

## Phytochemical Characterization of *Ficus Carica* L. Fruits and Leaves: Proximate Composition and LC-MS Analysis In Dual Ionization Modes

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### ABSTRACT

**Context:** *Ficus carica* L. (common fig; Anjeer) has long been valued in Ayurvedic traditional systems for its nutritive and therapeutic properties, especially in respiratory, digestive, and inflammatory disorders. These effects are attributed to its diverse phytoconstituents. **Objectives:** The present study aimed to integrate traditional knowledge with modern science through proximate analysis and LC-MS profiling of fruits and leaves extracts of *F. carica* under negative (NEG) and positive (POS) ionization modes. **Materials and Methods:** Fruits and leaves were extracted with hydroalcoholic solvent and subjected to proximate analysis for primary phytoconstituents. Comprehensive metabolite profiling was performed using Q-TOF LC-MS under optimized conditions in both NEG and POS ionization modes. **Results and Discussion:** Fruits exhibited higher moisture content ( $10.55 \pm 0.16\%$ ), alcohol-soluble extractives ( $19 \pm 0.17\%$ ), and phenolic content ( $31.39 \pm 1.4$  mg GAE/g extract). Leaves showed greater ash content ( $9.87 \pm 0.11\%$ ) and flavonoid content ( $15.73 \pm 2.8$  mg QE/g extract). LC-MS analysis in NEG ionization identified 259 compounds from 479 features, including threonate (C<sub>4</sub>H<sub>8</sub>O<sub>5</sub>, RT = 2.254 min), L-xylonate (C<sub>5</sub>H<sub>10</sub>O<sub>6</sub>, RT = 2.286 min), and dihydroferulic acid 4-O-glucuronide (C<sub>16</sub>H<sub>20</sub>O<sub>10</sub>; score = 99.28). In POS ionization, 851 compounds were identified from 1900 features, with major metabolites such as dulcitol (C<sub>6</sub>H<sub>14</sub>O<sub>6</sub>, RT = 2.185 min; score = 99.29), ephedrine (C<sub>10</sub>H<sub>15</sub>NO; RT = 2.622 and 4.078 min), and azoxystrobin (C<sub>22</sub>H<sub>17</sub>N<sub>3</sub>O<sub>5</sub>, RT = 21.597 min; score = 99.73). **Conclusions:** The findings demonstrate the phytochemical richness of *F. carica*, supporting its traditional Ayurvedic uses and indicating its potential for future therapeutic and integrative healthcare applications.

**Keywords:** *Ficus carica*, common fig, LC-MS profiling, NEG ionization, POS ionization

### INTRODUCTION

Medicinal plants have historically served as a fundamental part of traditional medical practices, providing numerous bioactive molecules with wide-ranging therapeutic applications. [1]. Among medicinal plants, *Ficus carica* L. (FC), commonly referred to as the fig tree, is well recognized in ethnomedicine for its diverse pharmacological activities [2]. A member of the Moraceae family, FC is a deciduous species cultivated extensively in tropical and subtropical areas. Traditionally, its fruits and leaves have been utilized to manage a variety of medical conditions, such as gastrointestinal problems, inflammatory disorders, and diabetes [3]. These therapeutic effects are attributed to the plant's rich phytochemical composition, comprising phenolics, flavonoids, alkaloids, and other secondary metabolites.

In recent years, advancements in analytical techniques have facilitated the detailed profiling of plant metabolites, providing a deeper understanding of their bioactive constituents. High sensitivity, specificity, and the capacity to analyse complicated combinations have made Liquid Chromatography-Mass Spectrometry or LC-MS a potent technique for phytochemical investigation [4]. The dual use of negative (NEG) and positive (POS) ionization modes in LC-MS offers a comprehensive approach to metabolite identification, as certain compounds ionize preferentially in one mode over the other [5]. This approach is particularly useful for profiling plant extracts with diverse chemical compositions. The current study focuses on the hydroalcoholic extracts of the fruits and leaves of FC, employing LC-MS analysis in both NEG and POS ionization modes. The choice of hydroalcoholic solvent ensures the extraction of a broad spectrum of polar and semi-polar compounds, enhancing the scope of metabolite identification [6]. While previous studies have explored the phytochemical and pharmacological properties of FC, the dual-mode LC-MS profiling of its extracts remains underexplored.

This research aims to bridge this gap by providing a detailed phytochemical profile of FC fruits and leaves, highlighting the differences in metabolite composition between the two plant parts. By identifying key bioactive compounds, the study seeks to validate the traditional uses of the plant and explore its potential applications in modern pharmaceutical formulations. The findings are anticipated to enhance the existing understanding its chemical variety and pharmacological importance along with the importance of advanced analytical techniques in natural product research, paving the way for the discovery of novel therapeutic agents derived from medicinal plants.

Metabolomics is an essential tool for understanding biochemical pathways and identifying biomarkers for diseases [6]. This study employs a Q-TOF-MS (Quadrupole Time-of-Flight Mass Spectrometry) platform to identify metabolites in two datasets processed under different ionization modes: negative (NEG) and positive (POS). The goal is to compare compound identification efficacy and explore key metabolites for pharmaceutical applications.

Furthermore, the use of dual ionization modes enhanced the detection and characterization of minor compounds, which might have been overlooked in a single-mode analysis [7,8]. This research sets the stage for further investigations into the bioactivity of individual compounds identified in the extracts and their potential synergistic effects. Furthermore, it is the expanding collection of evidence that backs the conventional applications of FC in ethnomedicine and its possible uses in contemporary pharmaceutical formulations. The investigation highlights the importance of use of sophisticated analytical methods with established knowledge to fully realize the benefits of medicinal plants.

