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Original Article

Pharmacognostic, Nutritional, Antioxidant, Anti-diarrheal and Vasoconstrictive Potential of *Solanum melongena* L. Leaf and Stem: *In vitro* and *in silico* Study

Asad Saleem Sial[1], Muhammad Mohtasheemul-Hasan[1], Khizar Abbas[2,*], Ambreen Aleem[3], Jahanzeb Mudassir[4], Iqra Islam[2], Imran Ahmad[5], Rizwana Manzoor[1], Usman Javaid[6], Adeel Usman[1], Syed Zia Ul Hasnain[1]

[1]Department of Pharmacognosy, Faculty of Pharmacy and Pharmaceutical Sciences, University of Karachi, Karachi, PAKISTAN.
[2]Department of Pharmacognosy, Faculty of Pharmacy, Bahauddin Zakaria University, Multan, PAKISTAN.
[3]Department of Pharmacology, Faculty of Pharmacy, Bahauddin Zakaria University, Multan, PAKISTAN.
[4]Department of Pharmaceutics, Faculty of Pharmacy, Bahauddin Zakaria University, Multan, PAKISTAN.
[5]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Bahauddin Zakaria University, Multan, PAKISTAN.
[6]Department of Pharmacology, Faculty of Pharmacy and Pharmaceutical Sciences, University of Karachi, Karachi, PAKISTAN.

ABSTRACT

Background/Purpose: Eggplant is one of the top ten vegetables with antioxidant capacity, traditionally used to cure gastrointestinal, cardiac, diabetic, and neurotoxic conditions. The purpose of the research is to carry out the Pharmacognostic, antioxidant, antidiarrheal and vasoconstrictive potential of the leaf and stem of *Solanum melongena* L. **Materials and Methods:** Pharmacognostic studies were carried out by organoleptic, physical, fluorescence and phytochemical analysis. Nutritional value was found by mineral analysis, and total phenolics and flavonoids were determined. Antioxidant potential was assessed using TAC, total reducing power, DPPH, H_2O_2 and FRAP methods. Isolated jejunum and aorta were used to determine antidiarrheal and vasoconstrictive potential, respectively, while network pharmacology and molecular docking were performed on important genes. **Results:** Phytochemical investigation showed diverse constituents; mineral analysis showed the presence of Ca, K, Cu, Mg, Na, and Zn. Leaf and stem possess appreciable phenolics, flavonoids, and strong antioxidant potential. Isolated jejunum demonstrated a spasmogenic effect from the leaf and a spasmolytic effect from the stem, while both exhibited contractile activity on isolated aorta. Hub genes were identified, with the top 3 showing promising binding with compounds. **Conclusion:** It is concluded that the leaf and stem of *Solanum melongena* L. possess considerable quantities of nutrients and diverse phytochemicals responsible for antidiarrheal and vasoconstrictive effects.

Keywords: Molecular docking, Spasmogenic, Standardization.

Correspondence:
Dr. Khizar Abbas
Associate Professor, Department of Pharmacognosy, Faculty of Pharmacy, Bahauddin Zakariya University, Multan, PAKISTAN.
Email: khizarabbas@bzu.edu.pk

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INTRODUCTION

Herbal remedies and pharmaceuticals have been effective in the treatment of several diseases. Despite excess of literature on their medicinal properties, there are no standard techniques for characterization of plant materials. Standardization of medicinal plants ensures consistency and therapeutic efficacy. Herbal goods are examined for identifying characteristics, effectiveness, and the purity of the extracts present, because it is vital to evaluate their therapeutic efficacy (Sharma *et al.*, 2021). *Solanum melongena* L. is a widespread plant around the world, sometimes called as eggplant and aubergine, predominantly in Asian nations, the Horn of Africa, and Mediterranean region. *Solanum melongena* L. is an commercial pinnacle plant of the family Solanaceae which contains seventy five genera and two thousand plus species and are grown mainly for food and medicinal purposes (Solanke & Tawar, 2019). Eggplants are categorized into three varieties based on their fruit form. It contains high fiber contents, minerals, vitamins C, thiamine, niacin, A, B6, D, B12, E, and K. Eggplant is traditionally utilized for managing a diversed conditions, such as arthritis, bronchitis, asthma, diabetes, and high cholesterol levels (Yarmohammadi *et al.*, 2021). Eggplant is a major vegetable crop grown for its fruits only. It is also called as brinjal. It is a non-tuberous species of high agronomic and economic significance. In 2017, global eggplant production reached 52.3 million tons, making it the world's sixth most-produced vegetable after tomatoes, onions, cucumbers, gherkins, and cabbages, conferring to the UN's Food and Agriculture Organization (FAO) (Alam & Salimullah, 2021). Due to the large utility and production, we have not found scientific study on the leaf and stem of this plant. Therefore, the present study planned to

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summarize the pharmacognostic features of leaf and stem and to find out the antioxidant, antidiarrheal and cardiac potential of eggplant along with networking and molecular docking.

MATERIALS AND METHODS

Chemicals and equipment's

Dragandroff's reagent, mayer's reagent, hager's reagent, wagner's reagent, Folin-Cicalto reagent, tannic acid, FeCl3 solution, gelatin solution, basic lead acetate, sodium hydroxide solution, 5% (w/v) glacial acetic acid, 5% (w/v) sodium nitrate solution, DPPH, Hydrogen peroxide and phosphomolybdenum were used for identification studies. Calcium chloride ($CaCl_2$), Sodium chloride (NaCl), Glucose ($C_6H_{12}O_6$), Potassium chloride (KCl), Magnesium chloride ($MgCl_2$), Sodium bicarbonate ($NaHCO_3$), Magnesium sulfate ($MgSO_4$), Potassium dihydrogen phosphate (KH_2PO_4), Sodium dihydrogen phosphate (NaH_2Po_4) was provided by Merck. Sigma Chemical Co. in St. Louis supplied, Atropine sulfate, Losartan potassium, verapamil HCl.

Collection, drying and preparation of extract

The *Solanum melongena* L. was collected from local fields of district Muzaffargarh, Punjab, Pakistan in the month of April 2023. The plant parts i.e., leaf and stem are cleaned, shade dried and pulverized after complete drying. Then ground material was macerated in ethanol, which was shaken after every 12 hr. After seven days the material was filtered and dried on rotary evaporator at 40°C. Weight of each dried extract was measured and stored in ambered glass container and stored in biomedical freezer. The percentage yield for leaf 21% and stem 16% was obtained.

Macroscopic Analysis

Macroscopic features such as, size, shape, color, odor, fracture, texture, external markings and other features were studied by using the standard methods described by Evans 2002.

Fluorescence Analysis

Fluorescence analysis of both powders was carried out according to the protocols described by Kitcher *et al.*, 2020.

Proximate Analysis

Association of Analytical Chemists (AOAC) methodologies were used to conduct the proximate composition analysis. Fat content was determined using the Soxhlet fat extraction technique. Moisture content was determined via air oven drying. Crude protein was evaluated using the Micro Kjeldahl technique. Hydrolysis was used to estimate crude fibre, and the ash content was assessed using a muffle furnace (Gaithersburg, 2000).

Phytochemical Evaluation

Phytochemical evaluation of crude extract of *Solanum melongena* Leaf (SML) and *Solanum melongena* Stem (SMS) of eggplant was carried out by using standard protocols as described by Agidew, 2022.

Analysis of Total Phenolic Content

It was estimated by technique of McDonalds *et al*, 2001, with minor changes. Different concentrations of 2.5-40 mL from the stock solution of leaf and stem were obtained in 5 different test tubes. In each tube 2.5 mL of Folin–Ciocalteu Reagent (FCR) and distilled water (final volume up to 10 mL) with 2 mL of sodium carbonate were incorporated. This mixture was left to stand for 30 min. The volume was adjusted to get concentrations that varied between 2.5-4.0 µg/mL with water. The solutions were then permitted to incubate at 30°C (30 min). The absorbance of the solutions was determined at 765 nm in contrast to blank reagent. It was subsequently determined as mg/g Gallic Acid (GAE/g) correspondent employing the subsequent equation (Izuegbuna *et al.*, 2019).

$$Y = 0.0052x, R^2 = 0.9846$$

Analysis of total flavonoid contents

Total flavonoid concentration was determined spectrophotometrically via an aluminum chloride colorimetric assay. Different concentrations of 2.5-40 ml after the standard solution were obtained in 5 different test tubes. Additions were made of 0.15 ml of 5% sodium nitrite and 2 mL of purified water. After the solution equilibrated at ambient temperature for 5 min, 0.15 mL of aluminium chloride (10%) was added and the blend was permitted to stand for a further 5 min. Subsequently, 1 mL of 4% NaOH was added, and the total volume was attuned to 5 mL with water. Finally, the samples were incubated for 15 min to allow for full color development. Then the absorbance was assessed at 420 nm. It was expressed as mg/g of quercetin equivalent employing the following equation (Izuegbuna *et al.*, 2019).

$$Y = 0.0029x\ R^2 = 0.997$$

Analysis of total tannin contents

It was calculated by Folin–Ciocalteu assay method described by Vijay and Bhambar, 2014.

Different concentrations of 2.5-40 mL from the stock solution of leaf and stem were obtained in 5 different test tubes. To each concentration, 0.5 mL of Folin–Ciocalteu reagent and 1 mL of Na_2CO_3 (4%) were added sequentially. The mixture was subsequently diluted to 10 mL with water. Following an incubation period, absorbance was made at 725 nm. A gallic acid standard curve was made under identical conditions. Results were stated as mg of Gallic Acid Equivalents per gram of analyte (mg/g GAE), calculated using the following equation (Izuegbuna *et al.*, 2019):

$$Y = 0.0122x \qquad R^2 = 0.9838$$

Antioxidant Analysis

Total Antioxidant Capacity (TAC)

The antioxidant capacity of the leaf and stem extracts under examination was assessed using a phosphomolybdenum-based assay, which includes the formation of green phosphomolybdate complexes in acidic media. Test samples with a greater absorbance at 645 nm have greater capacity to reduce Mo (VI) to Mo (V), implying a higher antioxidant capability. This is an essential technique since it analyzes the total antioxidant capability of test samples. The results are represented as ascorbic acid equivalents (Bahal *et al*., 2022).

DPPH radical scavenging assay

The DPPH radical-scavenging capacity of the leaf and stem extracts was measured using the method described by Gupta *et al*., (2021) with slight modifications. A 1 mL aliquot of 0.135 mM DPPH in methanol was added to 1 mL of either plant extract or gallic acid standard (0.25–40.0 mg/mL). After vortexing, the reaction mixtures were incubated in the dark at room temperature for 30 min. The absorbance was subsequently measured at 517 nm. Vitamin C and gallic acid served as positive controls. The DPPH radical scavenging activity was determined with the following formula:

$$\text{DPPH \% RSA} = \text{Abs con - Abs sam/ Abs con} \times 100$$

*where Abs con was the absorbance of DPPH radical + CH_3OH; Abs sam was the absorbance of DPPH radical + plant extract or standards.

