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Computational Screening and Biochemical Analysis of *Ricinus Communis Linn* Root

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ABSTRACT:

The goal of the current investigation was to computational screening and biochemical evaluation of *Riconus communis Linn's* root. The phytochemicals from the root of *Ricinus communis* were extracted using methanol and water. Via phytochemical screening with LC-MS, it was possible to identify the greater number of phytoconstituents in the *ricinus communis linn* root extracts. Potential sources of novel drugs and therapeutic leads included the plant's active phytoconstituents. The study's findings indicated that the methanolic extract of *Ricinus communis* root includes compounds with anticancer properties and some pharmacological active moieties. Esters, bioflavonoids and phenolic compounds have been estimated by chemical analysis and these were further identified with the help of LC-MS analysis. Thus, the raw root extracts of *Ricinus communis* may serve as fresh sources for the creation of novel plant-based medicines for the treatment of various illnesses. Since the plant already contains phenolic compounds, esters, and flavonoids, and the potential toxicity of a few specific components were investigated. It can be employed for the approaching research because it has been found that it is less dangerous and active.

KEYWORDS: Esters, bioflavonoids and phenolic compounds, LC-MS analysis, computational screening and biochemically evaluation.

INTRODUCTION

People from all around the world have been using herbal medicine to enhance medical regimens for millennia. The growing prevalence of adverse medication responses and the emergence of microbial resistance to currently available antimicrobials have led to an exponential increase in the importance of plant-based medicines for treating diseases. Moreover, there is a great chance of obtaining new chemicals[1]. Castor oil plant, scientifically named *Ricinus communis Linn*, is a type of flowering plant belonging to the *Euphorbiaceae* family. This soft-wooded

shrub grows widely in tropical climates[2]. The roots have few rootlets, are practically smooth, and are light in weight. However, they do have longitudinal wrinkles [3].

Because the plant's leaves, roots, and seed oil have been shown to be hepatoprotective, hypoglycemic, laxative, diuretic, and antibacterial, they have been utilized in Indian medicine to treat inflammation and liver problems. Roots can be used as a strong purgative and as a toothache paste when taken as a decoction or paste, respectively[4]. It has been found that distinct sections of *Ricinus communis Linn.* contain different phytoconstituents. The aerial portions of *Ricinus communis* contain alkaloids. The presence of ricinin (0.55%) and N Demethyl ricinin (0.016%), two alkaloids found in plant leaves[5].

When compared to an aqueous extract, the methanolic extract of *Ricinus communis Linn.* shown greater anti-microbial activity. The dermatophytic and pathogenic bacterial strains *Streptococcus progenies, Staphylococcus aureus,* and *Klebsiella pneumonia* were all successfully combated by *Ricinus communis*. Using the well diffusion method, the various solvent extracts of *Ricinus communis* roots exhibited antibacterial efficacy against pathogenic microbes. For instance: *Proteus vulgaris, Salmonella typhimurium, Pseudomonas aeruginosa, Escherichia coli,* and *Staphylococcus aureus*.[6] Because of its anti-allergic and mast cellstabilizing properties, *ricinus communis* root extract is useful in the treatment of asthma. Whereby flavonoids have bronchodilator and smooth muscle relaxant properties, and saponin has M. cell stabilizing properties[7]. Numerous investigations have demonstrated the antihistaminic properties of the *ricinus communis* root extract (ethanol/methanol).[8]

The lipid-lowering properties of the root and other portions of the *Ricinus communis* plant have been the subject of numerous investigations. According to findings, extracts from the roots of *Ricinus communis* may have hypolipidemic effects by lowering levels of triglycerides, lowdensity lipoprotein (LDL) cholesterol, and total cholesterol. An increase in high-density lipoprotein (HDL) cholesterol, which is thought to be advantageous for cardiovascular health, has also been observed in several studies[9]. Numerous chemicals found in the root of *Ricinus communis* have insecticidal effects. Among the most well-known substances is the poisonous protein called ricin, which is present in the seeds. But compared to the seeds, the roots have less ricin in them. In insects, ricin causes cell death by acting as a cytotoxin and interfering with the synthesis of proteins.[10]

Research has indicated that *Ricinus communis* root extracts can be useful in controlling a variety of insect pests. For instance, studies have shown that root extracts have insecticidal properties against leafhoppers, aphids, mosquitoes, and whiteflies. It has been demonstrated that these extracts cause death in the targeted insect species as well as feeding inhibition and decreased egg laying.[11]

The antiepileptic potential of *Ricinus communis* methanolic root extract was studied in mouse models by Raju G.M. et al. [12]. In order to investigate interactions with the active site utilizing PDB IDs 4MS4 (GABA agonists), 3WFG (glutamate antagonist), 5HCV (aspartate antagonist), and 6J8G (sodium channel antagonist), molecular docking studies were conducted by using Schrodinger software. Tounou *et al.* [13] assessed the feasibility of employing crude extracts from *Ricinus communis* leaves, roots, and seed kernels along with oil emulsion as a means of managing the diamond back moth, Plutella xylostella (L.) (Lepidoptera: Plutellidae). Jena and Gupta [14] proposed that the oil and the root of *Ricinus communis* were purgatives, effective against fever, rheumatism, inflammatory disorders, costiveness, and flatulence. The majority of compound medications used in rheumatic and neuralgic illnesses involve the root; seeds extracted from husks and germs and boiled in milk and water yield a decoction useful in rheumatism. According to Doshi A. K., *et al.* [15], the root of both wild and farmed forms of Ricinus communis Linn; Euphorbiaceae, often known as Eranda in the Ayurvedic medical system, is used as an analgesic and anti-inflammatory medication. In Swiss albino mice,

gentisic acid (GA) was found to have protective benefits against cyclophosphamide (CP)induced hepatotoxicity and genotoxicity, according to Nafees S., *et al.* [16]. The antiinflammatory and free radical scavenging properties of the methanolic extract of the root of *Ricinus communis (RCM) (Euphorbiaceae) Linn.* were investigated in Wistar albino rats by Ilavarasan R., *et al*.. The study's findings showed that in both acute and chronic inflammatory models in rats, the methanolic extract of *Ricinus communis* root exhibited strong antiinflammatory action. The presence of phytochemicals with diverse biological activities, such as flavonoids, alkaloids, and tannins, in the plant extract could be the cause of the observed pharmacological activity[17].