### MATERIALS AND METHODS

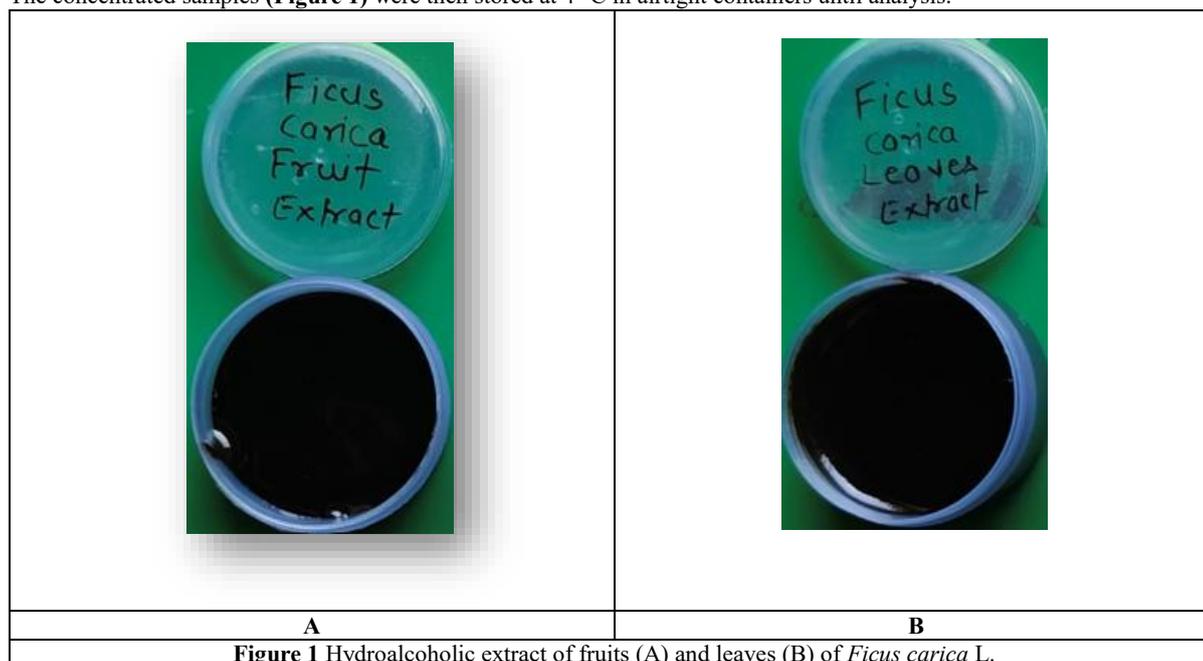
#### Plant material collection and preparation

The fruits and leaves of *Ficus carica* L. (FC) (Moraceae) (Anjeer/ Common Fig) were collected from a healthy, mature tree in Western/Sahyadri Ghat region of Pune, Maharashtra State of India. The plant material was authenticated by a qualified botanist, and a voucher specimen (BSI/WRC/Iden. Cer./2023/1001230007307) was deposited at the herbarium of Botanical Survey of India (B.S.I.), Pune, Maharashtra state of India. The gathered samples were meticulously cleaned with distilled water to eliminate dirt, air-dried in the shade for 7-10 days, ground using a mechanical grinder, and subsequently sieved through sieve no. 40, retaining the material on sieve no. 60 [9, 10].

#### Extraction Procedure

Powdered fruits and leaves of FC were extracted using a hydroalcoholic solvent mixture (70% ethanol and 30% water). In each case, 50 g of plant material was subjected to Soxhlet extraction for 12–15 hours with the solvent system [11]. The resulting extracts were passed through

Whatman No. 1 filter paper and then these filtrates underwent concentration under reduced pressure utilizing a rotary evaporator set at 40 °C. The concentrated samples (**Figure 1**) were then stored at 4 °C in airtight containers until analysis.



**Figure 1** Hydroalcoholic extract of fruits (A) and leaves (B) of *Ficus carica* L.

#### Proximate analysis

The powdered fruits and leaves of FC were assessed for physicochemical characteristics, including moisture content, total ash, acid-insoluble and water-soluble ash, alcohol-soluble and water-soluble extractive values, and foreign matter. Additionally, the concentrated extracts underwent preliminary phytochemical analysis to identify major classes of secondary metabolites [12, 13]. The extracts were additionally examined to ascertain Total Phenolic Content (TPC) and Total Flavonoid Content (TFC) determined using the Folin–Ciocalteu method and aluminum chloride colorimetric tests, respectively and Total Tannin Content (TTC) through a titrimetric approach [14, 15].

#### LC-MS instrumentation and analysis

A combined extract of FC fruits and leaves (1:1) was analysed by Liquid Chromatography–Mass Spectrometry (LC–MS) using an Agilent 6200 TOF/6500 Q-TOF B.09.00 (B9044.0) system at Venture Centre, Pune. Separation was achieved on a reverse-phase C18 column (100 mm × 2.1 mm, 1.7 μm) with a flow rate of 0.3 mL/min and an injection volume of 5 μL, maintaining the column temperature at 35 °C. The mass spectrometer was operated in both negative and positive electrospray ionization modes, with capillary voltages of 3.0 kV (NEG) and 3.5 kV (POS), a desolvation temperature of 350 °C, a nebulizing gas flow of 10 L/min, and an m/z scan range of 100–1000 [16, 17].

Compound identification was carried out by comparing the obtained spectra with published literature and online reference databases. Known standards of key phytochemicals were used for confirmation. A comparative assessment between fruits and leaves was performed to determine differences in phytochemical composition.