Hydrogen per-oxide radical scavenging assay

Using the technique outlined by Agrawal M., 2021, Leaf and stem extracts were assessed for hydrogen peroxide scavenging activity using a standard assay (Agrawal *et al*., 2021). Test solutions were prepared by mixing 4 mL of aqueous plant extract, vitamin C and gallic acid (0.25–40 mg/mL) with 0.6 mL of a 4 mM H_2O_2 solution in phosphate buffer (0.1 M, pH 7.4). Following a 10-min incubation at room temperature, the absorbance was calculated at 230 nm. The ratio of hydrogen peroxide scavenged was determined using the formula below:

$$H_2O_2\ \text{Abs con - Abs sam / Abs con} \times 100$$

*where Abs con was the absorbance of H_2O_2 radical + CH_3OH; Abs sam was the absorbance of the H_2O_2 radical + plant extract or standard.

Total Reducing Power (TRP)

The method as reported by Dahdouh, A., 2022 (Dahdouh *et al*., 2022). A 100 µL aliquot of sample (SML or SMS) was joint with 200 µL of phosphate buffer (pH 6.6) and 250 µL of potassium ferricyanide (1%) in a microcentrifuge tube. The mixture was vortexed and nurtured at 50°C for 20 min. Following incubation, 200 µL of Trichloroacetic Acid (TCA) (10%) was added and centrifugated at 3000 rpm (10 min). 50 µL of 0.1% ferric chloride was taken in respective 96 well plates and then 150 µL of supernatant from above centrifuged mixture and mixed thoroughly. The interpretations were made at 630 nm wavelength on microplate reader. 100 µL of stock solution of ascorbic acid (1 mg/mL) was given as positive control and respective solvent without sample was used as negative control.

Ferric Ion Reducing Antioxidant Potential (FRAP)

An improved method of Pastor, F. T., 2020 (Pastor *et al*., 2020) was adopted for the FRAP assay. The FRAP working reagent was made fresh by partying acetate buffer, 10 mM TPTZ (2,4,6-tripyridyl-s-triazine) in 40 mM HCl, and 20 mM $FeCl_3 \cdot 6H_2O$ in a 10:1:1 (v/v/v) ratio [25:2.5:2.5 mL] and pre-warmed to 37°C. Stock solutions of acetate buffer, TPTZ, and $FeCl_3$ were prepared as described previously [*or:* Acetate buffer (300 mM, pH 3.6) was prepared by dissolving 3.1 g of CH_3COONa in water, adding 16 mL of CH_3COOH, and regulating the final volume to 1 L. Separate stock solutions of 20 mM $FeCl_3$ and 10 mM TPTZ in 40 mM HCl were also prepared.] Aqueous extracts of leaves and stems (100 µL) at concentrations ranging from 0.25 to 40.00 mg/mL were allowed to react with 2.9 mL of the pre-warmed FRAP reagent in the dark for 30 min at 37°C. The absorbance of the resulting ferrous-tripyridyltriazine complex was then calculated at 593 nm. A normal curve was created using ferrous sulfate ($FeSO_4 \cdot 7H_2O$) solutions ranging from 200 to 1000 µM. The reducing antioxidant capacity was expressed as micromoles of ferrous equivalent per gram of dry extract (µM Fe (II)/g extract).

Nutritional Analysis

The A.O.A.C. technique was used to determine the mineral content (Horwitz & Latimer, 2000). 2-4 g of crushed materials have been placed in a crucible and combusted in a muffle furnace (550°C) for 6 hr. The subsequent ash was liquified in 10 mL of 10% (v/v) Nitric acid (HNO_3) with gentle heating for 20 min. After filtration, the obtained solution was analyzed to determine the mineral content. Ca, Mg, Cu, Se, Cr, Pb, and Zn were measured using an atomic absorption spectrophotometer, whereas Na and K were measured using a flame photometer in the filtrate.

Isolated tissue experimentation

Preparation of animals and housing condition

Albino rabbits (mixed-sex, 1.5–2.0 kg) were sourced from the Animal House of the Faculty of Pharmacy, BZU, Multan. The animals were held under typical laboratory conditions: ambient temperature of 23 ± 3°C, absolute humidity (30-70%), and a 12-hr light/dark cycle. They were provided with a conventional diet and water *ad libitum*.

Animals were allowed unrestricted access to water, but they weren't provided any food the night before the study. After

receiving a neck blow, rabbits were killed. The entire research followed all acceptable ethical guidelines outlined by "The Institute of Laboratory Animal Resources, Commission on Life Sciences" (NRC) and is approved by Institutional ethical committee of Bahauddin Zakaria University Multan, letter no 32/UREC/2023 (Council, 2011).

In vitro assays

Bio science isometrical force displacement transducers were connected to the Power lab data collecting system (AD Instruments, Bella Vista, NSW, Australia), which presented the results on a computer running Lab Chart software (version 6). In physiological settings, discrete tissue responses were seen. The percentage variation in the tissue response that was observed following the administration of test dosages was used to quantify the effect of the test drug (Iqbal *et al.*, 2023; Saqib *et al.*, 2021).

Isolated jejunum tissue preparation

Prepare the tissues after the abdominal cavity of rabbits was opened under anesthesia, pieces of the jejunum were dissected and chopped into lengths of about 1 cm. The jejunum fragments were then set vertically in an enclosed organ bath (15 mL volume) filled with Krebs-Henseleit buffer (KHS) having NaCl (118.2 mM), $NaHCO_3$ (25.0 mM), $CaCl_2$ (2.5 mM), KCl (4.7 mM), $MgSO_4$ (1.2 mM), and glucose (11.7 mM). Its higher end was wired to an isometric force transducer, and its lower end was coupled to a tissue holder in the organ bath (UF1 Isometric Transducer). It was kept under 1 g of stress. The KHS was continually oxygenated with a carbogen concoction (95% O_2 + 5% CO_2) and reserved at a temperature of 37°C. After stabilization, the tissue preparations were placed under 1g of strain for at least 30 min (e.g., until jejunum contractions became rhythmic). Segments with flimsy contractions were taken out of the protocol after stabilization. Different jejunum segment for every test were used (Chda *et al.*, 2023). On an equilibrated jejunal preparation, the potential spasmolytic and spasmogenic response of crude extracts was investigated through the cumulative addition of various extract dosages of leaf and stem. The response at each dose was normalized to the control contraction and plotted on a dose-response curve. The jejunum was precontracted with 80 mM KCl in order to measure the CCB (Calcium Channel Blockers) activity.

Isolated Aorta tissue preparation

Descending thoracic aortic rings (2–3 mm wide) were prepared and suspended in separate tissue organ baths. The baths contained Krebs-Henseleit solution (37°C) of the following composition (in mM): NaCl 118.2, $NaHCO_3$ 25.0, KCl 4.7, $CaCl_2$ 2.5, $MgSO_4$ 1.2, and glucose 11.7. The solution was continuously bubbled with carbogen (95% O_2 / 5% CO_2). Rings were equilibrated for 50 ± 10 min under an optimal resting tension of 2 g prior to experimentation. Plant extracts were progressively added to a baseline state of repose to better understand any potential vasodilator or vasoconstrictor effects (Janbaz *et al.*, 2015). Losartan and yohimbine were employed as prior treatments on isolated aortic rings to investigate the mechanism of contraction.

In silico approaches

Screening of the active ingredients

We obtained active ingredient information from online databases IMPPAT and Dr. Duke's Phytochemicals and Ethnobotanical Databases, which is a comprehensive database for active ingredients. We also used MolSoft, SwissADME, and Protox-II, which provide ideal information of the ADME&T properties of natural compounds (Ru *et al.*, 2014). The active compounds were screened based on Bioavailability (OB) and Drug-Likeness (DL), key indices for evaluating ADME characteristics using bioinformatics. Increasing OB can maximize efficacy while minimizing adverse effects (Wang *et al.*, 2017).

Identification of disease target genes

To get the disease targets, the GeneCards and OMIM databases were searched using the keywords "diarrhea, inflammatory bowel disease, constipation and cardiac diseases, i.e. IHD". The final disease target database was created by de-duplicating the targets in an Excel spreadsheet. The STITCH library was used to express the ultimate gene targets.

Identification of mutual disease effector targets

Using Venny 2.1.0, the active ingredient action targets were intersected with ailments targets to identify shared action targets between the two.

Analysis of Hub Gene and Development of PPI network

The connections between various kinds of mutual target proteins were studied via the String protein association database and Cytoscape software. The CytoHubba plug-in was utilized with network analysis techniques to identify important genes. The Degree method has a stronger prognostic consequence on genes and a greater advantage, so it was utilized in this work to screen key genes for the treatment of diarrhea and cardiac illnesses using the CytoHubba plug-in. Hub genes were found, and the rank file was stored (Liu *et al.*, 2023).

GO and KEGG path investigation

The standard targets were evaluated for the KEGG path and GO function enrichment using SRpolt. The top ten Biological Pathway (BP), Cellular Components (CC), Molecular Functions (MF), and cardiac and diarrhea-related signaling pathway were chosen based on their number of enriched genes.

Molecular docking

We selected the top six chemical compounds and the top three hub genes. To identify potential active compounds, a reverse docking approach was employed. The three-dimensional crystal structures of key protein targets, as identified in the network analysis, were retrieved from the Protein Data Bank. To choose the dynamic elements with the greatest bustle ranking, the structures of important chemicals were retrieved from the PubChem database. AutoDock Tools software was used for adjustments like as hydrogenation and charge balance. The receptor and ligand files were changed to the PDBQT format for docking. AutoDock Vina was used for molecular docking. The resulting poses were visualized and scrutinized using PyMOL software (version 2.2.0).

Statistical Analysis

All experimental data were collected in triplicates and results are expressed as Mean ± SD.

GraphPad Prism version 8 was used to prepare the graphs.

RESULTS AND DISCUSSION

Organoleptic evaluation is important parameter for standardization of herbal drugs, because, the majority of herbal products that are delivered to the market are distorted, twisted, rolled, and shrunken. Therefore, such medications are easily tampered or replaced. The use of pharmacognostic protocols will aid in determining the authenticity of pharmaceuticals because these tests provide results that are unique to a specific drug (Alam & Saqib, 2015). Our results of organoleptic evaluation which will help in proper identification of leaf and stem of *Solanum melongena* L. and are cited in Table 1.

With the aid of contemporary methods and the adoption of appropriate criteria and standards, the World Health Organization (WHO) has addressed the need to ensure quality inspections of medicinal plant materials. Fluorescence analysis and proximate analysis are two standardized parameters used in the current study. The fluorescence analysis is a tool for identifying plant components that provides a clear understanding of the chemical nature. It provides a hint as to whether powders are adulterated, making it a useful diagnostic tool for determining adulteration (Senthilkumar *et al.*, 2019). Our results presented in Table 2 showed different colors both in day light and UV light, forming a bench mark for its authentication.