Compared to alternative analytical methods, LCMS has a number of benefits. Because mass spectrometric detection and chromatographic separation are combined, it also provides selectivity and specificity.[18] Due to the molecular level of analysis; the main benefits of this technology are its sensitivity, specificity, and precision. It is also possible to decipher the analytes' structural features.[19]

The current study set out to biochemically analyze and computationally screen the root of *Riconus communis Linn.* using methanol and water, the phytochemicals from the *ricinus communis* root were extracted. The more phytoconstituents in the *ricinus communis linn* root extracts were found by phytochemical screening utilizing LC-MS.

MATERIALS AND METHODS

This part deals with the material and methods used for extraction, phytochemical screening and LCMS analysis of extracts of root of *Ricinus communis*.

Collection and authentication of plant:

The roots of the plant *Ricinus communis* were acquired from an online herbal store named www.indianjadibooti.com and were authenticated from Dr. Gaurav Dubey, Department of Pharmacognosy, NIMS Institute of Pharmacy **Storage:**

Dried roots of *Ricinus communis* plant was preserved in tightly closed air tight containers and stored in a suitable cool and dry place.

Chemicals used:

All the chemicals used for the study were analytical grade purchased from R.S. Enterprises, Jaipur, Rajasthan.

Extraction[18-22]:

Preparation of Methanolic Extract

At a temperature of 45±5°C, 20 gm of powdered *Ricinus communis* roots were extracted using 150 ml of methanol by a soxhlation process. This approach permits a continuous extraction process in order to achieve efficient extraction. Using a water bath, the produced organic extracts were dried and evaporated. This extraction method is cost-effective in terms of time, energy, and monetary outlays. To be used later, the extracts were stored in a refrigerator.

Preparation of Aqueous Extract

20 gm powdered material of **root**s of *Ricinus communis* were dried and extracted with 100 ml of water by soxhlation technique at a temperature of 60-80°C. The extracts were kept in a refrigerator for further use.

Prelimnary Phytochemical Screening [19-24]:

Phytochemical examinations were carried out for both the extracts of **root**s of *Ricinus communis* as per the standard methods as mentioned below.

Alkaloid:

Each extract was diluted in a little amount of hydrochloric acid before being filtered. To check for the presence of alkaloids, the filtrate was utilized.

Mayer's test:

Potassium mercuric iodide, the Mayer's reagent, was applied to the filtrates. Alkaloids were present when a yellow-colored precipitate formed.

Wagener's test:

Iodine in potassium iodide, Wagener's reagent, was applied to filtrates. When a brown or reddish precipitate formed, alkaloids were present.

Dragendroff's test:

Potassium bismuth iodide, the dragendroff's reagent, was applied to filtrates. The presence of alkaloids was shown by the formation of crimson precipitate.

Hager's test:

Saturated picric acid solution, Hager's reagent, was applied to the filtrates. The presence of alkaloids is verified by the precipitate's yellow coloration.

Flavonoids:

Alkaline reagent test: A few drops of sodium hydroxide solution were applied to the extracts. When diluted acid is added, the strong yellow color that formed before becoming colorless indicates the presence of flavonoids.

Lead acetate test:

A few drops of lead acetate solution were applied to the extracts. The presence of flavonoids was shown by the formation of a yellow-colored precipitate.

Tannins:

Ferric chloride test: In a test tube, 0.5 ml of extract and 10 ml of water were heated. After adding a few drops of 0.1% ferric chloride, the coloration was checked for brownish green or blue-black. This suggested that tannins were present.

Phenols

Test for Ferric Chloride:

Three to four drops of ferric chloride solution were applied to the extracts. The occurrence of bluish black coloration signified the existence of phenols.

Saponins:

Froth Test:

After diluting the extracts with 20 cc of distilled water, they were agitated for 15 minutes in a graduated cylinder. The presence of saponins was suggested by the formation of a 1 cm layer of foam. **Foam Test:**

Two milliliters of water were mixed with 0.5 grams of extract. Saponins were present if the foam generated lasted for 10 minutes or longer.

Glycosides:

Keller- Killiani test:

After boiling 0.5 ml of the extract in 5 ml of distilled water, 2 ml of glacial acetic acid with 1 drop of 0.5% ferric chloride solution was added. This was combined with 1 milliliter of sulfuric acid concentration. The presence of cardiac glycoside was suggested by the creation of a violet ring beneath the brown ring and a greenish ring slightly above the brown ring in the acetic layer, which subsequently spread throughout this layer.

Molisch's reagent test:

The extracts were combined thoroughly with two to three drops of the Molisch reagent. A few cautious drops of strong sulfuric acid were added to this. The presence of glycosides was shown by the formation of a reddish-purple colored ring at the intersection of two layers. **Terpenoids:**

Chloroform test:
After combining the extract with two milliliters of chloroform, three milliliters of concentrated H_2SO_4 were carefully added to create a layer. The interface takes on a reddish-brown coloration that indicates terpenoids are present and working well. **Carbohydrate: Fehling's reagent test:**
Two milliliters of the produced extract were placed in a sterile test tube, and then two milliliters each of Fehling's solutions A and B were added. For roughly ten minutes, the prepared solution was maintained in a bath of boiling water. The presence of carbohydrates was verified by the development of red precipitate.
Benedict's reagent test:
1 milliliter of the extract and 2 milliliters of Benedict's reagent were combined, and the mixture was cooked for 3 to 5 minutes in a boiling water bath. The presence of carbohydrates is confirmed by the formation of a brick-red-colored cuprous oxide precipitate.

