and 4.74±0.14µg/mL[8]. The crude extract of *M. haden* seeds showed scavenging activity of 94.65±0.83% and exhibited an IC_{50} of 1.03 µg/mL, and the methanolic extract showed scavenging activity of 95.85±3.04% with an IC_{50} of 1.08µg/mL at the concentration of 500µg/mL[7].

3.6.2 Reducing Power Assay

In the present research, the reducing power of ethanolic and aqueous extracts of *M. indica* seed kernels was determined by using Ascorbic acid as a standard, as given in Figure 4B. As the concentration of extracts was increased, the absorbance values increased, and a higher absorbance value indicates a stronger reducing power of the extracts. Among the extracts, the highest reducing power was shown by the ethanolic extract with an absorbance of 1.82±0.03 and the lowest was shown by the aqueous extract with an absorbance of 0.562±0.0 at the concentration of 100µg/mL. These values were compared with the standard Ascorbic acid, which exhibited an absorbance of 1.89, and both extracts showed less ferric reducing power than the standard. At lower concentrations (20–60 µg/mL), the aqueous extract showed significantly higher reducing power than the ethanolic extract and ascorbic acid, as reflected by non-overlapping letter groupings above the bars. At higher concentrations (80–100 µg/mL), ascorbic acid exhibited significantly greater reducing power than both extracts, whereas the ethanolic extract consistently showed the lowest activity at all concentrations. The methanol and ethyl acetate extract of *M. haden* seeds showed absorbance at 1.61±0.06, 1.50±0.04 and 1.58±0.07, respectively, at the concentration of 500µg/mL[7].

3.6.3 Phosphomolybdenum Assay or Total Antioxidant Capacity (TAC)

The TAC of ethanolic and aqueous extracts of *M. indica* seed kernels were estimated by using Ascorbic acid as

a standard, as given in Figure 4C. As the concentration of extracts was increased, the absorbance values increased, and a higher absorbance value indicates a stronger antioxidant capacity of the extracts. Among the extracts, the highest total antioxidant capacity was shown by the ethanolic extract with an absorbance of 0.481±0.001 and the lowest was shown by the aqueous extract with an absorbance of 0.396±0.004 at the concentration of 500µg/mL. These values were

compared with the standard Ascorbic acid, which exhibited an absorbance of 1.89, and both extracts showed less total antioxidant capacity than the standard. Ethanolic extract, aqueous extract, and the standard ascorbic acid demonstrate a clear, concentration-dependent increase in antioxidant activity, as measured by the optical density (OD) at 695nm. The highest absorbance was shown by ethyl acetate with 0.140±0.013, followed by methanol extract with 0.028±0.003 at the concentration of 500µg/mL[7].

3.7 Determination of Fat Content and Free Fatty Acids (Acid Value) of Kernel Oil

The extraction of fat from mango seed kernel was carried out by the Soxhlet extraction method. The petroleum ether was used as an extraction solvent. The fat or oil extracted from the mango seed kernel was yellowish in colour (Figure 1E). The fat yield was found to be 12.4%. The acid value of kernel oil in the present study was found to be 4.6± 0.3mg KOH/g oil. Earlier studies reported that the acid value of petroleum ether extract, hexane extract and ethanol extract was 0.15±0.08, 0.10±0.01 and 27.55±0.55 mg KOH/g oil, respectively. They suggested that mango seed kernel oil with low acid value can be stored with less deterioration[11]. The highest yield (9.88%) was obtained for kernel oil of *Dasehri* cultivar of mango, and the lowest (6.33%) was obtained for kernel oil of *Sindhri* cultivar of mango. Free fatty acid values of the tested mango cultivars *Laal Badshah*, *Sindhri*, *Safed Chaunsa*, *Dasehri*, *Langra*, *Fajri* and *Anwar Ratul* seed kernel oils varied from 0.50 to 3.9 mg/g, while the percentage acid values ranged from 1.00 to 7.70, with the *Fajri* cultivar showing the lowest values and the *Anwar Ratul* cultivar showing the highest[37].