In our study stem powder had higher moisture content compared to leaf powder and comparatively equal protein content as presented in Table 3. The ash content of stem is greater than leaf. Similarly, stem had significantly higher fat content compared to leaf, but fiber content of both parts was not significantly different as presented in Table 3. The large variance in proximate composition amongst the samples investigated showed that they have a comparative advantage over one another. Both leaf and stem have low moisture content. That leads a lengthy shelf life. The plant has a low protein content. Plants with low levels of crude protein make for less nutrient-dense foliage for creatures with high protein requirements. Low-fat components are also present in the plant. Consuming a great deal of crude fat can lead to health problems including cardiovascular diseases, atherosclerosis, cancer, and aging, thus it's best to consume it in moderation (Antia *et al.*, 2006). Ash content as a percentage serves as an indicator for the inorganic mineral components identified through research. The findings demonstrated that total ash is high than water insoluble ash but lower than acid insoluble ash. The abundance of minerals in the plants is shown by their high ash content. It contains fibers on higher level, which improves peristalsis, and helps in digestion and used to lowers blood cholesterol levels, which decreases the risk of heart attacks and strokes (Iheanacho & Udebuani, 2009).

Phytochemical compounds like, alkaloids, tannins, flavonoids, phenols and saponins are very important in the dealing of different diseases such as cancer, antimicrobial, inflammation and anti-helminthic. In our study both, leaf and stem extracts showed the presence of these metabolites which indicates the therapeutic potential of plant (Table 4).

Micronutrients are needed by humans and other organisms in varying levels throughout their lifetimes in order to regulate a wide range of physiological processes.

In our study *Solanum melongena* L. leaf and stem contains a good amount of Ca, and presence of Mg, K, Na, Cu, Zn, as presented in Table 5. The presence of these essential nutrients showed that

Table 1: Organoleptic evaluation of *Solanum melongena* L. leaf and stem.

Features	Leaf	Stem
Size	14 cm	85 cm
Shape	Elliptical	Cylindrical
External Color	Brown	Greenish brown
Internal color	N/A	Light green
Odor	Distinct	Distinct
Taste	Pungent	Pungent
Apex	Emarginate	N/A
Texture	Leathery	Rough
Margins	Sinuate	N/A
Venation	Reticulate	N/A
External markings	N/A	Nodules
Surface	Hairy/Pubescent	N/A
Fracture	Papery	Fibrous/Short
Fracture surface	Irregular	Uneven
Petiole size	1.5cm	N/A
Leaf base	Asymmetrical	N/A

leaf and stem can serve as a source of these nutrients in nutrient deficient individuals. The growth of bones and teeth depends on calcium. Additionally, it aids in the production of bodily fluids such as blood and extracellular and intracellular fluids (Olayiwola *et al.*, 2009). Magnesium and zinc are a crucial mineral element they serve as a cofactor of numerous enzymes. The presence of sodium and potassium in a reasonable amount is noteworthy because it aids in the generation of osmotic pressure between the cell and the tissues around it in the body and also controls fluid exchange between the cell and those tissues (Long *et al.*, 2007). Low amount of copper can cause high blood pressure and infertility. Selenium is a trace element that both people and animals require to survive (Junior & Dantas, 2016).

Quantitative analysis showed prominent results for the presence of phenolics, tannins and flavonoids as showed in Figure 1. Antioxidants have grown in popularity due to their ability to protect food and pharmaceutical items from oxidative degradation. Screening for antioxidant capabilities of plants and plant-derived elements demands the use of appropriate practices to investigate the mechanism of antioxidant activity and emphasis on the kinetics of events involving antioxidants. The DPPH radical is an inert organic compound, making it a powerful reagent for analyzing the free radical-scavenging powers of various substances (Sánchez-Moreno, 2002). The extracts showed good scavenging activity as showed in Figure 2A. Most enzymes are capable of being completely inactivated by hydrogen peroxide via oxidizing critical thiol (-SH) groups (PhD, 1999). H_2O_2 scavenging is relatively higher as showed in results Figure 2B. The TAC (phosphomolybdenum approach) relies on the creation of a Green Mo(V) complex with a maximum absorbance at 695 nm after Mo (VI) is reduced to Mo(V) by antioxidant chemicals. The extracts showed appreciable scavenging power in Figure 2C. The existence of reductants, which have been demonstrated to exercise antioxidant action by disrupting the free radical chain

Table 2: Fluorescence analysis of *Solanum melongena* L. leaf and stem powder.

Reagent	Leaf			Stem		
	Day light	254 nm	366 nm	Day light	254 nm	366 nm
Ethanol	Avo	Avo	Avo	Day	Gre	Gre
Methanol	Avo	Avo	Pig	Bai	Pag	Spg
Distilled water	Leg	Avo	Bea	Suc	Leg	Sag
Dil. H_2SO_4	How	Sag	Mog	Van	Leg	Bai
Conc. H_2SO_4	Reo	Med	Reo	Bea	Goc	Hav
Propanolol	Avo	Tar	Pig	Sos	Mig	Sim
Chloroform	Leg	Beq	Beq	Bai	Leg	Haw
Toluene	Pig	Mog	Avo	Reo	Bai	Wid
Dil. HCl	Spl	Tar	Ter	Riy	Haw	Bai
Conc. HCl	Hop	Beq	Leg	Pig	Avo	Tar
$FeCl_3$	Reo	Beq	Cha	Riy	Hav	Tar
Picric acid	Leg	Hav	Reo	Riy	Hop	Ham
Dil. NH_3	Riy	Beq	Ant	Pig	Sim	Haw
Iodine	Spl	Day	Avo	Ham	Ter	Bea
Benzene	Bai	Hab	Haw	Gold	Tar	Spl
Conc. HNO_3	How	Avo	Bea	Suc	Tar	Mor
Petroleum ether	Bag	Bea	Avo	Riy	Mdg	Ant
NaOH	Lim	Spl	Men	Wid	Lim	Ham
Acetic acid	Avo	Wid	Row	Coy	Haw	Tar
Acetone	Tar	Bea	Men	Hop	Gold	Med
Ethyl acetate	Leg	Hop	Tar	Sag	Reo	Mob

*Where, Ant=Antelope, Avo=Avocado, Bag=Beige green, Bai=Beige, Bea=Beachen, Beq=Becquer, Bod=Bodoir, Cac=Camel Cort, Cam=Camel, Cha=Charial, Cmo=Cameo, Coy=Corn yellow, Day=Daisy yellow, Dus=Dusty stone, Goc=Godcoin coconut, Gre=Green, Hab=Habitat, Hav=Havana, Haw=Hazle wood, Hom=Honey milk, Hop=Hopsack, How=Honey white, Leg=Leaf green, Lim=Limelight, Mdg=Mild green, Med=Medallion, Men=Mehndi, Mig=Mint green, Mob=Molten bronze, Mog=Moonsoon green, Mor=Morland, Pag=Par green, Pig=Pine green, Reo=Red oxide, Riy=Ribbon yellow, Sag=Sage green, Sas=Sand stone, Sim=Silver mist, Sis=Silk store, Sos=Soft silk, Spg=Spring green, Spl=Spring leaf, Suc=Sugar cane, Tar=Taracota, Ter=Tea rox, Thd=Thar dessert, Van=Vanilla, Wid=Wild Daffodil.

by surrendering a hydrogen atom, is necessary for a chemical to have reducing ability. The reduction of the ferric ion (Fe^{3+}) in the potassium ferricyanide multiplex to the ferrous state (Fe^{2+}) by antioxidants serves as the basis for measurement. Our results showed a correlation with the standard in Figures 2D & 2E. "Antioxidant power" is evaluated using a unique approach called the FRAP assay. A colorful ferrous-tripyridyltriazine multiplex is produced when ferric to ferrous ion drop occurs at a low pH. The results showed that extracts at different concentration showed a linear correlation against standard curve in Figures 2F & 2G.

In silico study

Screening for active compounds

We gathered active ingredient information from online databases. Out of 127 active compounds, only 6 demonstrated good ADMET characteristics (Figure 3). The supplemental materials include comprehensive data on active substances.

Screening of disease target genes

We employed the STITCH and Swiss target prediction database to evaluate prospective *Solanum melongena* L. targets. A total of 432 targets were discovered (refer to Supplementary Materials).

Table 3: Proximate Composition of *Solanum melongena* L. Leaf and Stem powder.

Parameters %	Leaf	Stem
Moisture	12.9±0.00	14.51±0.01
Protein	5.99±0.00	5.55±0.01
Ash	6.78±0.01	7.53±0.01
Water soluble ash	3.1±0.05	4.00±0.04
Acid insoluble ash	9.81±0.02	12.00±0.02
Fat	9.99±0.02	10.55±0.01
Fiber	34±0.02	37±0.01

Values are mean ± standard deviation of triplicate determination values in the same are not significant different at $p<0.05$.

Among these targets included Daturaolone (100), Ascorbic acid (46), Nicotinic acid (76), N-trans-p-Coumaroyloctopamine (100), riboflavin (10), and OPC-4:0 (100). Gene Cards and OMIM database were used to assess 41761 targets for diarrhea, IBD, constipation and heart disorders (see Supplementary Material). Top network candidates were constructed using the active chemicals and targets identified above.

Screening for common disease effector targets

The Venn plot was constructed between compounds targets and genes which showed 284 common unique elements, the overall unique elements are 24996, as showed in Figure 4.

Analysis of Hub Gene and Construction of PPI Network

We searched 432 similar molecules and 24993 targets related with diarrhea and heart disease. The union of chemical and disease targets produced 284 targets (Figure 4). The found targets were used as potential therapeutic targets. These 284 targets have been transmitted to the STRING database, and active protein interactions were picked from databases. The results have been uploaded into Cytoscape for further analysis. The top ten hub genes identified using CytoHubba's degree technique were TNF, EGFR, STAT3, HIF1A, ESR1, JUN, PPARG, HSP90AA1, PTGS2, and MAPK3. The hub gene is a key target in various biological processes (Zhang *et al.*, 2020). Cytoscape software was used to analyze the results, and Figure 5 depicts the resulting network which shows Daturaolone has 1 node and 100 edges, Ascorbic acid has 1 node and 46 edge, Nicotinic acid has 1 node and 76 edges, N-trans-p-Coumaroyloctopamine has 1 node and 100 edges. The top three genes i.e. TNF has 1 node and 121 edges, EGFR has 1 node and 102 edges and STAT3 has 1 node and 91 edges.

GO and KEGG Pathway Analyses

The hub genes were entered into the STRING library for GO and KEGG pathway enrichment analysis. Supplementary material displays the whole GO enrichment analysis results, whereas

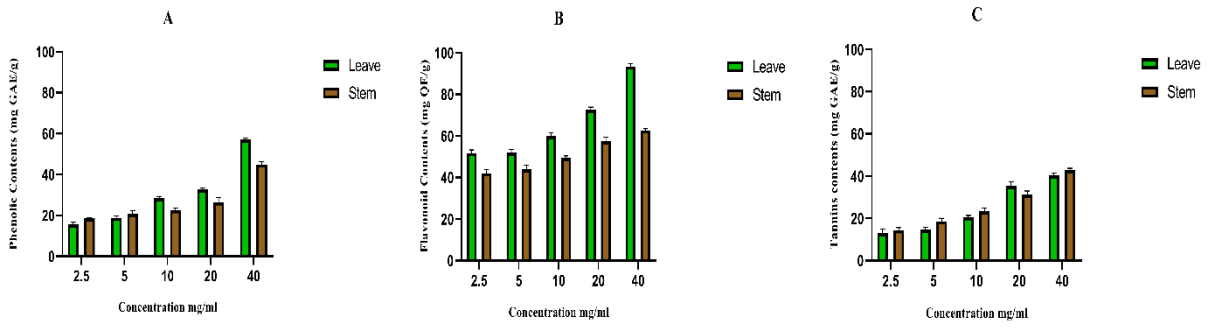


Figure 1: Quantitative analysis of: A) Total Phenolic Contents (TPC), B) Total Flavonoids Contents (TFC), C) Total Tannin Contents (TTC) of leaf and stem extract of *Solanum melongena* L.