Molisch's reagent test:
A tiny quantity of the extract needs to be combined thoroughly in a test tube with two to three drops of Molisch's reagent. To help a layer form and prevent mixing, a few drops of strong sulfuric acid were poured drop-wise along the test tube walls. An encouraging sign for carbohydrates is the emergence of a purple ring at the layer created by the concentrated acid.
Steroids:
Chloroform test:
After dissolving 2 milliliters of the extract in 2 milliliters of chloroform and treating it with strong acetic and sulfuric acids, the extract developed a greenish hue, which suggested the presence of steroids.
Fixed oils:
Spot test:
The test material was rubbed between the filter paper folds in this experiment. The emergence of a transparent area indicates that lipids are present in the sample.
Anthraquinones:
Bontrager's test:
Ten minutes were spent for boiling of one gram of extract in five to ten milliliters of diluted HCl over a water bath. After filtering the mixture, an equal volume of ammonia solution and CCl_4 or benzene were added to the filtrate extract. Following shaking, the presence of the anthraquinone moiety was revealed by the emergence of pink to red color.
Quantification of Bioactive Compounds
Analysis of total phenolic content:[20, 21]
With minor adjustments, the literature approach was used to calculate the extracts' total phenolic contents. A calibration curve was created by combining a 1 mL ethanol solution of gallic acid (0.025-0.400 mg/mL), 5 mL of tenfold-diluted Folin-Ciocalteu reagent, and 4 mL of sodium carbonate (0.7 M). At 765 nm, absorbance data were recorded, and a standard curve was created. The aforesaid reagents were combined with 1 mL of *Ricinus communis* root extract (5 g/L), and the absorbance was measured after 30 minutes to ascertain the total phenolic contents. All determinations were carried out in triplicate. By comparison with a gallic acid (GA) standard, an equation was obtained from the standard curve of GA and used to determine the phenolic compounds in the extracts of roots of *Ricinus communis* (milligram of the GA equivalent, mg GAE).
The flavonoid content analysis [22]

The colorimetric approach was utilized to ascertain the extracts' flavonoid concentration. To sum up, 30 minutes were spent at room temperature (RT) after 0.5 mL of the extract was combined with methanol, 10% aluminum chloride ($AlCl_3$), and 1 M potassium acetate. Utilizing a quercetin solution calibration curve and a spectrophotometer, the absorbance of the reaction mixture was determined at 415 nm. Micrograms of quercetin equivalent (QE) are used to represent the flavonoid content.

LCMS Analysis of the root extract of *R. communis:*

The Waters nano Acquity HSS T3, 1.8 µm, 100 µm × 100 mm column was used in the autosampler-equipped UHPLC system. 500 µL min^{-1} was the flow rate for the mobile phases, which were water 0.1 % formic acid (A) and 90% acetonitrile in water with 0.1 % formic acid (B). Following a 15-minute maintenance period, the LC conditions were as follows: 5% during 0–3 min, a linear increase from 5% to 20% during 3–25 min, 20–40% during 25–40 min, and 40–50% during 40–55 min. A Thermo Electron LTQ-Orbitrap XL mass spectrometer equipped with a nano-electro-spray ion source (Thermo Fisher Scientific, Bremen, Germany) and operated under Xcalibur 2.1 version software, was used in positive ionization mode for the MS analysis using data-dependent automatic switching between MS and MS/MS acquisition modes.

RESULTS & DISCUSSION

Preliminary Phytochemical Analysis

The preliminary phytochemicals were identified in the methanolic and aqueous extract of roots of *R. communis* using various chemical tests. The presences of phytochemicals are shown in **table 1.**

Table 1: Preliminary Phytochemical Analysis of Methanolic & Aqueous Extract of *R. communis* roots

Phytochemicals	**Test**	**Methanolic Extract**		**Aqueous Extract**	
		Observation	**Inference**	**Observation**	**Inference**
Carbohydrates	Fehling's test	Brick red ppt	+	Brick red ppt	+
Flavonoids	Sulfuric acid test	Orange tored color	+	Orange tored color	+
Glycoside	Keller-Killani test	Reddish brown color appears	+	Reddish brown color appears	+
Saponin	Foam test	Froth appears	-	Thick persistent Foam observed	+
Tannin	5% $FeCl_3$ test	Deep blue-black color	+	Deep blue-black color	+
Alkaloid	Dragendroff's test	Orange-brown ppt	+	No ppt formed	-
Steroid	Salkowski reaction test	Chloroform layer appear red and acid layer shows Greenish yellow color	+	No layer appeared	-

Protein	Million'stestfor protein	White ppt	+	No White ppt formed	-
Terpenoid	With acetic anhydride and sulphuric acid with chloroform	Deep red coloration	+	Orange coloration	-

+ Sign indicates presence and – sign indicates the absence of the phytochemical constituents
For aqueous extract (AE) and methanol (ME), the percentage yield was 5% and 6%, respectively. The methanolic extract of *R. communis* roots revealed the presence of carbohydrates, flavonoids, glycosides, tannins, alkaloids, steroids, protein, and terpenoids; however, saponin was not detected. The aqueous extract of *R. communis* roots was shown to include carbohydrates, flavonoids, glycosides, saponin, and tannins; however, alkaloids, steroids, protein, and terpenoids were found to be negatively associated with the extract.

Chemical Composition and Bioactive Compounds in RC

Bioactive compounds [23]

In terms of gallic acid equivalent, the total phenol levels was determined by the Folin-Ciocalteu reagent (standard curve equation: $y = 0.005x + 0.083$, $R^2 = 0.954$). Aqueous and methanolic extracts of *R. communis* roots showed a range of total phenols from 130 to 134 mg g^{-1} and 46 to 49 mg/g, respectively. Aqueous and methanolic extracts of *R. communis* roots showed the presence of flavonoid and it was 9.22 mg quercetin dihydrate equivalent (QE)/g DW (AE) and 8.24 mg quercetin dihydrate equivalent (QE)/g DW (ME).

The reported valued were compared with earlier reported data and results showed that the total phenolic content of the aqueous leaf extract of *Ricinus communis* L. was 48.39 mg gallic acid equivalent (GAE) per gram dry weight (DW). The flavonoid content was 9.76 mg quercetin dihydrate equivalent (QE)/g DW [24 &25]. Whole phenolic concentration Phenols are essential components of plants that are found in all plant species. The relationship between TPC and the extracts' overall antioxidant activity may be better understood with the use of the quantitative and qualitative analysis of the major phenolics in plants[24]. Individuals' mutagenesis and carcinogenesis are inhibited by polyphenolic compounds. TPC Chaharedhi *et al* [25] were calculated using the Folin-Ciocalteu method, and the results were expressed as gallic acid equivalents (mg gallic acid per gram of dry mass). This approach was chosen for measuring phenolics due to its speed and intensity. Excessive levels of free radicals contribute to aging. They are the cause of many illnesses. The absence of antioxidant activity is the cause. Plantbased antioxidants are thought to be superior to synthetic antioxidants. Antioxidants with small molecular masses exist. They are thought to be effective in preventing oxidative stress[26]. The purpose of the *Ricinus communis* leaf extract was to analyze the total flavonoid content. The extracts of benzene, ethanol, and methanol were taken. A range of 17 to 28 µg/ml of catechin equivalent activity was observed[27]. Analysis was done on *Ricinus communis* leaf extracts. The aqueous extracts, methanol, and petroleum ether were utilized. They demonstrated 23-37 µg/ml of catechin comparable activity[28]. Both the aqueous and methanol exhibited 32 µg/ml. The activity of the remaining extracts was lower than this. It is thought that *Ricinus communis* is a useful medicinal plant. Its antioxidant activity is good. Gallic acid equivalents in aqueous were 131 mg/mL, n-butanol was 127 mg/mL, ethyl acetate was 117 mg/mL, and control was 155 mg/mL. Extracts from *Ricinus communis* roots were found to provide less than the control, but they nevertheless shown good equivalent activity [22].