3.8 Antibacterial Activity

The antibacterial activity of ethanolic and aqueous extract of *M. indica* seed kernels, Streptomycin

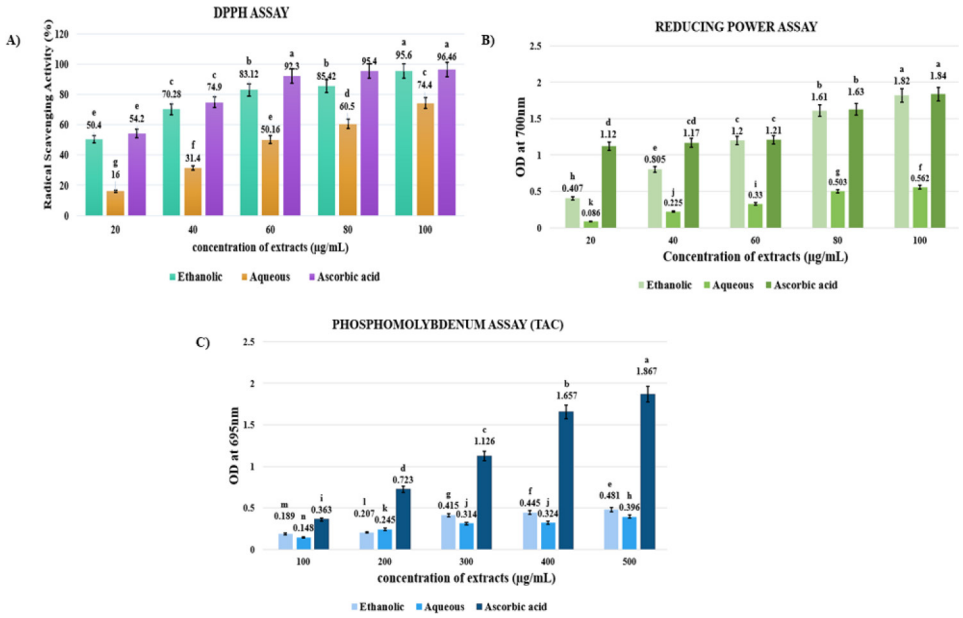


Figure 4. **(A).** DPPH radical scavenging activity in *M. indica* seed kernel extracts. **(B).** Reducing the power of *M. indica* seed kernel extracts. **(C).** Phosphomolybdenum assay in *M. indica* seed kernel extracts. Values are expressed as mean ± SD of the three replicates (n=3). Different letters above bars indicate statistically significant differences between treatment combinations, determined via two-way Analysis of Variance (ANOVA) followed by post hoc Least Significant Difference (LSD) tests ($p \leq 0.05$).

(5mg/mL) as positive control and ethanol, distilled water as negative control was tested against *K. pneumoniae* (Figure 5A), *S. aureus* (Figure 5B) and *E. coli* (Figure 5C) by using agar well diffusion method. As the concentration of extracts was increased, the antibacterial capacity of the extracts also increased. The aqueous extract showed slightly more zone of inhibition than the ethanolic extracts against all three bacterial strains, but exhibited less zone of inhibition than the positive control. At the highest concentration of 5mg/mL, aqueous extract showed the highest antibacterial activity with a mean zone of inhibition of 11.6±0.57mm, 12±0.4mm and 11.6±0.6mm for *E. coli, S. aureus* and *K. pneumoniae,* respectively. Ethanolic extract showed slightly lower antibacterial property with a mean zone of inhibition of 7.6±0.5mm, 10±0.0mm and 7.5±0.5mm for *E.coli*, *S. aureus* and *K. pneumoniae,* respectively, at the highest concentration of 5mg/mL. Distilled water (negative control) produced no inhibition zones against any test organism. Ethanol, also used as a negative control, produced small inhibition zones of 1.0±0.2mm, 0.9±0.33mm and 1.0±0.3mm against *E. coli*, *S. aureus* and *K. pneumoniae,* respectively. These values were subtracted from the inhibition zones of the corresponding ethanolic extracts. Antibacterial activity of the ethanolic and aqueous extracts against *E. coli*, *S. aureus* and *K. pneumoniae* was analysed using a two-way ANOVA with extract type and concentration as fixed factors, followed by a post-hoc Least Significant Difference (LSD) test ($p<0.05$). Increasing concentration significantly increased inhibition zone diameters for both extracts across all organisms, and aqueous extracts generally produced larger zones than ethanolic extracts. At all concentrations, the positive control produced significantly larger inhibition zones than either of the extracts, and LSD pairwise comparisons showed that, particularly for *K. pneumoniae* and *S. aureus*, the aqueous extract exhibited significantly higher activity than the ethanolic extract at most concentrations, whereas against *E. coli*, both extracts were less active overall, though inhibition zones still increased significantly with concentration. The mango seed ethanolic extract showed a zone of inhibition of 18mm and 20mm for *E. coli* and *S. aureus,* respectively, whereas the mango