Figure 7 shows the top ten results for the three aspects of BP, CC and MF. Biological Processes (BP) are primarily focused on (Figures 6 & 7 A) responding to cellular response to chemical stress, hemostasis, peptidyl–serine modification, peptidyl–serine phosphorylation, regulation of blood pressure, regulation of small molecule metabolic process, response to lipopolysaccharide, response to molecule of bacterial origin, rhythmic process and steroid metabolic process. Cell Component (CC) analysis (Figures 6 & 7 B) revealed that the targets mostly focused on azurophil granule lumen, caveola, cytoplasmic vesicle lumen, membrane microdomain, membrane raft, membrane region, nuclear envelope lumen, plasma membrane raft, secretory granule lumen and vesicle lumen. The Molecular Function (MF) study identified targets (Figures 6 & 7 C) that were closely connected to dioxygenase activity, icosanoid receptor activity, iron ion binding, ligand–activated transcription factor activity, nuclear receptor activity, oxidoreductase activity, acting on paired donors, with incorporation or reduction of molecular oxygen, prostaglandin receptor activity, prostanoid receptor activity, protein serine/threonine kinase activity and steroid binding.

The KEGG analysis findings are shown in the supplementary material. Figures 6 & 7 D depicts the 10 most prominent signal pathways. KEGG pathway enrichment analysis showed that target genes were implicated in many pathways, such as, Aldosterone–regulated sodium reabsorption, Bladder cancer, EGFR tyrosine kinase inhibitor resistance, HIF–1 signaling pathway, Insulin resistance, the PD-1/PD-L1 checkpoint pathway in cancer, proteoglycans in cancer, renal cell carcinoma, thyroid hormone signaling pathway and VEGF signaling pathway. Thus, *Solanum melongena* leaf and stem extract was found to regulate several pathways, potentially affecting GIT and CVS.

Molecular docking

Molecular docking investigations indicate that all six active components engage to the targets with a certain stability. *Solanum melongena* L. active constituents bind more effectively to target proteins, coexist with manifold interactions, and have a substantial contest with their active sites. These components may be key targets for treating diarrhea and cardiac problems.

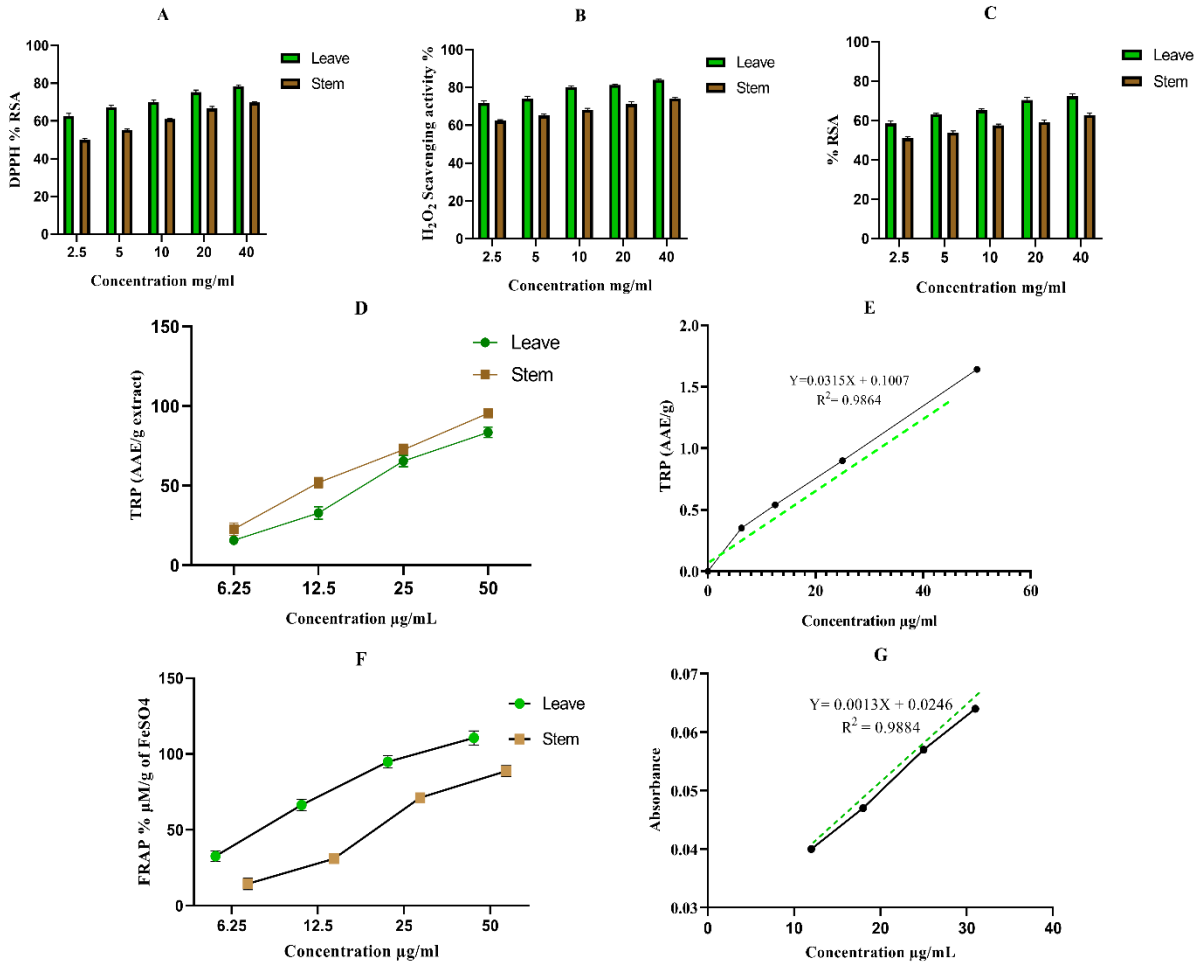


Figure 2: Antioxidant assay; A) DPPH assay B) H_2O_2 assay C) TAC assay D) TRP of SM extract (Leaf & stem) E) TRP standard curve F) FRAP of SM extract (Leaf & stem) G) FRAP standard curve.

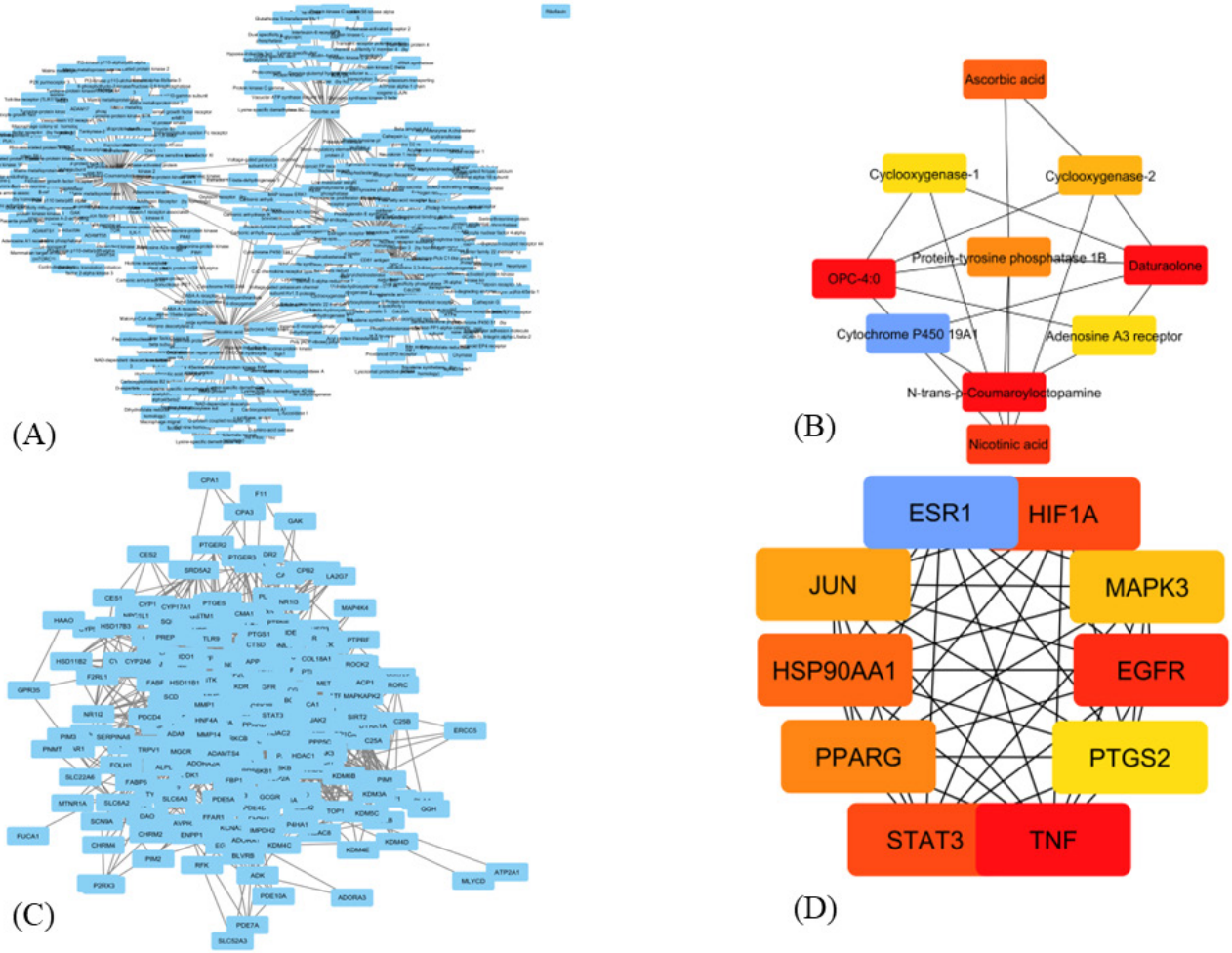


Figure 3: Network analysis; (A) Target compounds, (B) top ten compounds, (C) Target genes, (D) Top ten genes.