#### RESULTS AND DISCUSSION

The proximate analysis of powdered fruits and leaves of FC reveals significant differences in their physicochemical properties (**Table 1**).

**Table 1** Proximate analysis of powdered fruits and leaves of FC

Parameters	Physicochemical values of powdered <i>Ficus carica</i> Linn.	
	Fruits	Leaves
Moisture Content	10.55±0.16	8.61±0.08
Total Ash	3.9±0.85	9.87±0.11
Acid Insoluble Ash	0.57±0.21	0.98±0.02
Water Soluble Ash	2.29±0.17	1.84±0.11
Alcohol Soluble Extractive	19±0.17	10.29±1.03
Water Soluble Extractive	17.51±1.16	8.64±0.09
Foreign Organic Matters	0.06±0.31	0.19±0.07

\*Values are expressed in Mean % w/w ± S.D.

The moisture content is higher in fruits (10.55 ± 0.16%) compared to leaves (8.61 ± 0.08%), indicating their juicier nature, which could affect storage and stability [18]. The leaves exhibit significantly higher total ash content (9.87 ± 0.11%), suggesting a greater concentration of inorganic minerals. The acid-insoluble ash is higher in leaves viz. 0.98 ± 0.02%, reflecting a larger presence of siliceous impurities or substances, whereas fruits show higher water-soluble ash values (2.29 ± 0.17%), indicating more water-soluble minerals [19].

The alcohol-soluble extractive value is notably higher in fruits (19 ± 0.17%), pointing to a richer content of alcohol-soluble phytochemicals, such as flavonoids and other secondary metabolites as compared to leaves (10.29 ± 1.03%). Fruits also have a greater water-soluble extractive value (17.51 ± 1.16%), indicative of a higher presence of water-soluble constituents like sugars and tannins [20]. Both samples have minimal foreign organic matter, though slightly higher in leaves, reflecting their environmental exposure [19]. The differences in physicochemical parameters between the fruits and leaves of FC highlight the unique phytochemical and mineral profiles of each part. These findings support the distinct applications of fruits and leaves in herbal formulations and pharmacological research.

The preliminary properties of hydro-alcoholic test extracts of FC were mentioned **Table 2** reveals distinct characteristics.

**Table 2** Preliminary properties of test extract of FC

Parameters	Hydro-Alcoholic Extracts of <i>Ficus carica</i> Linn.	
	Fruits	Leaves
Colour	Dark Brown	Brownish Black
Odour	Aromatic	Aromatic
Taste	Characteristics	Characteristics
Nature	Viscous	Viscous
Solubility	Miscible	Miscible
% Moisture	2.60% w/w	1.56% w/w
% Ash Content	2.55% w/w	2.80% w/w

The hydro-alcoholic extracts of FC fruits and leaves demonstrate consistent aromatic, taste, and solubility properties. The extract of fruits is dark brown, whereas the extract from leaves is brownish black. The darker color in the leaves could indicate a higher concentration of certain pigments or tannins [11]. Both extracts exhibit an aromatic odor, characteristic of the plant's phytochemical profile. Both extracts share characteristic taste profiles, suggesting similar secondary metabolites contributing to the taste. Both extracts are viscous, indicative of a dense phytochemical composition and solvent retention. Both extracts are miscible in the solvent system, reflecting good solubility of bioactive constituents in the hydro-alcoholic medium. The moisture content is higher in fruit extracts (2.60% w/w), possibly due to the juicier nature of fruits, which retain more water during extraction. The ash content is slightly higher in leaf extracts viz. (2.80% w/w), suggesting a marginally higher concentration of inorganic mineral residues compared to fruits (2.55% w/w) [13].

The **Table 3** represents the results of preliminary phytochemical analysis of hydro-alcoholic extracts of fruits and leaves of FC. The analysis highlights the presence (+) and absence (-) of specific phytochemical constituents in the test extracts.

**Table 3** Preliminary phytochemical constituents in test extracts of FC

Sr. No.	Hydro-Alcoholic Extracts of <i>Ficus carica</i> Linn.		
	CHEMICAL TEST ↓	Fruits	Leaves
1		<b>TEST FOR ALKALOIDS</b>	
a)	Mayer's Test	+	-
b)	Hager's Test	+	-
c)	Wagner's Test	+	-
2		<b>TEST FOR CARBOHYDRATE</b>	
A		<b>General Test</b>	
a)	Molisch's Test	+	+
B		<b>Test for Reducing Sugar</b>	
b)	Fehling test	+	+
c)	Benedict's test	+	+
3		<b>TEST FOR STEROIDS</b>	
a)	Salkowski reaction	+	+
4		<b>TEST FOR GLYCOSIDES</b>	
A		<b>Test for Cardiac Glycoside</b>	
a)	Baljet's Test	+	+
b)	Keller-killiani Test	+	+
B		<b>Test for Anthraquinone Glycosides</b>	
a)	Brontrager's Test	+	-
C		<b>Test for Saponin Glycosides</b>	
a)	Foam Test	+	+
5		<b>TEST FOR FLAVONOIDS</b>	
a)	Lead acetate test	+	+
b)	Shinoda test	+	+
6		<b>TEST FOR FAT AND OILS</b>	
a)	Solubility Test	-	+
b)	Filter Paper Test	-	+
7		<b>TEST FOR TANNIN AND PHENOLIC COMPOUND</b>	
a)	Potassium Permanganate Test	+	+
b)	Lead acetate solution Test	+	+
c)	Bromine Water Test	+	+
8		<b>TEST FOR PROTEIN</b>	
a)	Biuret test	+	+
9		<b>TEST FOR AMINO ACID</b>	
a)	Ninhydrin test	+	+
10		<b>TEST FOR GUMS AND MUCILAGE'S</b>	
a)	Hydrolyze Test (Gums)	+	-
b)	Ruthenium Red Test (Mucilage)	+	-