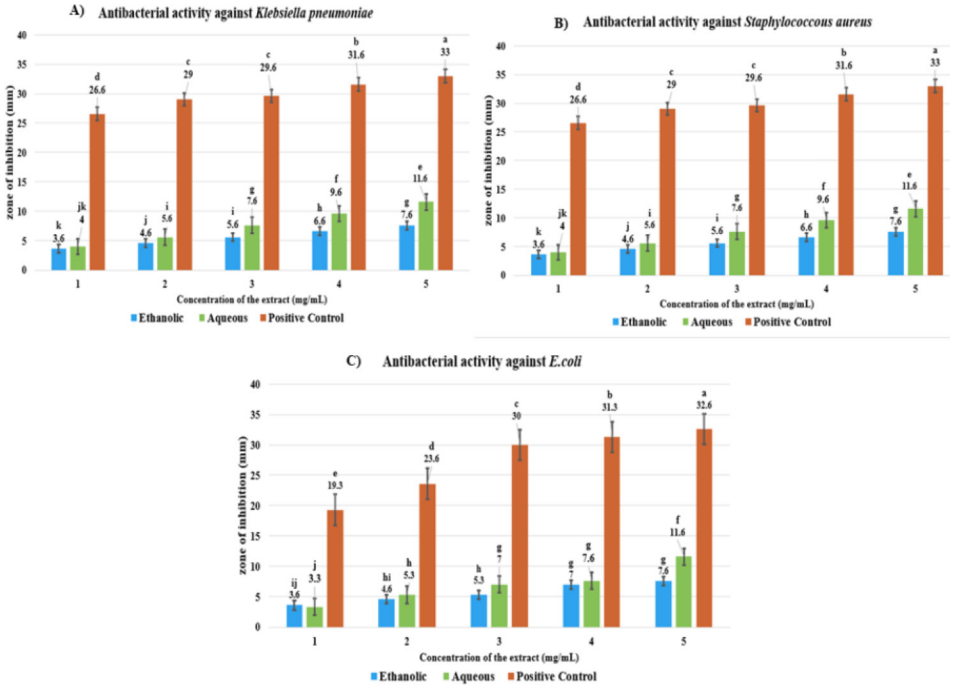


Figure 5. Antibacterial activity of *M. indica* seed kernel extract against **(A).** *Klebsiella pneumoniae,* **(B).** *Staphylococcus aureus* and **(C).** *Escherichia coli.* Values are expressed as mean ± SD of the three replicates (n=3). Different superscript letters above the bars represent statistically significant differences among treatment combinations, as assessed by two-way analysis of variance (ANOVA) followed by post-hoc Least Significant Difference (LSD) test ($p \leq 0.05$).

Table 4. Antibacterial activity of kernel butter formulation of *M. indica* seed kernel on bacterial strains

Volume of butter in the well (µL)	Zone of inhibition (mm)*	
	Escherichia coli	*Staphylococcus aureus*
60	7±0.5	4±0.4
80	9±0.51	6±0.5
100	12±0.15	7±0.6

* Mean ± SD, N=3

seed acetone extract showed a zone of inhibition of 18mm for both *E. coli and S. aureus*[26]. The mango seed kernel ethanolic extract of cultivars Blackgold, Waterlily and Lemak showed zone of inhibition of 17mm,15mm and 20mm for *S. aureus,* respectively and 14mm, 15mm and 16mm for *E. coli,* respectively, at the concentration of 0.10M[38].

3.9 Antibacterial Activity of Kernel Butter Formulation

The mango seed kernel butter was prepared from mango kernel pieces (Figure 1F) and virgin coconut oil and stored at 4ºC for further use. To prove its antibacterial property by agar well diffusion method, 60, 80, and 100µL of butter formulation was loaded into wells in nutrient agar plates spread with bacterial strains. The antibacterial activity of the kernel butter formulation is given in Table 4. Kernel butter formulation showed the highest zone of inhibition of 12±0.15mm and 7±0.6mm against Gram positive *S. aureus* and Gram negative *E. coli,* respectively, at the highest volume of 100µL, which was comparatively lower than the positive control. Streptomycin (5mg/mL) was used as a positive control, and coconut oil was used as a negative control was tested against *S. aureus* and *E. coli* by using the agar well diffusion method. When 20µL of kernel oil was loaded in agar wells, it showed a zone of inhibition of 20mm against *Proteus vulgaris* (Gram-negative) and *K. pneumoniae* (Gram-negative) bacterial strains[39].

3.10 LC-MS Analysis of Ethanolic Extract and Identification of Bioactive Compounds

LC-MS analysis of the ethanolic extract of mango kernel was carried out using an HPLC model Waters 2965 (Conquer Scientific, USA) furnished with two solvent delivery modules, a thermoautosampler, a column oven, a diode array detector, and a degasser. Ethanolic extract exhibited better results in enzymatic studies, therefore analysed in order to identify the presence of key compounds.