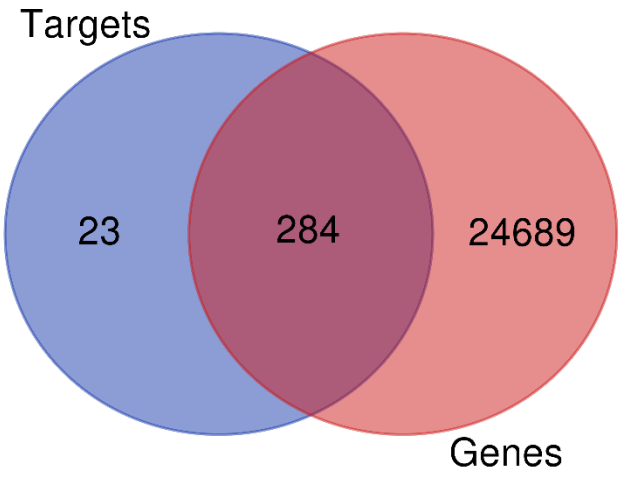


Figure 4: Venn plot analysis for compound targets and genes.

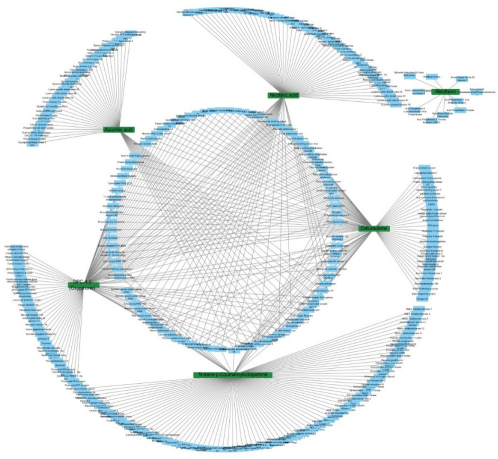
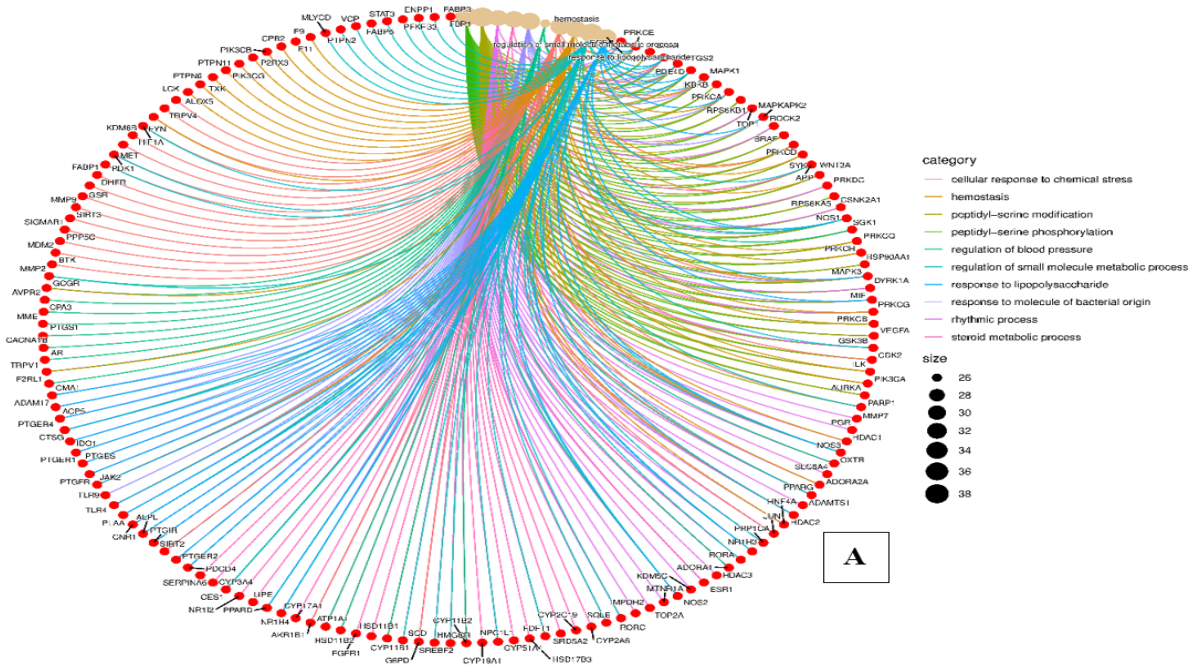


Figure 5: PPI network of compounds and target Genes for *Solanum melongena* in the treatment of diarrhea and cardiac diseases.


hemostasis
category
cellular response to chemical stress
hemostasis
peptidyl–serine modification
peptidyl–serine phosphorylation
regulation of blood pressure
regulation of small molecule metabolic process
response to lipopolysaccharide
response to molecule of bacterial origin
rhythmic process
steroid metabolic process
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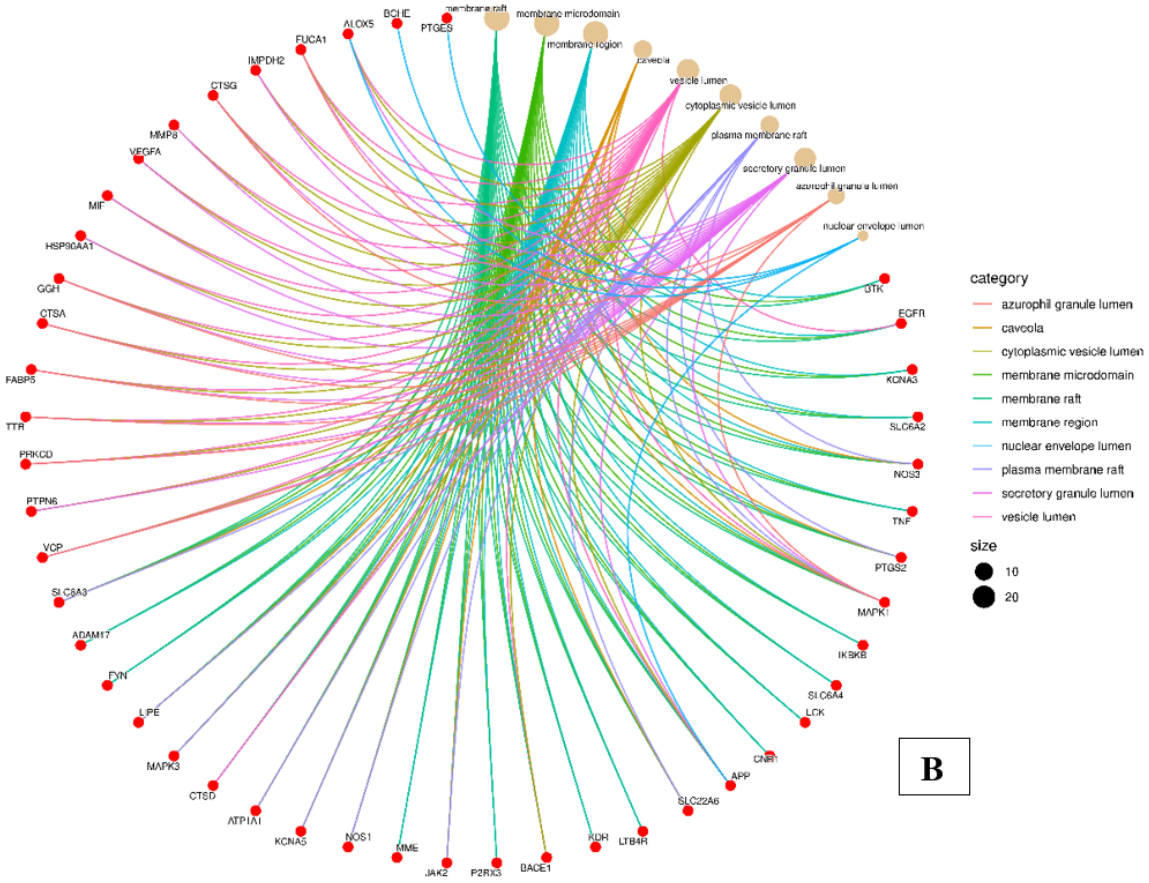
membrane raft
membrane microdomain
membrane region
caveola
vesicle lumen
cytoplasmic vesicle lumen
plasma membrane raft
secretory granule lumen
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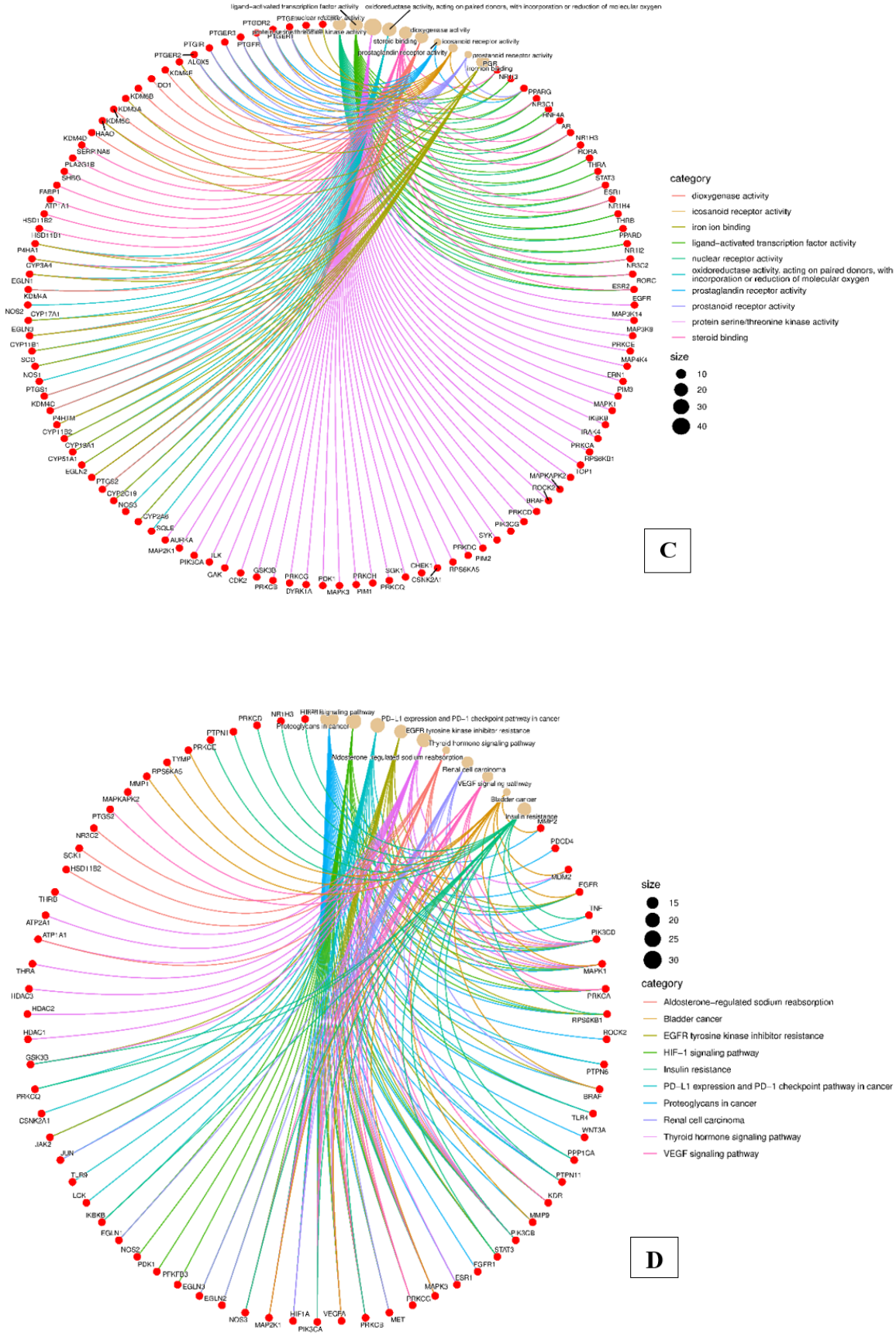

Figure 6: Map enrichment analysis of biological process; (A) GO BP analysis (B) GO CC analysis (C) GO MF analysis (D) KEGG pathway of target genes.