\*Presence (+) and absence (-)

The exclusive presence of Alkaloids in fruits indicates potential therapeutic roles, as alkaloids often possess pharmacological properties like analgesic and anti-inflammatory effects [21]. The carbohydrates and reducing sugars presence in both fruits and leaves suggests their contribution to energy storage and structural components, which might be exploited in nutraceuticals [22]. Steroids are detected in both fruits and leaves, indicating potential applications in anti-inflammatory and immunomodulatory therapies [23]. Cardiac glycosides consistent presence could be important for cardiovascular health [24]. Anthraquinone glycosides, present only in fruits, highlight its potential for laxative properties [25]. Saponin glycosides presence may relate to cholesterol regulation and immune-boosting effects [26]. Universal presence of Flavonoids in both fruits and leaves suggests antioxidant properties, enhancing the plant's role in disease prevention [27]. The absence of fats and oils in fruits and presence in leaves is noteworthy. Consistent presence of Tannins and Phenolic Compounds highlights astringent and antimicrobial properties, supporting traditional uses in wound healing and infection control [28]. Proteins and Amino Acids presence reflects a nutritional advantage, with possible contributions to cell repair and enzymatic functions [29]. Fruits showing positive results for both Gums and Mucilages suggest their use in emulsification, stabilization, and potential as dietary fibers [30]. This comprehensive analysis underscores FC phytochemical diversity, indicating its potential as a source for pharmaceuticals, nutraceuticals, and functional foods. Further research and isolation of active compounds could validate its traditional uses and explore new therapeutic applications.

The total phenolic, flavonoid and tannin content of hydro-alcoholic extracts of FC fruits and leaves was estimated and presented in **Table 4**.

**Table 4** TPC, TFC, TTC values of test extracts of FC

Sr. No.	Parameters	Hydro-Alcoholic Extracts of <i>Ficus carica</i> Linn.	
		Fruits	Leaves
1	Total Phenolic Content (TPC)	31.39±1.4	1.97±2.9
2	Total Flavonoid Content (TFC)	8.97±2.9	15.73±2.8
3	Total Tannin Content (TTC)	1.08±2.10	3.01±0.07

\*Values are expressed as mg.100 gm<sup>-1</sup>

The phenolic content in the fruits was found to be 31.39 ± 1.4 mg GAE/g extract which is markedly higher than in the leaves (1.97±2.9 mg GAE/g extract). Phenolic compounds are known for their antioxidant activity and play a crucial role in preventing oxidative stress [31]. The high phenolic content in FC fruits indicates their potential as a natural source of antioxidants, which can be beneficial for health and the food industry. However, the total flavonoid content was also assessed, and a contrasting trend was observed. Unlike the phenolic content, the flavonoid content in the leaves viz. 15.73 ± 2.8 mg QE/g extract was significantly higher compared to the fruits. Flavonoids are another group of bioactive compounds with well-established antioxidant, anti-inflammatory, and anticancer properties [32]. The elevated levels of flavonoids in the leaves suggest their potential use in herbal formulations or dietary supplements.

The tannin content in the leaves of FC was recorded as 3.01 ± 0.07 mg/100 gm, which is considerably higher compared to the tannin content in the fruits. The relatively high standard deviation observed in the fruit extract (1.08 ± 2.10) indicates variability, possibly due to differences in maturity, environmental conditions, or extraction efficiency.

These variations may be attributed to differences in the biosynthesis, distribution, and accumulation of secondary metabolites in plant tissues [33]. Environmental factors, maturity stages, and extraction methods could also influence the observed results. Further studies focusing on the individual phenolic and flavonoid compounds and their bioactivities are recommended to better understand their therapeutic potential. Overall, both fruits and leaves of FC serve as valuable sources of bioactive compounds, each with distinct applications depending on the targeted therapeutic or industrial purpose.

The retention time and scores of identified compounds in NEG and POS ionization modes were recorded in LC-MS analysis of hydroalcoholic mixture of extracts of fruits and leaves of FC (Table 5 and 6). Table 5 LC-MS data-NEG ionization mode for compounds identified in hydroalcoholic extract of fruit and leaves of FC