Total phenolics (mg of GAE*/g DW**)=130 to 134 mg g^{-1} (AE) and 46 to 49 mg/g (ME).
Total flavonoids (mg of QE***/g DW**) =9.22 (AE) AND 8.24 (ME).

*GAE: Gallic acid equivalent.
**DW: Dry weight.
***QE: Quercetin equivalent.

LCMS Analysis of Methanolic Extract

Figures 1 and 4 display the LC-MS chromatogram of the *Ricinus communis* methanolic extract, whereas figures 2 & 3 and 5-10 display the mass spectrum of the chemicals that were identified. It was noted that various retention times were used to generate the various peaks. By employing the molecular weight, the compounds are clarified using the standard reference graphs. Chromatogram of Methanolic extract of *R. Communis Linn* (Positive and negative ions) with the highest peak at that specific retention time and all the compounds are listed in tables 2 & 3, figures 1 & 4.

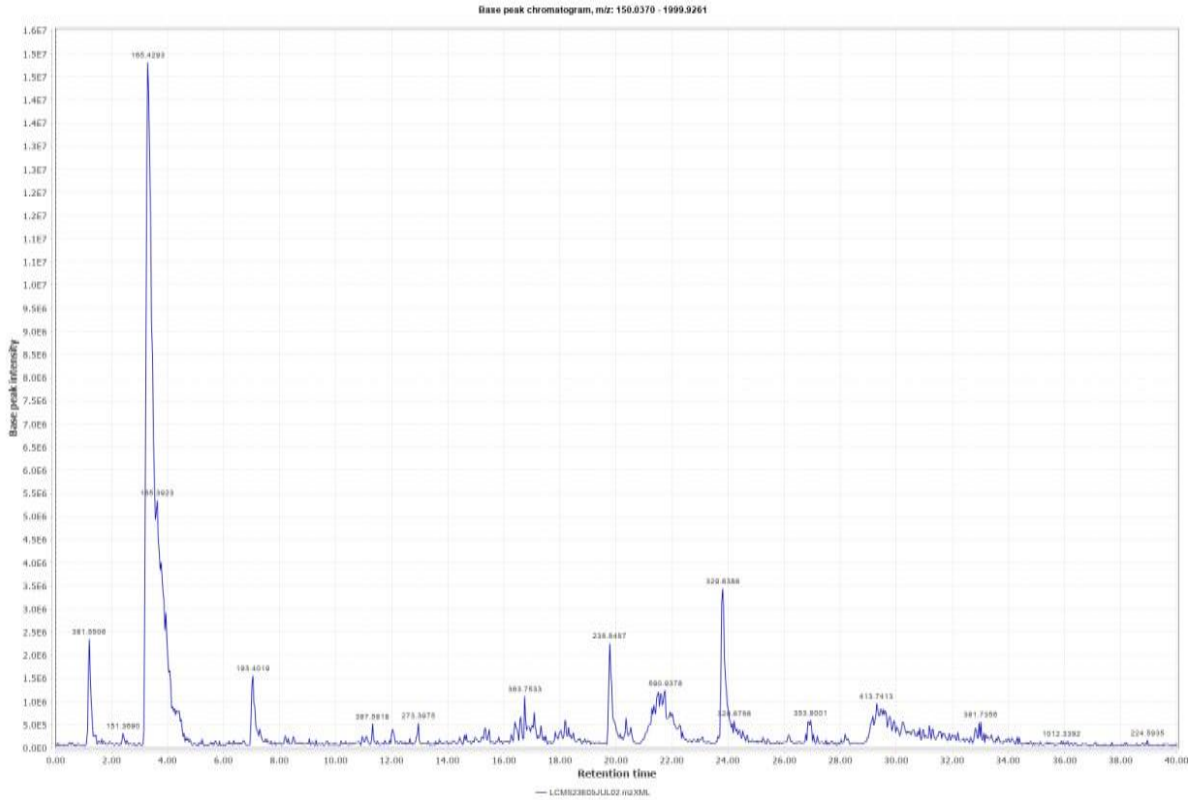

Figure 1: Chromatogram of Methanolic extract of *R. Communis Linn* (Positive ion)

Table 2: List of Compounds Reported from LCMS Analysis of Methanolic extract of *R. communis Linn* (Positive ion)

R. Time (min)	Score	Compound Name	Type of Ion	Formula	Exact Mass	Observed Mass	Mass Difference
1.21	0.731	**Zeatin-9-glucoside**	Positive	$C_{16}H_{23}N_5O_6$	381.164	381.5506	-0.3866
3.77	0.99	**D-Carnitine hydrochloride salt**	Positive	$C_7H_{15}NO_3$	161.105	165.4293	-4.3243
3.94	0.982	**L-Carnitine**	Positive	$C_7H_{16}NO_3$	162.113	165.4293	-3.3163

4.08	**0.987**	**Alpha-Methyl-DL-histidine dihydrochloride**	Positive	$C_7H_{11}N_3O_2$	169.085	165.4293	3.6557
7.05	**0.988**	**Caffeine, Anhydrous**	[M+H]+	$C_8H_{10}N_4O_2$	194.19	193.4019	0.7881
16.74	**0.83**	**Guanosine-5'-monophosphate**	Positive	$C_{10}H_{14}N_5O_8P$	363.057	363.7533	-0.6963
19.78	**0.613**	**1-Isothiocyanato-8-(methyl sulfinyl)octane**	Positive	$C_{10}H_{19}NOS_2$	233.09	235.5457	-2.4557
21.52	**0.21**	**Uridine-5'-diphospho-Nacetylglucosamine sodium salt**	Positive	$C_{17}H_{27}N_3O_{17}P_2$	607.081	678.9996	-71.9186
23.77	**0.634**	**Adenosine-3',5'-cyclic monophosphate**	[M+H]+	$C_{10}H_{12}N_5O_6P$	329.21	329.6016	-0.3916
23.80	**0.606**	**Malvidin Chloride**	Positive	$C_{17}H_{15}O_7$	331.081	329.6386	1.4424
23.84	**0.626**	**Malvidin Chloride**	Positive	$C_{17}H_{15}O_7$	331.081	329.6016	1.4794
29.30	**0.608**	**Solasodine**	Positive	$C_{27}H_{43}NO_2$	413.329	413.7413	-0.4123

All the peaks of chromatogram (**fig. 1**) of methanolic extract of *R. Communis Linn* (Positive ion) were observed and the highest peak was found out at the retention time of 4.08 min for the compound of Alpha-Methyl-DL-histidine dihydrochloride with mass of 169.085 followed by RT at 1.21min, 19.78 min and 23.77min.