Different interactions with gene TNF (Figure 8), EGFR (Figure 9), STAT3 (Figure 10) are displayed while binding energies and H-bonding are elaborated in Table 6.

Table 4: Phytochemical analysis of leaf and stem extract of *Solanum melongena* L.

Class	Tests	Leaf	Stem
Alkaloids	Dragendorff's test	++	+
	Mayer's test	++	+
	Hager's test	++	+
	Wagner's test	++	+
	Tannic acid test	++	+
Tannins	FeCl3 test	+	+
	Gelatin test	++	+
Flavonoids	Lead acetate test	++	+
	Alkaline reagent test	++	+
Phenols	FeCl3 test	++	+
	Ellagic acid test	+	+
Saponins	Froth formation	-	-

*Where ++ = strongly present; + = present; - = absent.

Isolated tissue experimentation

The extracts of *Solanum melongena* L. leaf and stem were tested on isolated jejunum tissue samples. The jejunum is utilized because smooth muscles are highly reactive.

Solanum melongena Stem (SMS) produced a spasmolytic reaction when administered to spontaneously constricting isolated jejunum tissue at cumulative doses ranging from 0.003 to 3 mg/mL, with an EC_{50} value of 0.3722 mg/mL (95% CI: 0.1561 to 0.9179, n=3). To evaluate relaxant activity, tissue preparations were pre-contracted with a high-K^+ (80 mM) solution to induce depolarization. Subsequent cumulative addition of the stem

Table 5: Mineral elemental analysis of *Solanum melongena* L. leaf and stem.

Mineral/Elemental	Leaf	Stem
Calcium (Ca) %	5.82	3.42
Magnesium (Mg) %	0.020	0.029
Potassium (K) %	0.372	0.362
Sodium (Na) %	0.2207	0.0113
Copper (Cu) (ppm)	17.00	2.00
Zinc (Zn) (ppm)	0.03	0.09
Lead (Pb) (ppm)	0.06	0.05

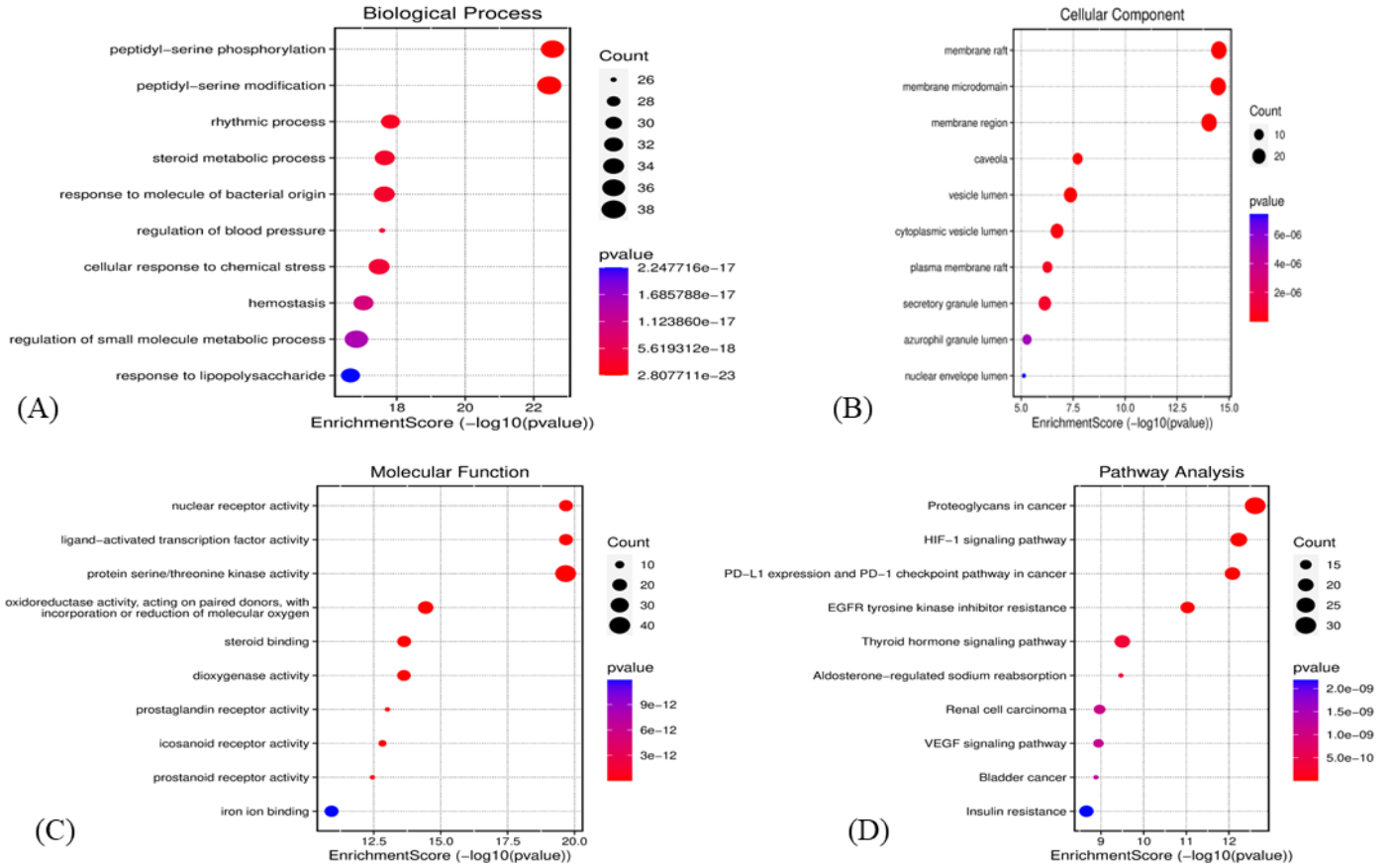

Figure 7: Gene ontology biological process; (A) GO BP analysis, (B) GO CC analysis, (C) GO MF analysis, (D) KEGG pathway of target genes.

extract (SMS) induced a complete, concentration-dependent relaxation of these evoked contractions (0.003–3 mg/mL). The half-maximal Effective Concentration (EC_{50}) was 0.1372 mg/mL (95% confidence interval: 0.05469–0.3296; n=3) (Figure 11A). *Solanum melongena* Leaf (SML) increased contractile response, but its spasmogenic action was inhibited by atropine (1 µM) pretreatment (Figure 11 B).

Isolated tissue is used for the research of underlying mechanism since it is untouched by nervous or hormonal stimuli and only retorts spontaneously. A brief increase or decrease in free Ca++ in the cytosol is the main trigger for smooth muscle spontaneous contraction. This easily accessible cytosolic Ca++ intermingles with the muscle's contractile elements to produce a momentary activation or deactivation of those elements. Antispasmodic medications treat conditions with hyperactive gastrointestinal symptoms by disrupting this system (Gilani *et al.*, 2006) Several studies have indicated that the Ca++ antagonistic consequence of curative herbs is the fundamental source of their means of action (Saqib & Janbaz, 2021). The SMS extract reduced spontaneous contractions at doses of 3 mg/mL, via inhibiting calcium input into the cell. To further investigate the anti-spasmodic method of action of stem extract, rabbit jejunum tissue was subjected to protracted constriction with high-K+ (80 mM). Elevated extracellular potassium (K^+) concentrations are known to induce

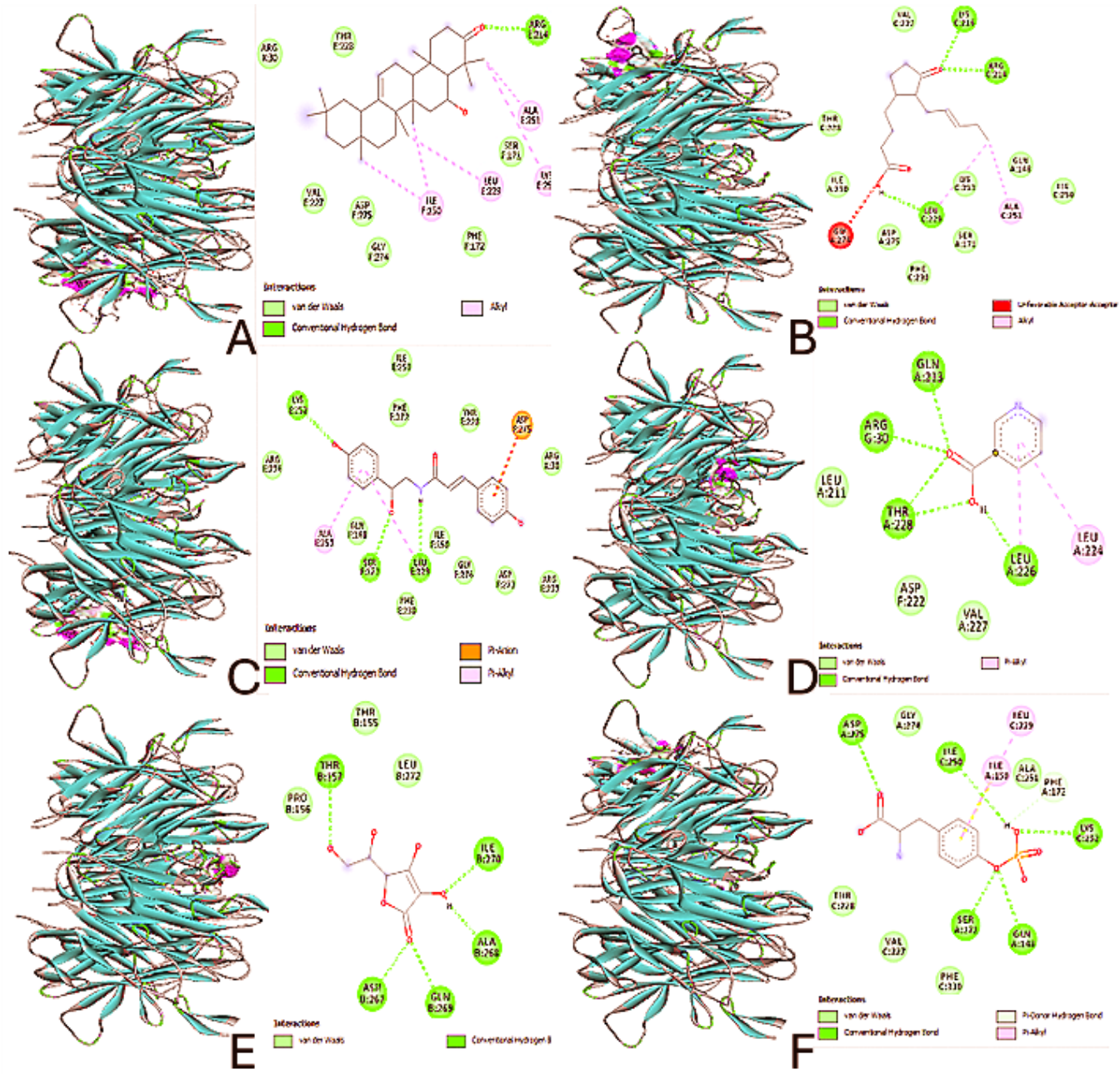

Figure 8: Molecular docking Gene TNF (3D & 2D) (A) Daturalon, (B) OPC-4:0 (Oxypinone), (C) N-trans-p-Coumaroyloctopamine, (D) Nicotinic acid, (E) Ascorbic acid, (F) Protein-Tyrosine phosphatase.