Sr. No.	Name	Formula	RT	Mass	CAS	Score (DB)
1	Threonate	C4 H8 O5	2.254	136.0377	70753-61-6	98.19
2	L-Xylonate	C5 H10 O6	2.286	166.0485		96.17
3	Gluconic acid	C6 H12 O7	2.305	196.0589	526-95-4	98.09
4	D-Fructose	C6 H12 O6	2.318	180.0640	57-48-7	96.87
5	3-b-Galactopyranosyl glucose	C12 H22 O11	2.336	342.1162	28447-38-3	94.58
6	D-Tartaric acid	C4 H6 O6	2.353	150.0164	147-71-7	97.79
7	Ethyl glucuronide	C8 H14 O7	2.356	222.0743	17685-04-0	98.51
8	2-Dehydro-D-xylonate	C5 H8 O6	2.362	164.0327		97.16
9	5'-Butyrylphosphouridine	C13 H19 N2 O10 P	2.376	394.0785		90.92
10	threo-Isocitric acid	C6 H8 O7	2.592	192.0279		94.89
11	3'-Methoxyfukiic acid	C12 H14 O8	9.217	286.0696		97.89
12	Dihydroferulic acid 4-O-glucuronide	C16 H20 O10	9.795	372.1057		99.28
13	Dihydroferulic acid 4-O-glucuronide	C16 H20 O10	10.134	372.1065		94.80
14	Cis-5-Caffeoylquinic acid	C16 H18 O9	10.471	354.0951		99.79
15	Benzoquinoneacetic acid	C8 H6 O4	10.722	166.0269	10275-07-7	98.78
16	Methyl salicylate O-[rhamnosyl-(1->6)-glucoside]	C20 H28 O12	10.894	460.1575		98.60
17	Monomethyl phthalate	C9 H8 O4	11.127	180.0427	4376-18-5	96.67
18	Rustoside	C26 H28 O15	11.224	580.1420	83144-68-7	97.14
19	5a,6a-Epoxy-7E-megastigmene-3a,9e-diol 3-glucoside	C19 H32 O8	11.364	388.2092	189351-14-2	96.27
20	dTDP-D-mycarose	C17 H28 N2 O14 P2	11.615	546.1009		96.03
21	Monomethyl phthalate	C9 H8 O4	11.646	180.0425	4376-18-5	98.07
22	Diglycolic acid	C4 H6 O5	11.667	134.0219		98.59
23	Apigenin 6-C-glucoside 8-C-arabinoside	C26 H28 O14	11.685	564.1476		96.69
24	Mono-trans-p-coumaroylmesotartaric acid	C13 H12 O8	11.705	296.0535	27174-06-7	97.62
25	Furocoumarinic acid glucoside	C17 H18 O9	11.758	366.0948		99.13
26	5a,6a-Epoxy-7E-megastigmene-3a,9e-diol 3-glucoside	C19 H32 O8	11.845	388.2093	189351-14-2	98.84
27	1-O-E-Cinnamoyl-(6-arabinosyl)glucose	C20 H26 O11	12.341	442.1466	181373-66-0	97.76
28	Violarvensin	C27 H30 O14	12.372	578.1622		95.13
29	Rutin	C27 H30 O16	12.439	610.1521	153-18-4	95.47
30	Furocoumarinic acid glucoside	C17 H18 O9	12.856	366.0948		98.56
31	Ptelatoside A	C19 H26 O10	12.923	414.1521	90899-20-0	97.63
32	Torachryson 8-glucoside	C20 H24 O9	13.244	408.1412	64032-49-1	97.22
33	PG(16:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C44 H73 O10 P	13.769	792.4948		92.34
34	PG(16:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C44 H73 O10 P	14.170	792.4952		91.33
35	3-O-Sulfogalactosylceramide	C48 H93 N O12 S	14.890	907.6433	151122-71-3	90.15
36	Traumatic Acid	C12 H20 O4	17.517	228.1368	6402-36-4	97.40
37	Nordihydrocapsiate	C17 H26 O4	20.506	294.1839		95.72
38	Epicatechin-(4beta->8)-gallocatechin	C30 H26 O13	20.797	594.1374		98.24
39	Lauryl hydrogen sulfate	C12 H26 O4 S	23.034	266.1560	151-21-3	95.68

\*The phytoconstituents are evaluated on the basis of their registered mass spectra m/z databases. The phyto-constituents mentioned in table are main compound some other natural compounds are also present as isomeric forms or as isobaric compounds with the same molecular weight but different elemental composition.

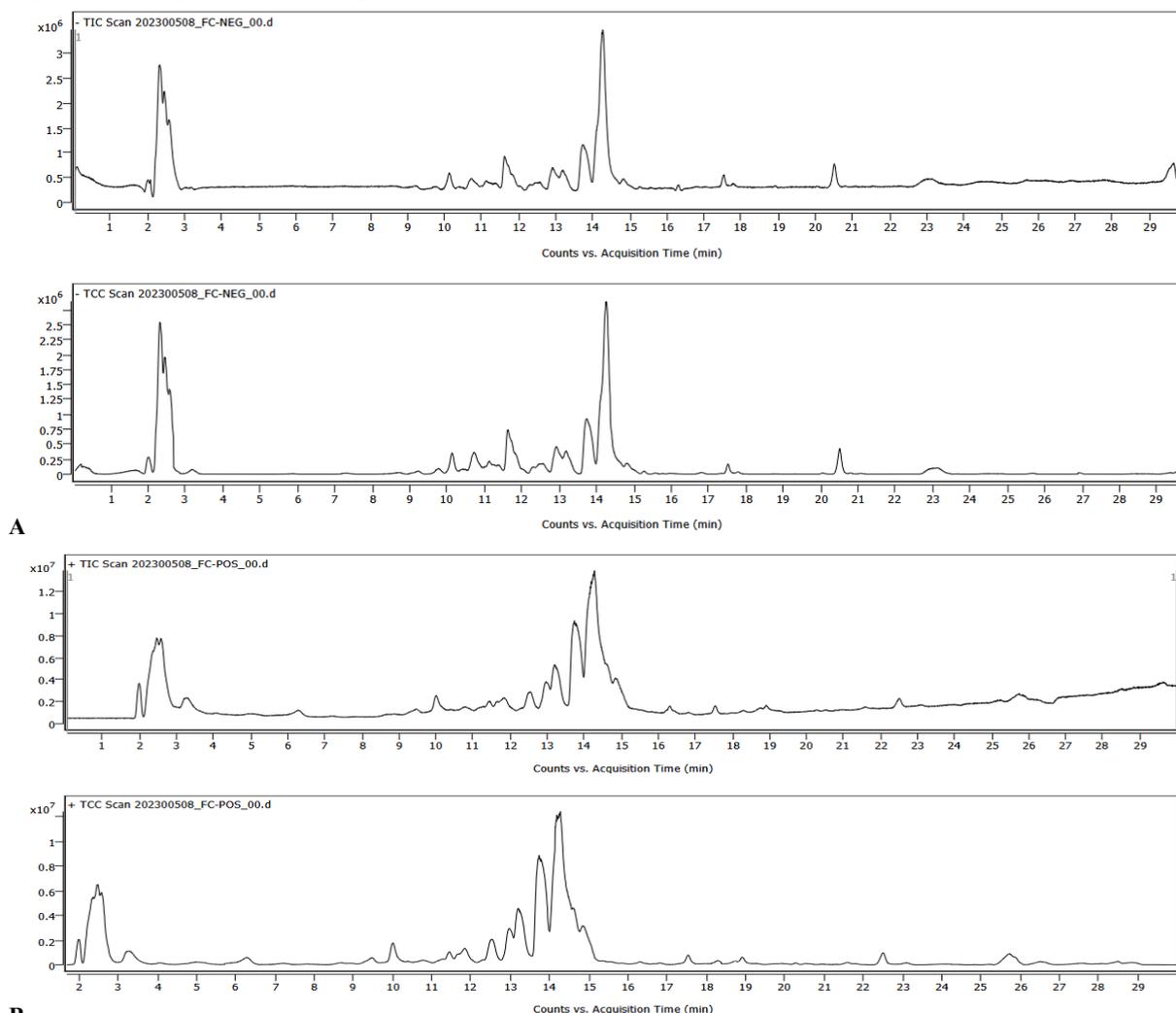
**Table 6** LC–MS data-POS ionization mode for compounds identified in hydroalcoholic extract of fruit and leaves of FC