Table 5. Characterisation of major bioactive compounds present in the ethanolic extract

Retention time (minutes)	m/z ratio	Bioactive compounds
1.12	118-144	Small polar phenolics or sugar fragments
1.82	179	Caffeic acid
2.22	169.24	Gallic acid
2.3	197.23	Syringic acid
6.8	197	Ethyl gallate

In the negative ion mode of the spectra (Figures 6A and B), the prominent peak at retention time (RT) of 2.22 min (with maximum area of 45%) may correspond to m/z (mass/charge ratio) of 169.24 for Gallic acid (deprotonated), which is a commonly observed phenol in the mango kernel extracts ($C_7H_6O_5$ MW=170.12 g/mol). Another prominent separation of a phenol at m/z of 179 (Caffeic acid, $C_9H_8O_4$, 180 g/mol, deprotonated) was noted at retention time 1.82 min. The presence of Ethyl gallate with RT 2.21 was noted at m/z of 197. The presence of a fragment of another phenol, Syringic acid, with RT at 2.2-2.3 min was noted at m/z of 197.23 (syringic acid has the molecular weight of $C_9H_{10}O_5$, i.e., 198.17, here it is deprotonated). Other smaller intensity separations were also noted in the negative ion mode with m/z ratios of 243.33, 321.46, 387.55, 393.59 and 470.02, which may correspond to hydrolysed tannins or mon/di/tri galloyl glucose derivatives with overlapping RT at 2.22 min, which is the major area in the spectrum (Table 5). The m/z ratio of 341.55 may indicate the presence of hexose (like sucrose =MW: 342.29 g/mol) or others, which is normally seen in mango kernel extracts (at RT of 1.12 to 1.8 min).

In the positive ion mode of the spectra (Figures 6A and C), there may be the presence of small molecular weight phenol fragments, small organic acids/ amino acid derivatives (with m/z of 118-199), either protonated or sodium adducts. Additionally, glycosylated adducts of

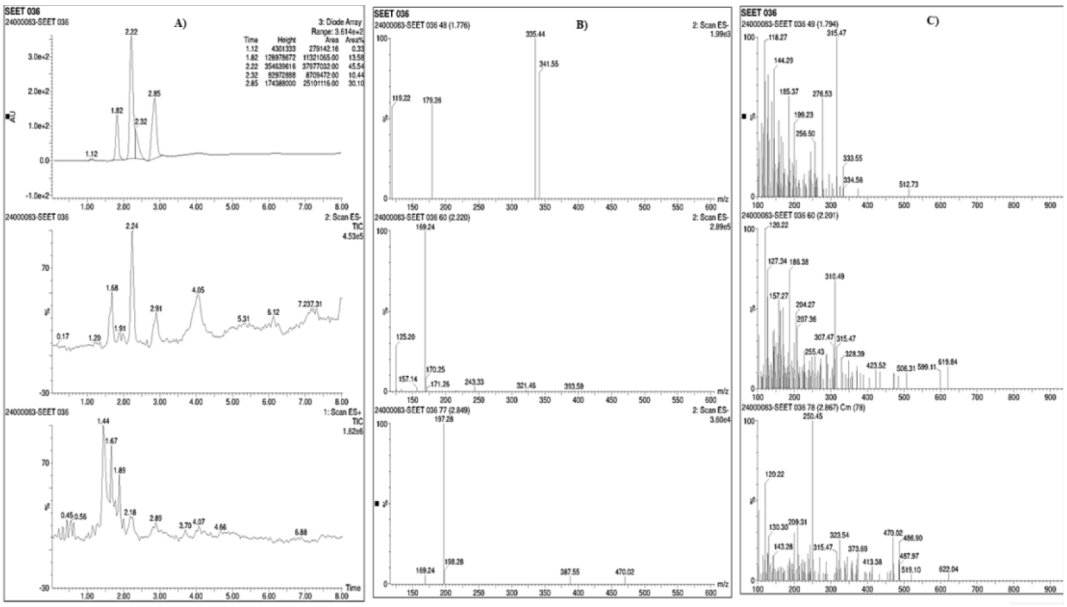


Figure 6. **(A).** LC chromatogram with retention time and area of mango seed kernel ethanolic extract. **(B).** Negative ion mode of LC-MS of mango kernel ethanolic extract. **(C).** Positive ion mode of LC-MS of mango kernel ethanolic extract.