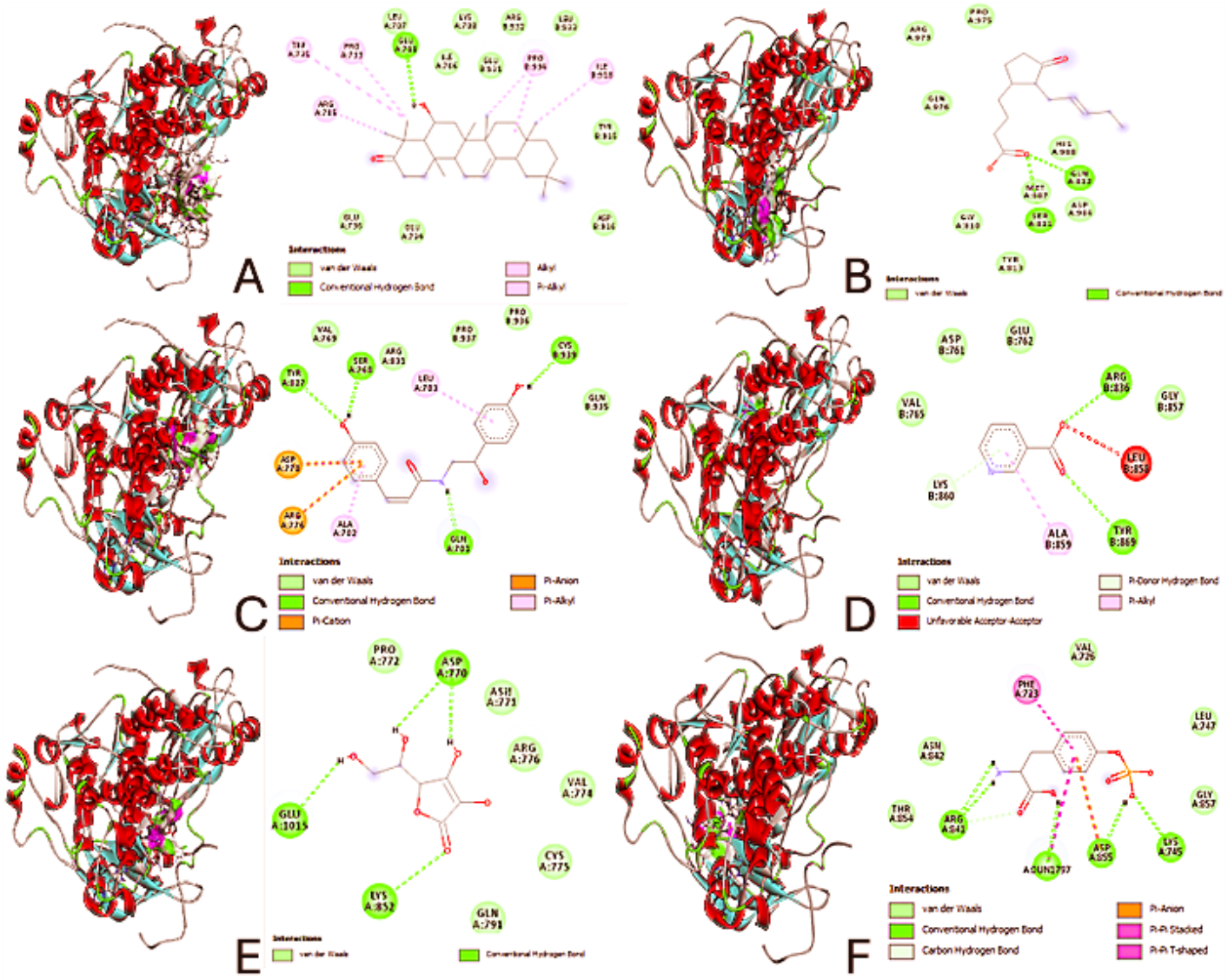

Figure 9: Molecular docking Gene EGFR (3D & 2D) (A) Daturalon (B) OPC-4:0 (Oxypinone) (C) N-trans-p-Coumaroyloctopamine (D) Nicotinic acid (E) Ascorbic acid (F) Protein-tyrosine Phosphatase.

sustained smooth muscle contraction. This occurs through the depolarization of the membrane potential, which activates Voltage-Dependent Calcium Channels (VDCCs). The subsequent influx of free Calcium ions (Ca^{2+}) into the cytosol triggers and maintains the contractile response (Iqbal *et al.*, 2023). Stem extract relaxed high k induced contractions at doses 0.003-3 mg/mL (Figure 11A). This result shows that Ca++ channel blockers exist in plants because they are useful in situations where the gut is hyperactive (Saqib & Janbaz, 2021). Leaf extract produced spasmogenic response at doses range from 0.1-1 mg/mL which was masked when tissue was pretreated with Atropine, a muscarinic blocker (Figure 11B). Studies suggest that activation of the M3 muscarinic receptor stimulates PLC, which in turn promotes the hydrolysis of phosphatidylinositol 4,5-bisphosphate to produce the secondary messenger's inositol 1,4,5-trisphosphate (IP3) and Diacylglycerol (DAG). The IP_3-induced release of Ca^{2+} from the SR elevates cytosolic Ca^{2+}. This ion serves a dual role: it cooperates with DAG to activate Protein Kinase C (PKC) and, more directly, binds to calmodulin. The resulting Ca^{2+}/calmodulin complex activates Myosin Light-Chain Kinase (MLCK), which phosphorylates Myosin Light Chains (MLCs) to promote contraction. A contractile response is then produced by an interaction network between phosphorylated MLCs and actin (Wahid *et al.*, 2021).

Furthermore, *Solanum melongena* L. leaf and stem extract demonstrated contractile action on isolated aortic tissues in tissue bath concentration range of 0.03-5.0 mg/mL and 0.01-5 mg/mL, which was found to be minimized when isolated rabbit aortic preparations were pre-treated with yohimbine for stem extract (Figure 12A) and was clinched to be arbitrated through activation of α-adrenergic receptors and pretreatment with

Table 6: Binding energies and interactions of the phytochemicals with genes in *Solanum menolgena* L.

Compound	Genes	Pose	Binding energy	Hydrogen bonds	Hydrophilic bonds
Daturaolone	TNF	1	-8.2	Arg214	Arg30, Thr228, Ala251, Ser171, Lys252, Leu229, Phe172, Ile150, Gly274, Asp275, Val227.
	EGFR	1	-8.7	Glu711	Arg705, Trp731, Pro733, Leu707, Lys708, Ile706, Glu931, Arg932, Pro934, Leu933, Ile918, Tyr915, Asp916, Glu734, Glu736.
	STAT3	6	-5.1	Lys57	Pro32, Arg58, Lys31, Ser54, Glu61, Leu18,
OPC_40 (Oxypinone)	TNF	3	-5.2	Lys216, Arg214, Leu229.	Thr228, Val227, Gln148, Lys252, Ile250, Ala251, Ser171, Phe230, Asp275, Ile150.
	EGFR	1	-4.0	Gln812, Ser811.	Gln976, Arg973, Pro975, His988, Met987, Asp984, Tyr813, Gly810.
	STAT3	1	-3.8	Lys109, Val102.	Lys21, Tyr25, His22, Lys98, Asp101, Phe105, Arg106.
N-trans-p-Coumaroyloctopamine	TNF	1	-6.4	Lys252, Leu229, Ser171.	Arg214, Phe172, Ile250, Thr228, Asp275, Arg30, Arg231, Asp273, Gly274, Ile150, Phe230, Gln148, Ala251.
	EGFR	4	-5.6	Tyr827, Ser768, Cys939.	Val769, Arg831, Leu703, Pro937, Pro936, Gln935, Ala702, Arg776, Asp770.
	STAT3	3	-5.9	Asp101, Gln100, Arg76.	Tyr83, Glu104, Phe103, Phe79, Ser80.
Nicotinic acid	TNF	7	-3.9	Arg30, Gln213, Leu226, Thr228.	Leu224, Val227, Asp222, Leu211.
	EGFR	3	-4.4	Arg836, Tyr869.	Val765, Asp761, Glu762, Gly857, Leu858, Ala859, Lys860.
	STAT3	7	-3.1	Leu290, Gln288, Gln291.	Ser292, Phe289.
Ascorbic acid	TNF	3	-4.6	Thr157, Ile270, Ala268, Gln269, Asn267.	Pro156, Thr155, Leu272,
	EGFR	1	-5.0	Asp770, Lys852, Glu1015.	Pro772, Asn771, Arg776, Val774, Cys775, Gln791.
	STAT3	1	-3.5	Glu61, Arg58.	Leu18, Lys57, Ser54, Thr55.
Protein tyrosine phasphatase	TNF	1	6.0	Asp275, Ile250, Lys252, Gln148, Ser171.	Gly274, Ile150, Leu229, Ala251, Phe172, Phe230, Val227, Thr228.
	EGFR	4	-5.8	Lys745, Asp855, Oun1797, Arg841.	Asn842, Phe723, Val726, Leu747, Gly857, Thr854.
	STAT3	1	5.2	Lys109, Arg106, Asp101, Lys98.	His22, Tyr25, Leu99, Val102, Phe105