Sr. No.	Name	Formula	RT	Mass	CAS	Score (DB)
1	Dulcitol	C6 H14 O6	2.185	182.0787	608-66-2	99.29
2	3-Galactosyllactose	C18 H32 O16	2.248	504.1682	32694-82-9	96.27
3	Sucrose	C12 H22 O11	2.252	342.1163	57-50-1	98.74
4	D-1-[(3-Carboxypropyl)amino]-1-deoxyfructose	C10 H19 N O7	2.263	265.1166	10003-63-1	98.01
5	Malonylcarnitine	C10 H18 N O6	2.263	248.1138	853728-01-5	98.57
6	Choline chloride	C5 H13 N O	2.269	103.1002	67-48-1	98.09
7	Trimethylammonioacetate	C5 H12 N O2	2.357	118.0867		99.91
8	Ephedrin	C11 H19 N O6	2.470	261.1215	126050-09-7	97.77
9	N-(1-Deoxy-1-fructosyl)valine	C11 H21 N O7	2.473	279.1321		98.57
10	L-Pipecolic acid	C6 H11 N O2	2.500	129.0794	3105-95-1	97.58
11	Methoxamine	C11 H17 N O3	2.590	211.1208	390-28-3	91.23
12	Pirbuterol	C12 H20 N2 O3	2.593	240.1472	38677-81-5	99.30
13	N-(1-Deoxy-1-fructosyl)isoleucine	C12 H23 N O7	2.598	293.1479	87304-79-8	98.24
14	Ephedrine	C10 H15 N O	2.622	165.1151	299-42-3	99.07
15	Ethyl beta-D-glucopyranoside	C8 H16 O6	3.078	208.0944	3198-49-0	99.07
16	N-(1-Deoxy-1-fructosyl)tyrosine	C15 H21 N O8	3.123	343.1265	34393-22-1	91.23
17	N-(1-Deoxy-1-fructosyl)leucine	C12 H23 N O7	3.295	293.1477	34393-18-5	98.62
18	3-(3,4,5-Trimethoxyphenyl)propanoic acid	C12 H16 O5	3.314	240.0996	25173-72-2	99.20
19	Ilicifolinolide A	C11 H20 O7	3.612	264.1205		94.97
20	Ephedrine	C10 H15 N O	4.078	165.1151	299-42-3	97.91
21	(S)-Angelica	C15 H16 O6	4.991	292.0945	49624-66-0	99.40
22	N-(1-Deoxy-1-fructosyl) phenylalanine	C15 H21 N O7	4.997	327.1313	87251-83-0	98.64
23	N-(Heptan-4-yl)benzo[d][1,3] dioxole-5-carboxamide	C15 H21 N O3	7.193	263.1518	745047-51-2	98.89
24	1,8-Diazacyclotetradecane-2,9-dione	C12 H22 N2 O2	8.635	226.1682		99.83
25	Tetrahydropentoxylone	C17 H22 N2 O7	8.835	366.1423	154204-09-8	98.70
26	De-O-methylsimmondsin	C15 H23 N O9	8.861	361.1373	135105-75-8	94.59
27	Ricinine	C8 H8 N2 O2	9.447	164.0589	524-40-3	98.83
28	1-(3-Methylbutanoyl)-6-epiosylglucose	C16 H28 O11	9.553	396.1626	467242-31-5	94.49
29	Tyrosyl-Valine	C14 H20 N2 O4	9.903	280.1423		99.23
30	1,8-Diazacyclotetradecane-2,9-dione	C12 H22 N2 O2	9.967	226.1683		99.68
31	Cincassiol B	C20 H32 O8	9.991	400.2106	73599-13-0	97.67
32	Carbendazim	C9 H9 N3 O2	10.013	191.0701	10605-21-7	96.91
33	trans-p-Menthane-1,7,8-triol 8-glucoside	C16 H30 O8	10.285	350.1937	217962-29-3	97.49
34	(2R,6x)-7-Methyl-3-methylene-1,2,6,7-octanetetrol 2-glucoside	C16 H30 O9	10.393	366.1886	219814-32-1	95.32
35	Diflorasone	C22 H28 F2 O5	10.401	410.1911	2557-49-5	97.32
36	Apiosylglucosyl 4-hydroxybenzoate	C22 H24 O12	10.697	432.1264	223261-31-2	96.87
37	2-[4-(3-Hydroxypropyl)-2-methoxyphenoxy]-1,3-propanediol 1-glucoside	C19 H30 O10	10.701	418.1836	68340-35-2	92.89
38	trans-p-Menthane-1,7,8-triol 8-glucoside	C16 H30 O8	11.093	350.1940	217962-29-3	95.94
39	Benzyl gentiobioside	C19 H28 O11	11.103	432.1628	56775-64-5	90.20
40	Cyanidin 3-sambubioside	C26 H29 O15	11.228	581.1495	33012-73-6	97.01
41	Apigenin 6-C-glucoside 8-C-arabinoside	C26 H28 O14	11.308	564.1470		97.67
42	Biochanin A 7-(6-methylmalonylglucoside)	C26 H26 O13	11.679	546.1362	34232-19-4	96.91
43	Apigenin 6-C-glucoside 8-C-arabinoside	C26 H28 O14	11.680	564.1476		98.45
44	Furocoumarinic acid glucoside	C17 H18 O9	11.763	366.0949		97.57
45	Furocoumarinic acid glucoside	C17 H18 O9	11.768	366.0947		98.12
46	5-Methyl-2,5-di-1-pyrrolidinyl-2-cyclopenten-1-one	C14 H22 N2 O	11.844	234.1734	97826-64-7	98.41
47	5a,6a-Epoxy-7E-megastigmen-3a,9e-diol 3-glucoside	C19 H32 O8	11.860	388.2095	189351-14-2	91.34
48	L-Menthyl acetoacetate	C14 H24 O3	11.863	240.1726	59557-05-0	98.87
49	2,3-Naphthalenedicarboxylic acid	C12 H8 O4	11.937	216.0420		98.70
50	Pelargonidin 3-rhamnoside 5-glucoside	C27 H31 O14	12.376	579.1699	53925-32-9	95.06
51	Cyanidin 3-glucogalactoside	C27 H31 O16	12.445	611.1595	142562-01-4	94.07
52	Furocoumarinic acid glucoside	C17 H18 O9	12.857	366.0947		98.71
53	1,4-Dihydroxy-6-naphthoate	C11 H8 O4	12.861	204.0421		99.23
54	Ptelatoside A	C19 H26 O10	12.918	414.1522	90899-20-0	98.55
55	Ptelatoside A	C19 H26 O10	12.924	414.1519	90899-20-0	98.34
56	Torachrysone 8-glucoside	C20 H24 O9	13.054	408.1414	64032-49-1	97.84
57	2,3-Naphthalenedicarboxylic acid	C12 H8 O4	13.178	216.0421		98.77
58	Coroloside	C35 H54 O12	13.255	666.3607	57361-71-4	92.05
59	(+)-7-epi-Syringaresinol 4'-glucoside	C28 H36 O13	13.319	580.2143		90.33
60	5-Megastigmen-7-yne-3,9-diol 9-glucoside	C19 H30 O7	13.336	370.1987	62512-26-9	98.44
61	Carpaine	C28 H50 N2 O4	13.781	478.3762	3463-92-1	91.21
62	Calenduloside G methyl ester	C43 H68 O14	13.783	808.4597	155740-15-1	94.44
63	Calenduloside G methyl ester	C43 H68 O14	14.240	808.4594	155740-15-1	94.87
64	Erythromycin ethylsuccinate	C43 H75 N O16	14.534	861.5083	1264-62-6	95.53
65	beta-Solamarine	C45 H73 N O15	14.782	867.4956	3671-38-3	91.78
66	PC(18:2(9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C48 H81 N O8 P	15.645	830.5706		97.07
67	gamma-2-Solamarine	C39 H63 N O11	15.646	721.4381	11034-34-7	93.24
68	4'-O-methyl(-)-epicatechin	C16 H16 O6	15.837	304.0941		97.28
69	Flazine	C17 H12 N2 O4	16.166	308.0793	100041-05-2	99.04
70	Valacyclovir	C13 H20 N6 O4	16.467	324.1544	124832-27-5	97.12
71	4,4-Difluoropregn-5-ene-3,20-dione	C21 H28 F2 O2	16.816	350.2065		95.75
72	Psoralen	C11 H6 O3	17.541	186.0317	66-97-7	99.34
73	2,2,4,4,-Tetramethyl-6-(1-oxopropyl)-1,3,5-cyclohexanetrione	C13 H18 O4	18.292	238.1204		98.41