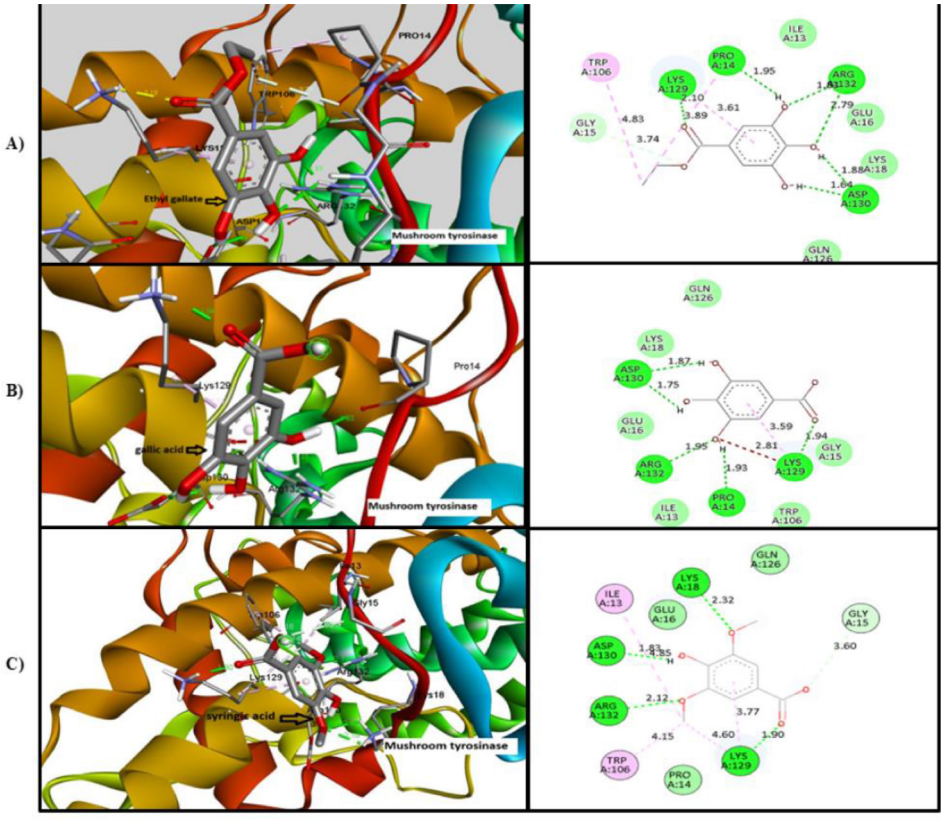


Figure 7. Docked complexes: **(A).** Ethyl gallate-Mush tyrosinase, **(B).** Gallic acid-Mushroom tyrosinase, **(C).** Syringic acid-Mushroom tyrosinase.

either phenols or monoacylglycerols may be observed at m/z of 307-333. The separation of diacyl glycerol adducts/ larger galloyl oligomers may be noted at m/z of 413-523, and the presence of larger tannins may be noted at (m/z of

599.11-622.04). The separation of mostly lipids and larger adducts is noted in the positive ion mode[40-42].

3.11 Molecular Docking

As per the literature and LC-MS chromatogram, three bioactive compounds were chosen for docking with the mushroom tyrosinase enzyme. Ethyl Gallate (Figure 7A), Gallic Acid (Figure 7B), Syringic Acid (Figure 7C).

Among the docked complexes, Ethyl gallate exhibited the strongest binding affinity with Mushroom Tyrosinase (−6.14 kcal/mol), followed by gallic acid (−6.10 kcal/mol). Syringic acid showed a moderately lower affinity (−5.54 kcal/mol). The interaction of the three ligands revealed a highly conserved binding pattern within the active site. As shown in the figures, Lys129, Asp130, and Arg132 consistently participate in hydrogen bonding with all three ligands, indicating their central role in stabilising ligand binding. Pro14 contributes to hydrogen bond formation only in the Ethyl gallate and gallic acid complexes, while Lys18 interacts only with syringic acid, suggesting a slight variation in ligand positioning within the pocket. Trp106 interacts hydrophobically with both Ethyl gallate and syringic acid, whereas Ile13 interacts only with syringic acid to form a hydrophobic bond. Additionally, residues such as Ile13, Gly15, Glu16, Lys18, and Gln126 were involved in van der Waals interactions, providing further non-specific stabilisation across the complexes. Docking analysis correlates with the *in vitro* anti-tyrosinase activity by demonstrating that the above-stated bioactive compounds bind within the mushroom tyrosinase active site through multiple hydrogen bonds and hydrophobic interactions with key amino acid residues and prevent substrate access. This disturbs the enzymatic oxidation of L-DOPA to dopaquinone. These interactions likely contribute to the concentration-dependent inhibition observed experimentally, supporting the role of these phenolic compounds as the major bioactive constituents of the ethanolic extract. The findings suggest that these bioactive compounds present in mango seed kernel can bind the active site of mushroom tyrosinase enzyme and thereby inhibit its activity in the melanin synthesis pathway. Mango seed kernels may serve as an alternative medicine for skin hyperpigmentation, where the tyrosinase activity is elevated and for addressing scars and dark spots within the cosmetic industry. Mango seed kernels could be beneficial in storage applications by helping to reduce the browning of fruits and vegetables.

