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The nutrient-rich profile of wonder cane: A comprehensive phytochemical and elemental analysis of Co 86032 sugarcane variety

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Abstract

Sugarcane (*Saccharum officinarum* L.) is a key crop, cultivated globally for its significant contributions to sugar production and renewable bioenergy. Beyond its industrial uses, sugarcane juice is also valued for its nutritional benefits. Nutritional attributes and flavor profiles are influenced by various factors including plant variety, soil quality, cultivation techniques, geographic location and humidity levels. This study examines the Co 86032 sugarcane variety, known as wonder cane, recognized for its high yield and disease resistance. Using GC-MS, ICP-MS and metabolite analysis, we comprehensively profiled its phytochemical and elemental composition. Phytocomponent screening identified alkaloids, carbohydrates, saponins, tannins, phenols, and glycosides. GC-MS revealed 25 different volatile organic compounds and bioactive phytochemicals, while ICP-MS detailed 16 essential and trace elements, highlighting nutritional and potential toxicological aspects. The metabolite analysis offered a distinct perspective on the metabolic profile and its pathways. Biological assays showed significant antimicrobial activity against pathogens, strong antioxidant capacity, and potential anticancer properties attributed to specific compounds identified through GC-MS. Moreover, the beneficial properties of sugarcane juice, which is packed with essential nutrients and bioactive substances, were emphasized, showcasing its role in promoting hydration and supporting overall health. This comprehensive profiling and bioactivity assessment underscore Co 86032 variety as a valuable high-yield crop and a source of phytochemicals with pharmaceutical, nutraceutical, and functional food applications.

1. Introduction

Sugarcane, a hybrid plant from the *Saccharum* species in the Poaceae family, is known for its high water and nutrient requirements, long growth period, and substantial biomass production. This tropical perennial grass produces multiple stems, reaching heights of 3 to 4 meters with a diameter of about 5 centimeters, by generating lateral shoots at its base. As a perennial crop, sugarcane can be harvested every 12 to 18 months from the same plants for up to five years, though yield typically decreases over time (Singh *et al*., 2015). Sugarcane accounts for about 86% of sugar crops, with sugar beets making up the remaining 14%. It plays a crucial role in the global sugar market, making up about 95% of worldwide sugar production and 80% of the total sugar produced. In 2022, India became the largest producer and consumer of sugar, with productivity rising from 81.98 tonnes per hectare in 2021-22 to 84.0 tonnes per hectare in 2022-23, surpassing the global average of 77 tonnes per hectare. For the 2023/24 season, Brazil reclaimed its position as the world's largest producer and exporter of sugar, providing over 60% of the global raw sugar supply.

India has become the world's largest consumer and the second-largest producer and exporter of sugar. Sugarcane is extensively grown in several Indian states, including Tamil Nadu, Karnataka, Andhra Pradesh, Maharashtra, Madhya Pradesh, Gujarat, Uttarakhand, Uttar Pradesh, Punjab, Haryana and Bihar. Covering approximately 5.15 million hectares, sugarcane cultivation accounts for about 2.50% of India's total cropped area. The country produces over 468.79 million tonnes of sugarcane, with a productivity rate of 83.89 tonnes per hectare. India is expected to see substantial recovery due to favorable weather and increased plantings, with production projected to rise by 5.1 million tonnes to 35.6 million tonnes by 2030. In 2024, India will assume the chairmanship of the International Sugar Organization (ISO), leading the global sugar industry. The country is notable for paying the highest prices to its sugarcane farmers worldwide while providing the cheapest sugar to its citizens despite record-high global sugar prices (FAOSTAT, 2022).

Global sugar consumption is projected to increase at an annual rate of 1.4%, reaching 196 million tonnes by 2030, driven by population and income growth. During this period, the average global per capita consumption is anticipated to rise from 22 kg to 23 kg, though there will be considerable regional and country-specific differences. In the 2023/24 season, global sugar consumption exceeded 176 million

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metric tonnes, with India alone consuming around 31 million metric tonnes. By 2030, India is projected to be the world's most populous country, with an estimated population of 1.51 billion people. According to the FAO, global food production must increase by 70% by 2050 to meet the needs of a growing global population and the evolving consumption patterns of the expanding middle class. (OECD-FAO, 2021).

Sugarcane originating from tropical South and Southeast Asia, exhibits a wide variety of species within its genus. The tropical cane variety Co 86032, often referred to as "Wonder cane," is a prominent cultivar in India, covering 6.176 lakh hectares. It is highly favoured by growers because of its remarkable characteristics and suitability for industrial purposes. Today's cultivated sugarcanes are complex hybrids involving multiple species, primarily *S. officinarum* (the noble cane) and *S. spontaneum*, with genetic contributions from *S. sinense, S. robustum, S. barberi* and other related grass genera. Sugarcane is a crucial crop, offering renewable and natural agricultural resources such as sugar, biofuel, fiber, fertilizer, and numerous by-products, contributing to ecological sustainability. Beyond refined sugar, processing sugarcane juice produces by-products like brown sugar, molasses, and jaggery. Key by-products from the sugar industry include bagasse, used in the paper industry, and molasses, which is used to produce ethanol (Ali *et al*., 2019).