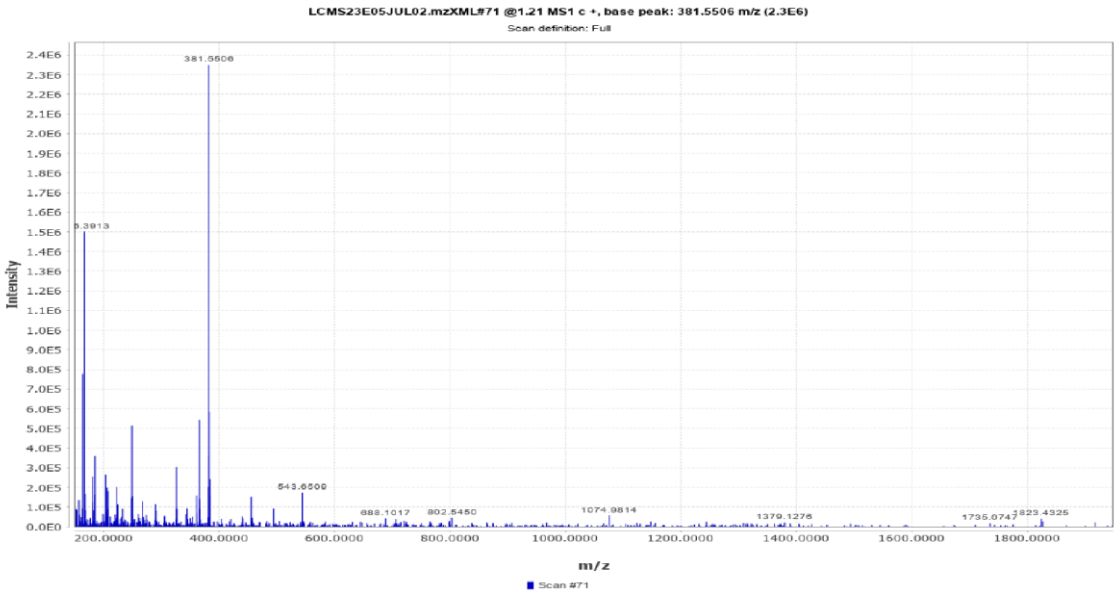

Figure 2: Mass spectrum at the retention time 1.21 (base peak 381.55m/z)

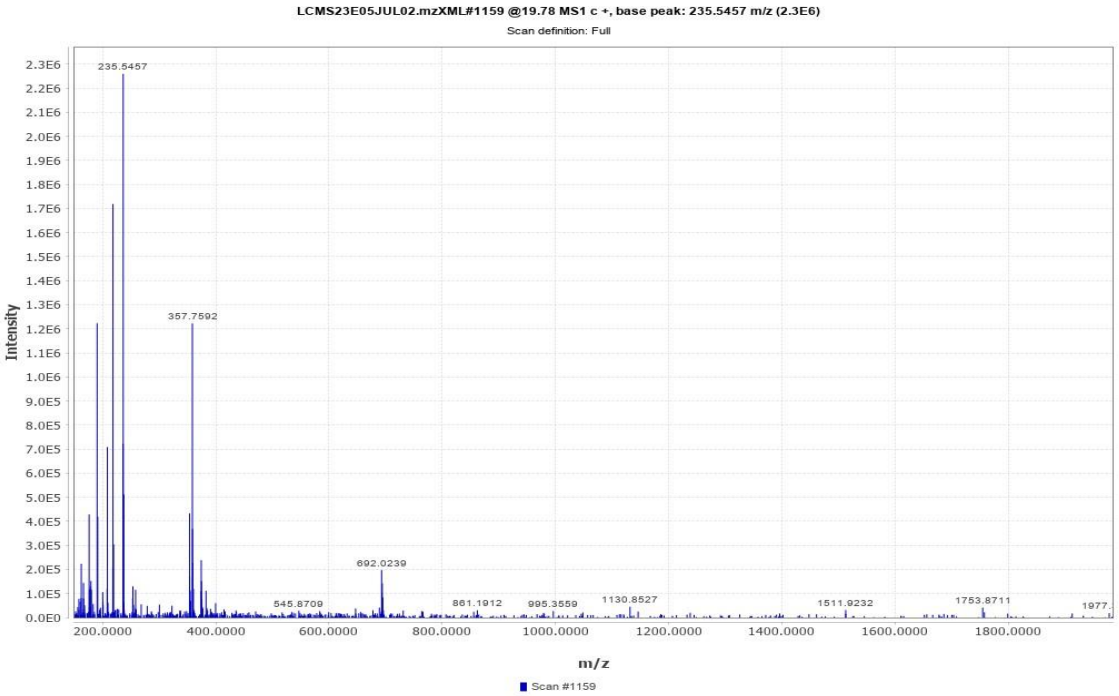

Figure 3: Mass spectrum at the retention time 19.78 (base peak 235.5457 m/z)