4. Conclusion

Mango, a widely appreciated seasonal fruit, is rich in bioactive compounds and antioxidants that contribute to various health benefits. Phytochemical analysis of the ethanolic and aqueous extracts from the seed kernels of the *Bellare* cultivar of *M. indica* L. revealed the presence of bioactive phenolics, flavonoids, tannins, proteins and carbohydrates. Both extracts exhibited strong antioxidant activity, indicating their potential as value-added ingredients in the food and pharmaceutical industries. Notably, the ethanolic seed kernel extract showed significant anti-tyrosinase activity, suggesting its use as a natural tyrosinase inhibitor for addressing skin issues and as a skin lightening agent in cosmetics. The mango seed kernel oil demonstrated a higher yield and lower acid value, making it suitable for prolonged storage. Furthermore, aqueous extract displayed antibacterial activity against common pathogens, with phenolic compounds in the mango seed showing the ability to inhibit microbial growth, thereby addressing various medical and industrial challenges.

5. Acknowledgements

The authors gratefully acknowledge the support and facilities provided by Alva's College (Autonomous), Moodbidri, Mangalore, Karnataka, India, for carrying out this research work. The authors sincerely thank Dr Raghavendra Rao, Professor, and Dr Jayadev K., Associate Professor, PG Department of Biotechnology, Alva's College (Autonomous), Moodbidri, for their continuous support and suggestions throughout the study.

6. References

1. Nithitanakool S, Pithayanukul P, Bavovada R, Saparpakorn P. Molecular docking studies and anti-tyrosinase activity of Thai mango seed kernel extract. Molecules. 2009; 14(1):257-265. https://doi.org/10.3390/molecules14010257 PMid:19136913 PMCid:PMC6254019.
2. Orijajogun J, Batari L, Aguzue O. Chemical composition and phytochemical properties of mango (*Mangifera indica*) seed kernel. Int J Adv Chem. 2014; 2(2):185-187. https://doi.org/10.14419/ijac.v2i2.3549