74	Helinorbisabone	C14 H18 O4	18.754	250.1207	201288-95-1	99.34
75	Tetrahydrofurfuryl cinnamate	C14 H16 O3	18.755	232.1098	65505-25-1	98.88
76	2,3-Naphthalenedicarboxylicacid	C12 H8 O4	18.917	216.0425		98.64
77	9,10,13-Trihydroxystearic acid	C18 H36 O5	20.055	332.2572	50439-74-2	95.98
78	(+)-Setoclavine	C16 H18 N2 O	20.279	254.1419	519-12-0	98.55
79	Azoxystrobin	C22 H17 N3 O5	21.597	403.1166	131860-33-8	99.73
80	(p-Aminobenzyl)penicillin	C16 H19 N3 O4 S	21.599	349.1086		90.31
81	$\epsilon$ -Rhodomycinone	C22 H20 O9	21.787	428.1102	21288-60-8	98.90
82	Octhilimone	C11 H19 N O S	21.818	213.1184	26530-20-1	97.62
83	Tebuconazole	C16 H22 Cl N3 O	22.426	307.1448	107534-96-3	98.53
84	4,4'-Bis(dimethylamino)benzo phenone	C17 H20 N2 O	22.503	268.1580	90-94-8	98.25
85	C14:1n-9	C14 H26 O2	23.015	226.1929		98.81
86	p-Hydroxyphenethyl trans-ferulate	C18 H18 O5	23.102	314.1151	84873-15-4	98.64
87	Epicatechin-(2beta->7,4beta->6)-catechin	C30 H24 O12	25.213	576.1254		95.35
88	Austrobailignan 7	C20 H22 O5	25.731	342.1471	55890-25-0	97.83
89	4,5-Dihydro-1-benzoxepin-3(2H)-one	C10 H10 O2	25.741	162.0684	35783-10-9	98.47
90	Stigmatellin Y	C29 H40 O6	26.460	484.2817		97.26
91	Stigmatellin Y	C29 H40 O6	26.499	484.2815		96.96
92	Alpha-CEHC	C16 H22 O4	26.546	278.1518	4072-32-6	99.22
93	Acetyl tributyl citrate	C20 H34 O8	28.068	402.2248	77-90-7	98.92
94	Stigmatellin Y	C29 H40 O6	28.447	484.2819		94.95
95	Polidocanol	C30 H62 O10	28.690	582.4337	3055-99-0	97.78