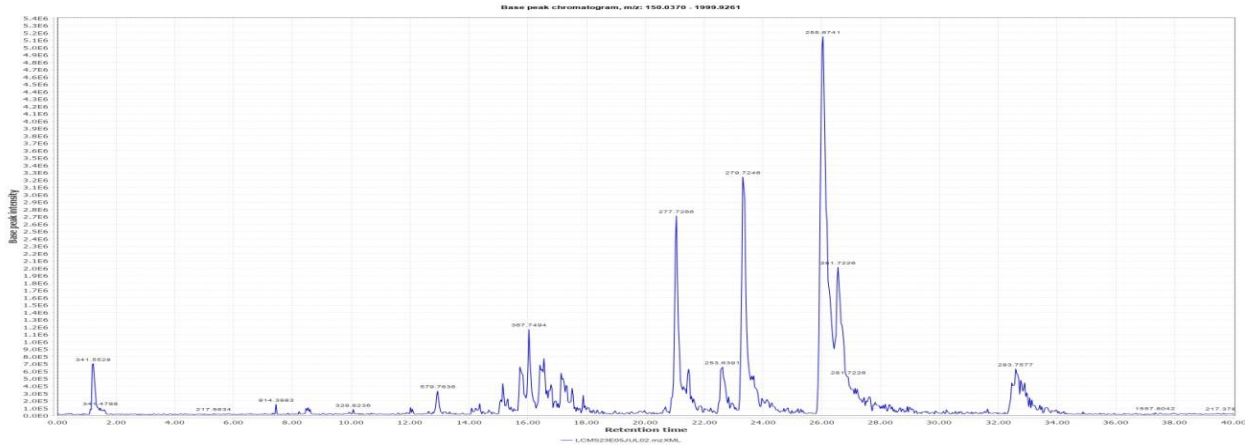

Figure 4: Chromatogram of Methanolic extract of *R. communis Linn* (Negative)

Table 3: List of Compounds Reported from LCMS Analysis of Methanolic extract of *R. communis Linn* (negative ion)

R. Time (min)	Score	Compound Name	Type of Ion	Formula	Exact Mass	Observed Mass	Mass Difference
1.23	**0.949**	**Galactinol Dihydrate**	negative	$C_{12}H_{22}O_{11}$	342.116	341.5528	0.56
15.73	**0.937**	**Petunidin**	negative	$C_{16}H_{13}O_7$	317.066	311.6932	5.37
16.04	**0.813**	**Lignoceric Acid**	negative	$C_{24}H_{48}O_2$	368.365	367.7494	0.62

16.55	**0.941**	**2'-Deoxyadenosine-5'monophosphate**	negative	$C_{10}H_{14}N_5O_6P$	331.068	325.7165	5.35
21.06	**0.975**	**6-Phosphogluconic acid Barium salt hydrate**	negative	$C_6H_{13}O_{10}P$	276.024	277.7266	-1.7
22.63	**0.916**	**D-Glucosamine-6-phosphate sodium salt**	negative	$C_6H_{14}NO_8P$	259.045	253.6391	5.41
23.31	**0.975**	**6-Phosphogluconic acid Barium salt hydrate**	negative	$C_6H_{13}O_{10}P$	276.024	279.7246	-3.7
23.38	**0.974**	**Gamma-Linolenic acid**	[M-H]-	$C_{18}H_{30}O_2$	278.43	279.7616	-1.33
26.04	**0.974**	**2'-Deoxyinosine**	negative	$C_{10}H_{12}N_4O_4$	252.085	255.6741	-3.59
26.55	**0.895**	**Luteolin**	negative	$C_{15}H_{10}O_6$	286.047	281.7226	4.32
26.69	**0.876**	**Gamma-Linolenic acid**	[M-H]-	$C_{18}H_{30}O_2$	278.43	281.7966	-3.37
32.56	**0.929**	**Acacetin**	negative	$C_{16}H_{12}O_5$	284.068	283.7577	0.31

All the peaks of chromatogram (**fig. 4**) of methanolic extract of *R. Communis Linn* (negative ion) were observed and the highest peak was found out at the retention time of 26.55 min for the compound of Luteolin with mass of 281.722 followed by RT at 23.31min, and 23.38min.