3. Tam DTT, Nhan TC, Phuong NNM. Antimicrobial activity of phenolic-rich extracts from mango seed kernel on microorganisms. Microbiol Biotechnol Lett. 2023; 51(4):416-424. https://doi.org/10.48022/mbl.2310.10009
4. Ruchika S, Bhat PR, Ravishankar KV. Qualitative and quantitative assessment of wild genotypes of mango (*Mangifera indica* L.) in coastal districts of Karnataka, India. J Hortic Sci. 2024; 18(2):271-275. https://doi.org/10.24154/jhs.v18i2.1769
5. Somkuwar DO, Kamble VA. Phytochemical screening of ethanolic extracts of stem, leaves, flower and seed kernel of *Mangifera indica* L. Int J Pharm Bio Sci. 2013; 4(2):383-389.
6. Yatnatti S, Vijayalakshmi D, Chandru R. Processing and nutritive value of mango seed kernel flour. Curr Res Nutr Food Sci. 2014; 2(3):170-175. https://doi.org/10.12944/CRNFSJ.2.3.10
7. Nwafor MN, Anosike AC, Onodugo CA, Yau M, Babandi A. Antioxidant, phytochemical composition and proximate analysis of *Mangifera haden* seeds. Int J Scholar Res Chem Pharm. 2022; 1(1):11-23. https://doi.org/10.56781/ijsrcp.2022.1.1.0022
8. Namngam C, Boonyuen S, Pinsirodom P. Fractionation, antioxidant and inhibitory activity of Thai mango seed kernel extracts. Czech J Food Sci. 2018; 36(1):8-15. https://doi.org/10.17221/225/2017-CJFS
9. Petrillo A, González-Paramás AM, Era B, Medda R, Pintus F, Santos-Buelga C, Fais A. Tyrosinase inhibition and antioxidant properties of *Asphodelus microcarpus* extracts. BMC Complement Altern Med. 2016; 16(1):453-462. https://doi.org/10.1186/s12906-016-1442-0 PMid:27829416 PMCid:PMC5103440.
10. Maisuthisakul P, Gordon MH. Antioxidant and tyrosinase inhibitory activity of mango seed kernel by product. Food Chem. 2009; 117(2):332-341. https://doi.org/10.1016/j.foodchem.2009.04.010
11. Kittiphoom S, Sutasinee S. Mango seed kernel oil and its physicochemical properties. Int Food Res J. 2013; 20(3):1145-1149.
12. Oudah I. Evaluation of aqueous and ethanolic extraction for coriander seeds, leaves and stems and studying their antibacterial activity. Iraq Natl J Nurs Spec. 2010; 23(1):1-7. https://doi.org/10.58897/injns.v23i1.65
13. Balamurugan V, Fatima S, Velurajan S. A guide to phytochemical analysis. Int J Adv Res Innov Ideas Educ. 2019; 5(1):236-245.
14. DuBois M, Gilles KA, Hamilton JK, Rebers PA, Smith F. Colorimetric method for determination of sugars and related substances. Anal Chem. 1956; 28(3):350-356. https://doi.org/10.1038/168167a0 PMid:14875032.
15. Krishnaveni S, Balasubramanian T, Sadasivam S. Sugar distribution in sweet stalk sorghum. Food Chem. 1984; 15(3):229-232. https://doi.org/10.1016/0308-8146(84)90007-4
16. Miller GL. Use of Dinitrosalycylic acid reagent for determination of reducing sugar. Anal Chem. 1959; 31(3):426-428. https://doi.org/10.1021/ac60147a030
17. Lowry OH, Rosebrough NJ, Farr AL, Randall RJ. Protein measurement with the Folin phenol reagent. J Biol Chem. 1951; 193(1):265-275. https://doi.org/10.1016/S0021-9258(19)52451-6 PMid:14907713 PMCid: PMC11896512.
18. Kuganesan A, Thiripuranathar G, Navaratne AN, Paranagama PA. Antioxidant and anti-inflammatory activities of peels, pulps and seed kernels of three common mango (*Mangifera indica* L.) varieties in Sri Lanka. Int J Pharm Sci Res. 2017; 8(1):70-78. https://doi.org/10.13040/IJPSR.0975-8232.8(1).70-78
19. Phuyal N, Jha PK, Raturi PP, Rajbhandary S. Total phenolic, flavonoid contents, and antioxidant activities of fruit, seed, and bark extracts of *Zanthoxylum armatum*. Sci World J. 2020; 20(2):878-884. https://doi.org/10.1155/2020/8780704 PMid:32256249 PMCid:PMC7102453.
20. Kamtekar S, Keer V, Patil V. Estimation of phenolic content, flavonoid content, antioxidant and alpha amylase inhibitory activity of marketed polyherbal formulation. J Appl Pharm Sci. 2014; 4(9):61-65.
21. Saxena V, Mishra G, Saxena A, Vishwakarma KR. A comparative study on quantitative estimation of tannins in *Terminalia chebula*, *Terminalia bellirica*, *Terminalia arjuna* and *Saraca indica* using spectrophotometer. Asian J Pharm Clin Res. 2013; 6(3):148-149.
22. Shen Z, Wang Y, Guo Z, Tan T, Zhang Y. Novel tyrosinase inhibitory peptide with free radical scavenging ability. J Enzyme Inhib Med Chem. 2019; 34(1):1633-1640. https://doi.org/10.1080/14756366.2019.1661401 PMid:31496313 PMCid:PMC6746264.
23. Nishaa S, Vishnupriya M, Sasikumar JM, Hephzibah PC, Gopalakrishnan VK. Antioxidant activity of ethanolic extract of *Maranta arundinacea* L. tuberous rhizomes. Asian J Pharm Clin Res. 2012; 5(4):85-88.
24. Tariq AL, Reyaz AL. Antioxidant activity of *Camellia sinensis* leaves. Int J Curr Microbiol Appl Sci. 2013; 2(5):40-46.
25. Cox HE, Pearson D. The chemical analysis of foods. New York: Chemical Publishing Co. Inc. 1962; p. 420-421.
26. Ahmed EF. Antimicrobial and antibiofilm activity of mango seeds extract. Iraqi J Sci. 2015; 56(4B):3121-3129.
27. Satheeshan KN, Seema BR, Manjusha AM. Development of virgin coconut oil-based body lotion. Pharma Innov J. 2020; 9(5):96-101.
28. Tian W, Chen C, Lei X, Zhao J, Liang J. CASTp 3.0: Computed atlas of surface topography of proteins. Nucleic Acids Res. 2018; 46(W1):W363-W367. https://doi.org/10.1093/nar/gky473 PMid:29860391 PMCid:PMC6031066.
29. Morris GM, Huey R, Lindstrom W, Sanner MF, Belew RK, Goodsell DS, Olson AJ. AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. J Comput Chem. 2009; 30(16):2785-2791. https://