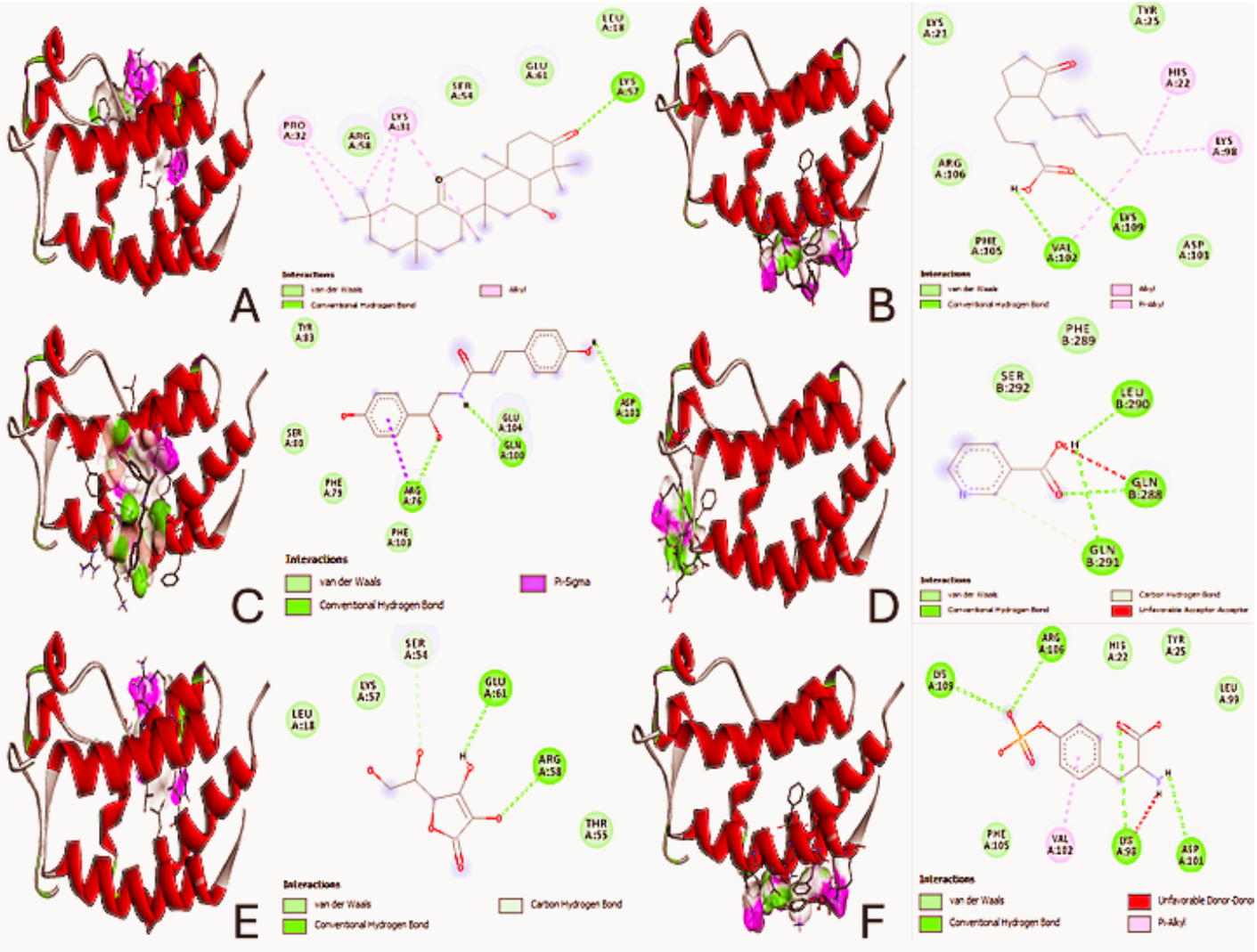

Figure 10: Molecular docking Gene STAT3 (3D & 2D) (A) Daturalon (B) OPC-4:0 (Oxypinone) (C) N-trans-p-Coumaroyloctopamine (D) Nicotinic acid (E) Ascorbic acid (F) Protein-Tyrosine phosphatase.

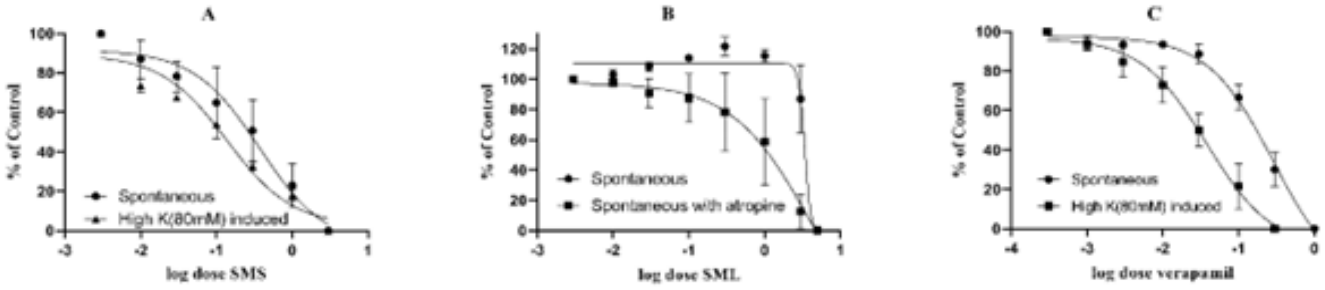

Figure 11: A) Graded relaxant response of the stem extract (SMS) on both spontaneous and high-K^+ (80 mM)-induced contractions in isolated rabbit jejunum preparations (*n*=3). B) Graded relaxant response of the leaf extract (SML) on spontaneous and atropine-pretreated contractions in isolated jejunum tissue preparations (*n*=3). C) Inhibitory effect of verapamil on spontaneous and high-K^+ (80 mM)-induced contractions in isolated rabbit jejunum. Data represent mean ± SEM (*n*=3).

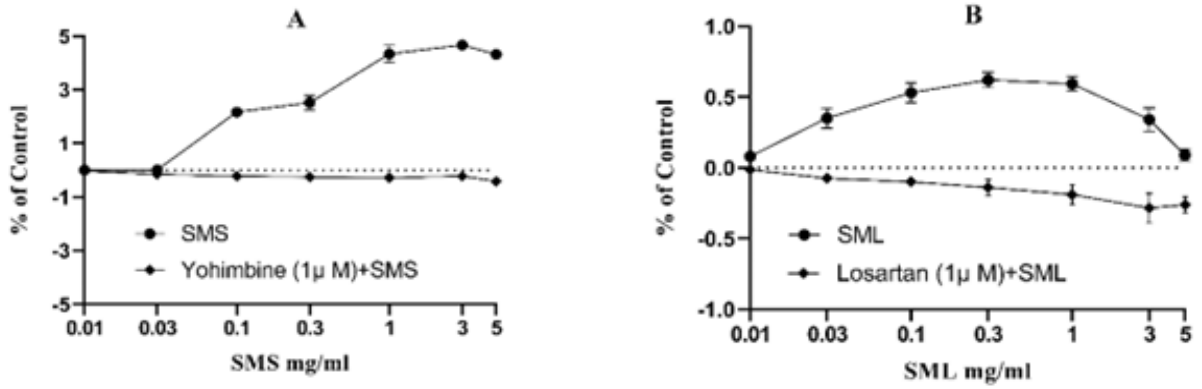

Figure 12: A) Dose response relationship of stem on isolated aortic rings with and without pretreatment with yohimbine (*n*=3). B) Dose response relationship of leaf on isolated aortic rings with and without pretreatment with Losartan (*n*=3).

losartan reduced leaf extract activity, which was attributed to activation of angiotensin II receptors (Figure 12B) (Bolton, 1979).

The antidiarrheal activity observed in the isolated jejunum assay suggests that several bioactive compounds previously identified in *Solanum melongena* L.—such as daturaolone, ascorbic acid, riboflavin, nicotinic acid, luteolin, and oxypinone—may contribute to this effect. The pharmacological basis for this activity likely involves interactions with key regulatory pathways in gut motility. Specifically, modulation of calcium channel function and inhibition of H^+/K^+-ATPase could underlie the extract's antimotility effect, potentially by reducing intracellular calcium influx and altering acid secretion, thereby diminishing peristaltic movement (Qazi *et al.*, 2022). The known antidiarrheal mechanisms of these compounds involve the dual inhibition of Cyclooxygenase (COX) and Lipoxygenase (LOX) enzymes, coupled with calcium channel blocking activity, all of which contribute to reduced intestinal motility and secretion. (Wahid *et al.*, 2022). Luteolin has been reported to exert antidiarrheal activity by reducing the volume and weight of small intestinal contents. This effect may be mediated through the upregulation of Na^+/K^+-ATPase and Creatine Kinase (CK) activity and gene expression, thereby enhancing electrolyte reabsorption and normalizing intestinal ion concentrations (Dong *et al.*, 2021). Recent research indicates that flavonoids and phenolic acids—including quercetin, luteolin, nicotinic acid, and ferulic acid—may have therapeutic potential against diarrheal disorders. Their proposed mechanisms involve the modulation of key pathways in gut smooth muscle contraction, such as inhibition of L-type voltage-gated calcium channels, antagonism of M3 muscarinic receptors, or interference with downstream signaling proteins like Phospholipase C (PLC). These findings collectively suggest that the antidiarrheal activity of *Solanum melongena* L. is likely mediated through a combination of antisecretory and antimotility actions.

This aligns with the established multi-modal mechanisms of many medicinal plant extracts, which have been shown to alleviate diarrhea through one or more pathways, including anti-secretory effects, enhanced intestinal absorption, reduced gut motility, antimicrobial activity, and direct antispasmodic action. The therapeutic relevance of these mechanisms has been consistently demonstrated in various *in vivo* studies (Rawat *et al.*, 2017) and are related to our results.

CONCLUSION

Pharmacognostic studies concluded in our research showed that leaf and stem contain different types of chemical compounds and minerals/micronutrients which are responsible for therapeutic potential. Furthermore, the antidiarrheal effects of *Solanum melongena* L. parts were produced by regulatory genes of calcium-mediated smooth contraction and contractile effect on aorta was mediated by angiotensin II receptors.

ACKNOWLEDGEMENT

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ABBREVIATIONS

SML: *Solanum melongena* leaf; **SMS:** *Solanum melongena* stem; **TPC:** Total Phenolic Content; **TFC:** Total Flavonoid Content; **TTC:** Total Tannin Content; **GAE:** Gallic acid equivalent; **QE:** Quercetin equivalent; **TAC:** Total antioxidant capacity; **DPPH:** 2,2-diphenyl-1-picrylhydrazyl; **FRAP:** Ferric ion reducing antioxidant potential; **TRP:** Total reducing power; **AOAC:** Association of Analytical Chemist; **FCR:** Folin–Ciocalteu reagent; **KHS:** Krebs-Henseleit buffer; **CCB:** Calcium channel blockers; **VDCCs:** Voltage-dependent calcium channels; **BP:** Biological pathway; **CC:** Cellular components; **MF:** Molecular functions; **GO:** Gene Ontology; **KEGG:** Kyoto Encyclopedia of Genes and Genomes; **PPI:** Protein-Protein Interaction; **OB:** Bioavailability; **DL:** Drug-likeness; **ADMET:** Absorption, Distribution, Metabolism, Excretion, and Toxicity.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

SUMMARY

The paper offers an in-depth analysis of the Pharmacognostic, nutritional, antioxidant, antidiarrheal, and vasoconstrictive effects of the *Solanum melongena* L. leaf and stem. The study is combination of *in vitro* and *in silico* methodologies to describe the conventional application of this plant. The finding showed that the leaf and stem of *Solanum melongena* L. have been rich sources of nutrients and various phytochemicals with valuable antioxidant, antidiarrheal (calcium channel blockade and muscarinic actions) and vasoconstrictive (angiotensin II and angiotensin I receptors) characteristics. The *in silico* analyses provide mechanistic platform, major bioactive compounds, protein targets and the biological pathways. This research scientifically justified the traditionally uses of eggplant in treating the gastrointestinal and cardiovascular diseases.

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