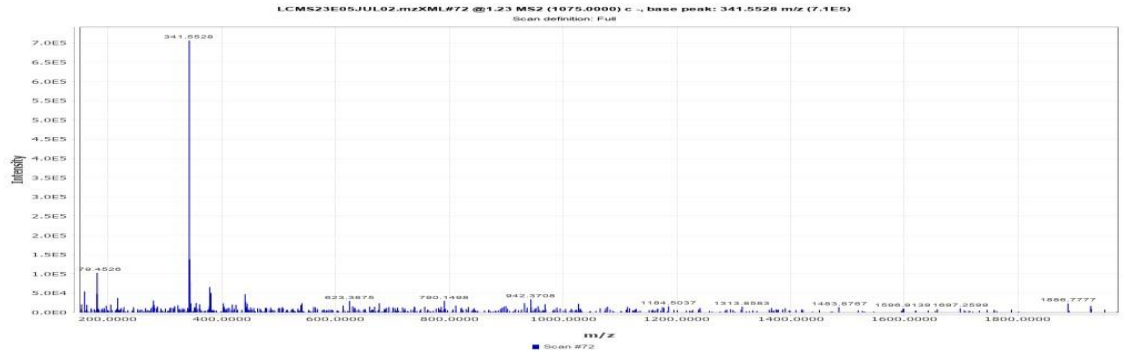

Figure 5: Mass spectrum at the retention time 1.23

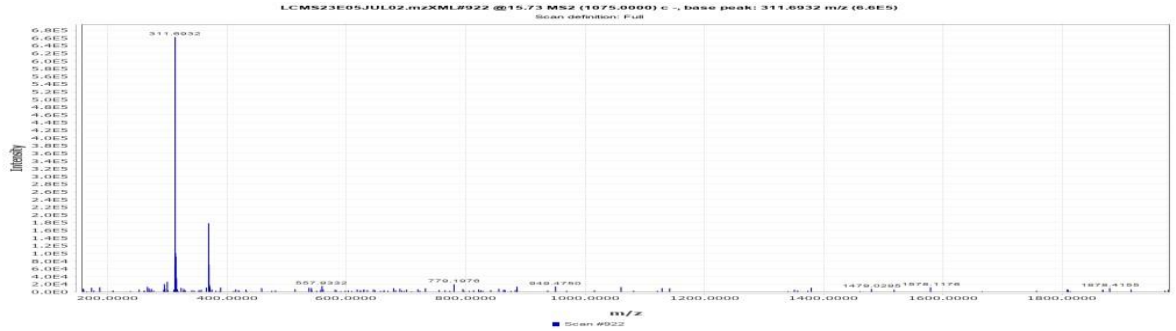

Figure 6: Mass spectrum at the retention time 15.73

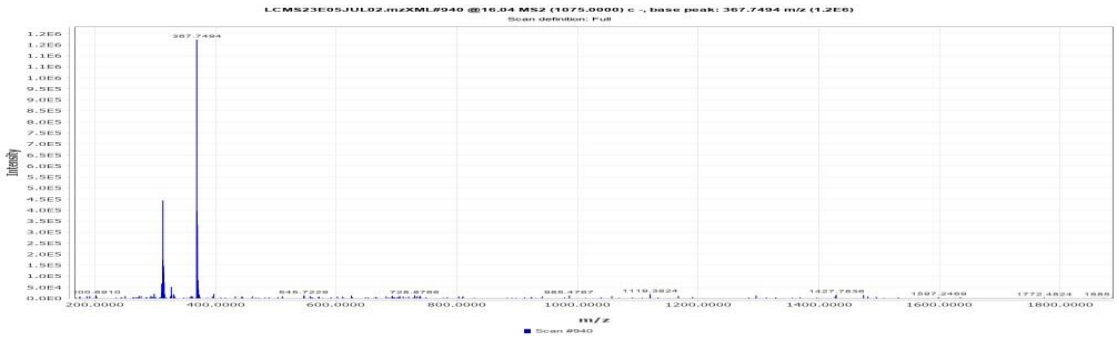

Figure 7: Mass spectrum at the retention time 16.04

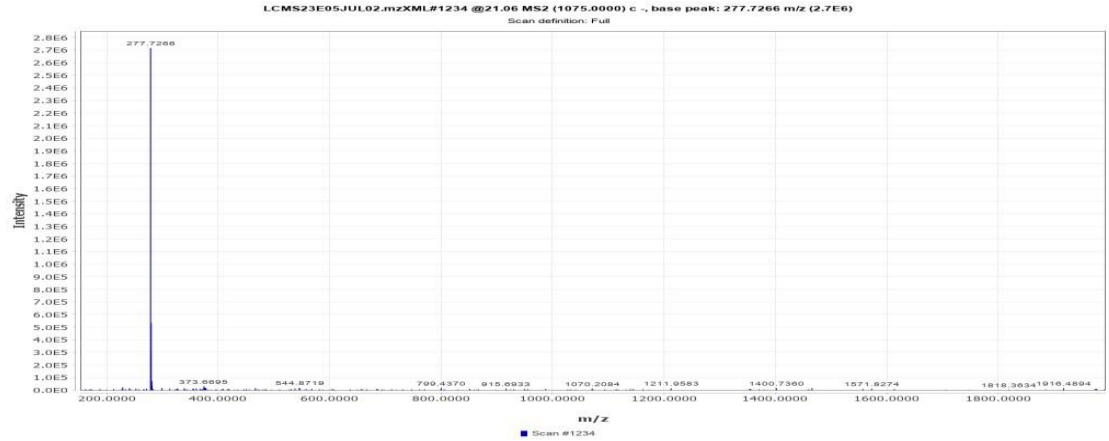

Figure 8: Mass spectrum at the retention time 21.06

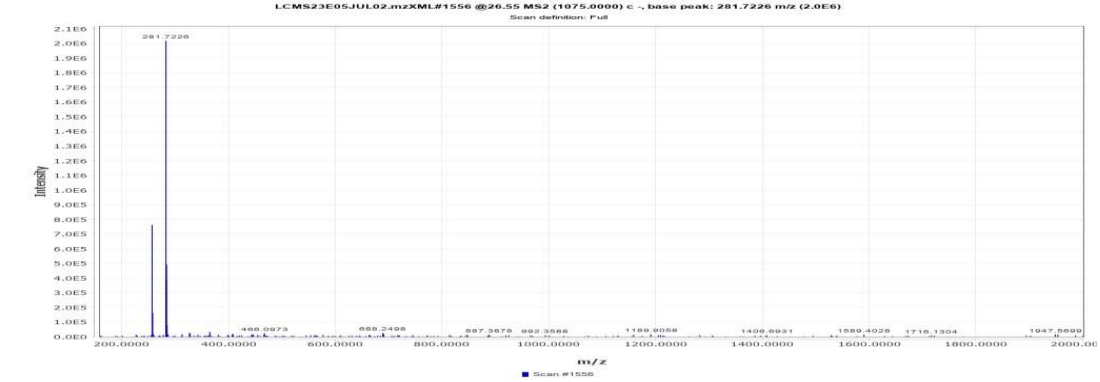

Figure 9: Mass spectrum at the retention time 26.55

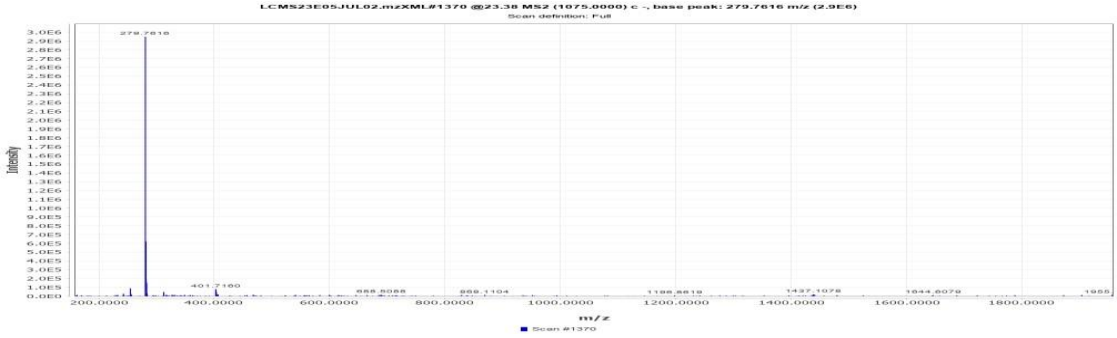

Figure 10: Mass spectrum at the retention time 26.69

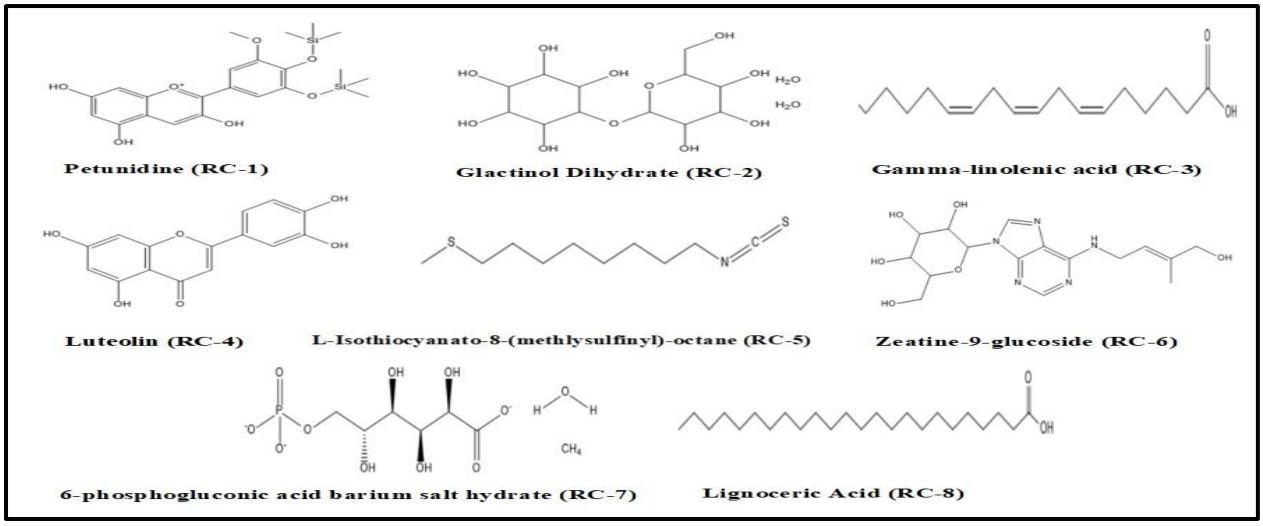

Figure 11: Structures of some isolated compounds

Since the plant already contains flavonoids, esters, and phenolic chemicals, we conducted toxicological investigations on a few selected components. We investigate the anticancer activity based on this. We discovered that the molecule is less hazardous and active; therefore we can use it in our future research.

Computational study of the following compounds