\*The phytoconstituents are evaluated on the basis of their registered mass spectra  $m/z$  databases. The phyto-constituents mentioned in table are main compound some other natural compounds are also present as isomeric forms or as isobaric compounds with the same molecular weight but different elemental composition.

The high precision and reliability of the data were supported by the database match scores, most exceeding 90 percent, indicating strong confidence in compound identification. NEG ion mode mass spectroscopy is the most commonly used tool in phyto-analysis. NEG mode mass spectrometry is widely utilized in phytochemical analysis. The electrospray process generates ( $M-H^-$ ) ions, enabling accurate determination of the mass-to-charge ( $m/z$ ) ratio of sample molecules. Electrospray ionization in negative mode is particularly effective for detecting low-molecular-weight ketones and carboxylic acid derivatives. [34]. In POS ionization in mass spectroscopy involves the formation of POS ions, for the determination of the mass to charge ratio of the sample molecule [ $M+H^+$ ]. The chromatograms of identified phytoconstituents in the samples of plant materials presented in the **Figure 2 A and B**.



**Figure 2** TIC and TCC scan of sample FC in LC-MS Analysis by *NEG* ionization mode (**A**) identified 259 (479 found) compounds and by *POS* ionization mode (**B**) identified 851 (1900 found) compounds.

The LC-MS analysis of FC hydroalcoholic extracts revealed a diverse array of bioactive compounds in both fruits and leaves. Using both NEG and POS ionization modes, a total of 1110 phytochemicals were identified, including flavonoids, phenolic acids, alkaloids, and tannins etc. Most identifications scored above 90, indicating reliable compound matches against the database.

The analysis using LC-MS in the NEG ionization mode identified several metabolites with high precision. A total of 39 unique compounds with retention times from 2.254 to 23.034 minutes. Key findings are Dihydroferulic acid 4-O-glucuronide (99.28, RT= 9.795 min), Cis-5-Caffeoylquinic acid (99.79, RT= 10.471 min), and Furocoumarinic acid glucoside (99.13, RT = 11.758 min). The diverse compounds ranged from simple acids like Threonate (RT= 2.254 min) to complex glycosides like Methyl salicylate O-[rhamnosyl-(1→6)-glucoside] (RT= 10.894 min) and Rutin (RT= 12.439 min). The POS ionization mode in LC-MS analysis identified 95 unique compounds with retention times (RT) ranging from 2.185 to 28.690 minutes. Key findings are Dulcitol (99.29, RT= 2.185 min), Sucrose (98.74, RT= 2.252 min), Ephedrine (99.07 and 97.91, RT= 2.622 and 4.078 min), Cyanidin 3-sambubioside (97.01, RT=11.228 min), Azoxystrobin (99.73, RT= 21.597 min).

Few compounds were identified at two distinct retention times, suggesting isomeric or adduct formation. The detection of compounds like Cis-5-Caffeoylquinic acid with a near-perfect score 99.79 highlights the sensitivity of the LC-MS method and is known for its antioxidant properties, could be significant for further functional or pharmaceutical studies [35]. Several complex glycosides were detected, Rutin and Furocoumarinic acid glucoside, often associated with bioactive properties, including anti-inflammatory and UV-protective effects. The dataset revealed a diverse array of compounds spanning various chemical classes, including carbohydrates and derivatives, amino acid derivatives, flavonoids and phenolic compounds etc. The identified metabolites align with expected profiles in similar samples but also provide novel insights, warranting further validation and exploration of bioactivity.

### CONCLUSION

The research effectively characterized hydroalcoholic extracts of FC fruits and leaves through LC-MS analysis in both NEG and POS ionization modes. The outcomes lend scientific credibility to the plant's traditional medicinal applications and emphasize its potential as a valuable source of natural therapeutic compound. The comprehensive identification of bioactive compounds sets the stage for future studies focusing on the isolation, bioactivity, and mechanism of action of individual phytochemicals.

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**LIST OF ABBREVIATIONS:**

**FC-** *Ficus carica* L.

**LC-MS-** Liquid Chromatography-Mass Spectrometry

**NEG-** Negative

**POS-** Positive

**Q-TOF-** Quadrupole Time-of-Flight Mass Spectrometry

**DB-** Data Base

**RT-** Retention Time

**TPC-** Total Phenolic Content

**TFC-** Total Flavonoid Content

**TTC-** Total Tannin Content

**ESI-** Electrospray ionization