doi.org/10.1002/jcc.21256 PMid:19399780 PMCid: PMC2760638.
30. Gopinath PP, Parsad R, Joseph B, Adarsh VS. GRAPES: General Rshiny-based analysis platform empowered by statistics [software]. Version 1.0.0. 2020 [cited 2026 Jan 22]. https://www.kaugrapes.com/home https://doi.org/10.5281/zenodo.4923220
31. Roa-Tort A, Meza-Márquez OG, Osorio-Revilla G, Gallardo-Velázquez T, Ramos-Monroy OA. Extraction and microencapsulation of phytochemical compounds from mango peel (*Mangifera indica* L.) var. Kent and assessment of bioaccessibility through *in vitro* digestion. Processes. 2024; 12(1):154-172. https://doi.org/10.3390/pr12010154
32. Rajan S, Surya D, Vijaya P, Prabhu K, Thirunalasundari T. Pharmacognostical and phytochemical studies of *Mangifera indica* seed kernel. J Pharm Res. 2011; 4(11):4272-4275.
33. Mutua JK, Imathiu S, Owino W. Evaluation of the proximate composition, antioxidant potential, and antimicrobial activity of mango seed kernel extracts. Food Sci Nutr. 2017; 5(2):349-357. https://doi.org/10.1002/fsn3.399 PMid:28265370 PMCid:PMC5332260.
34. Dandwate AM, Joshi BH, Dhingani RM. Standardization of hot airdrying parameters and their impact on total phenolics and oil content of mango seed kernel. J Appl Hortic. 2024; 26(1):21-26. https://doi.org/10.37855/jah.2024.v26i01.04
35. Dhingra S, Kapoor AC. Nutritive value of mango seed kernel. J Appl Hort. 1985; 36(8):752-756. https://doi.org/10.1002/jsfa.2740360817
36. Namngam C, Pinsirodom P. Antioxidant properties, selected enzyme inhibition capacities, and a cosmetic cream formulation of Thai mango seed kernel extracts. Trop J Pharm Res. 2017; 16(1):9-10. https://doi.org/10.4314/tjpr.v16i1.3
37. Zahoor S, Anwar F, Qadir R, Soufan W, Sakran M. Physicochemical attributes and antioxidant potential of kernel oils from selected mango varieties. ACS Omega. 2023; 8(25):22613-22622. https://doi.org/10.1021/acsomega.3c01155 PMid:37396275 PMCid:PMC10308537.
38. Mirghani MES, Yosuf F, Kabbashi NA, Vejayan J, Yosuf ZBM. Antibacterial activity of mango kernel extracts. J Appl Sci. 2009; 9(17):3013-3019. https://doi.org/10.3923/jas.2009.3013.3019
39. Mounica MV, Subbiah V. Extraction and characterization of mango seed kernel oil and its antimicrobial activity. Int J Adv Inf Sci Technol. 2014; 21(21):25-29.
40. Lim KJA, Cabajar AA, Lobarbio CFY, Taboada EB, Lacks DJ. Extraction of bioactive compounds from mango (*Mangifera indica* L. var. Carabao) seed kernel with ethanol-water binary solvent systems. J Food Sci Technol. 2019; 56(5):2536-2544. https://doi.org/10.1007/s13197-019-03732-7 PMid:31168135 PMCid:PMC6525705.
41. Alañón ME, Pimentel-Moral S, Arráez-Román D, Segura-Carretero A. HPLC-DAD-Q-ToF-MS profiling of phenolic compounds from mango (*Mangifera indica* L.) seed kernel of different cultivars and maturation stages as a preliminary approach to determine functional and nutraceutical value. Food Chem. 2021; 337:127764. https://doi.org/10.1016/j.foodchem.2020.127764 PMid:32795857.
42. García-Mahecha M, Soto-Valdez H, Carvajal-Millan E, Madera-Santana TJ, Lomelí-Ramírez MG, Colín-Chávez C. Bioactive compounds in extracts from the agro-industrial waste of mango. Molecules. 2023; 28(1):458. https://doi.org/10.3390/molecules28010458 PMid:36615647 PMCid:PMC9823791.

Author Contribution

Conceptualisation, Megha D. Sawanth and Rama Bhat P.; Methodology, Megha D Sawanth; Investigation, Megha D. Sawanth.; Resources, Megha D Sawanth and Rama Bhat P.; Molecular docking, Thejaswi Bhat and Megha D Sawanth.; Writing—original draft preparation, Megha D Sawanth; Writing—review and editing, Megha D Sawanth.; supervision, Rama Bhat P. All authors have read and agreed to the published version of the manuscript.