2D and 3D structure of computational study of the 2 compounds of Luteolin and Zeatin-9glucoside were conducted and it was mentioned in fig. 12 and 13.

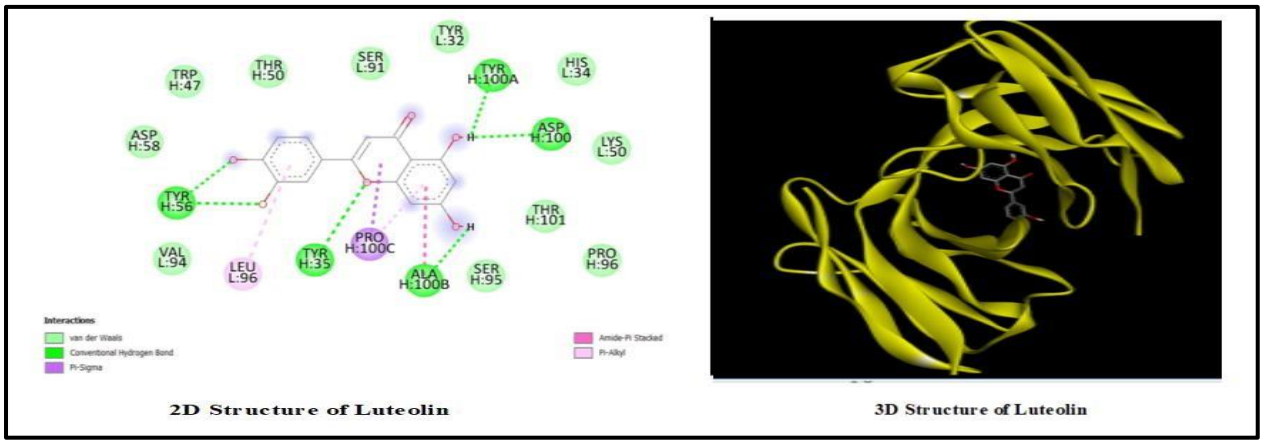

Figure 12: 2D Structure of Luteolin & 3D Structure of Luteolin

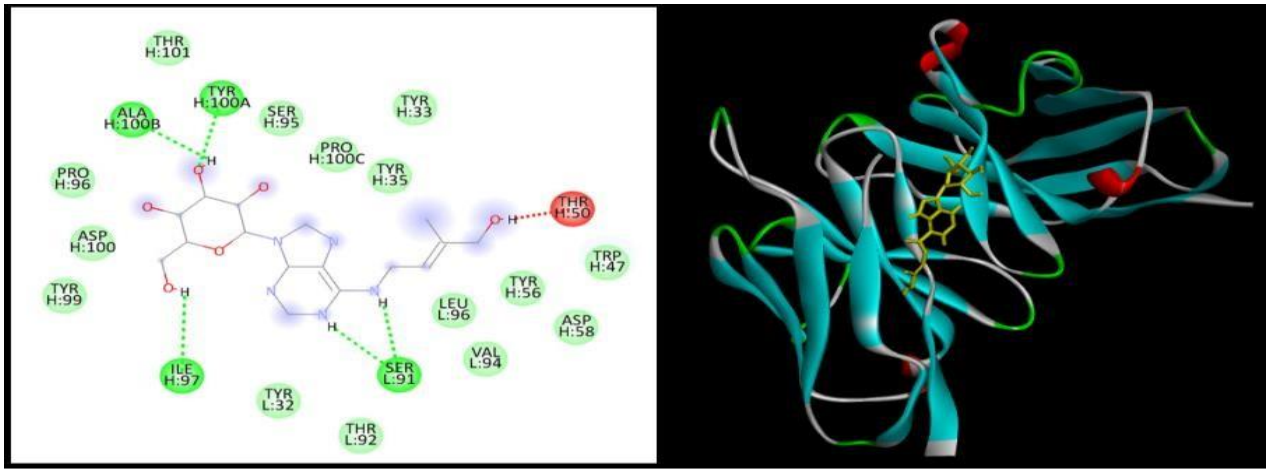

Figure 13: 3D Structure of Zeatin-9-glucoside & 3D Structure of Zeatin-9-glucoside

CONCLUSION

The plant's active phyto-constituents offered a potential source for novel medicinal and pharmaceutical possibilities. The study's findings demonstrated the presence of pharmacologically active compounds with anticancer potential in a methanolic extract of *Ricinus communis* root. The existence of esters, bioflavonoids, and phenolic compounds has been revealed by the LC-MS analysis. As a result, *Ricinus communis* root crude extracts may provide new opportunities for the development of novel plant-based therapies for the treatment of a variety of illnesses.

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