Sugarcane juice, a common beverage often commercialized using crushers, serves as a nutritional supplement. It primarily consists of 70-75% water, 13-15% sucrose, and 10-15% fiber. The juice's color components can be categorized into polyphenolic compounds, plant pigments, caramels and degradation products from sugar-amine reactions. While high in natural sugars, it should be consumed in moderation. Sugarcane juice is the primary ingredient for refined sugar production, and its wax offers a cost-effective alternative to carnauba wax used in cosmetics and pharmaceuticals. The juice contains various phytochemicals, including phenolics, terpenoids, sterols, policosanols and lignins which are common in plant waxes and oils. Beyond its industrial uses, sugarcane juice is also valued for its nutritional benefits. It is a rich source of essential nutrients, including vitamins C and B, and minerals like calcium, magnesium, potassium, and iron. These components contribute to its nutritional value and are linked to several biological effects such as antihyperglycemic, antihepatotoxic, analgesic, anti-inflammatory, diuretic, antithrombotic, and antihypercholesterolemic properties (Hewawansa *et al*., 2024). Additionally, sugarcane juice contains antioxidants and has a high glycemic index, providing a quick source of energy. Its natural sugars and phytonutrients make it a refreshing and health-boosting beverage.

With the growing popularity of antioxidant-rich supplements and fortified beverages in India's market, as well as the recognized therapeutic value of blackstrap molasses, interest in the antioxidant properties of sugarcane has increased. The sugarcane plant contains a high concentration of polyphenols, which has spurred research into optimizing the extraction processes for these polyphenolic fractions and evaluating their potential properties (Jamir *et al*., 2021; Carvalho *et al*., 2021). This study aims to perform phytochemical screening, GC-MS, ICP-MS along with pathway and enrichment analysis on sugarcane juice samples from the Co 86032 variety. The goal is to accurately identify the volatile phytocompounds and multiple elements in the samples, thereby evaluating their potential biological and pharmacological activities.

2. Materials and Methods

2.1 Collection of plant material

Mature stems (twelve months old) of the sugarcane variety Co 86032, which covers about 80% of the cane cultivation area in Tamil Nadu and has distinctive characteristics (Table 1), were harvested close to the ground at a plantation in Vallanadu, Trichy district, Tamil Nadu from Kothari Sugars and Chemicals Ltd., Kattur sugar mill area in January 2024 (Figure 1). Dr. M. Shanmuganadhan (Sugarcane breeder, Tamil Nadu Agricultural University) validated the plant material and a specimen of the plant material was deposited in the Herbarium of the Department, Genetics and Plant Breeding, ADAC & RI, Trichy (ADACRI/TRY/GPB/GP/SC/24/003). Once they arrived at the laboratory, the stems were cleaned and peeled for juice extraction.

Table 1: Special features of Co 86032 variety

Parentage	Co 62198 X CoC 671
Released	1996
Soil type	Medium to deep black, fertile, well drained
Duration (month)	10-12
Season	Mid-late
Sucrose at 12 months (%)	19.2
Cane yield (t/ha)	110.0
CCS % and CCS (t/ha)	13.0 and 15.1
Cane yield (t/ha)	110.0
Characters / features	• Performs well in all soil types and can be grown throughout the year • High cane and CCS yield • Gives higher recovery • Jaggery: A-1 quality (golden yellow) • Sparse flowering and easy de-trashing • Profuse tillering and good ratoonability • Amenable for wide row spacing • Drought tolerant and moderately resistant to smut, red rot, wilt and grassy shoot disease

2.2 Preparation of juice sample

Sugarcane juice was extracted using a power-operated sugarcane crusher machine without any additives. The extracted juice was then filtered through a double sieve and muslin cloth to eliminate any impurities. This filtered juice was subsequently used for GC-MS, ICP-MS and phytochemical screening.

Figure 1: Field view and harvested cane bundle of Co 86032 variety.

2.3 Gas chromatography-mass spectrometry (GC-MS)

The filtered cane juice was collected in the head space sample vials and covered with O-ring and then air tightened using moulded screw cap. The head space vial was loaded in the GC-MS facility available in Agricultural College and Research Institute, Madurai. Using Shimadzu QP 2020 model GC-MS attached with column: Rtx-SMS, helium flow of 1 ml/min with pressure of 61.3 kPa and temperature of 70°C, hold for 1 min and increase to 225°C @ 5°C, increase and hold for 3 min, and final temperature of 280°C @ 5°C, increase with a total running time of 45 min. The basic principle of head space analysis is briefed in Figure 2. The compounds eluted were compared with NIST library software.

Phases of the headspace vial

G = the gas phase (headspace)

The gas phase lies above the condensed sample phase.

S = the sample phase

The sample phase contains the compound(s) of interest.

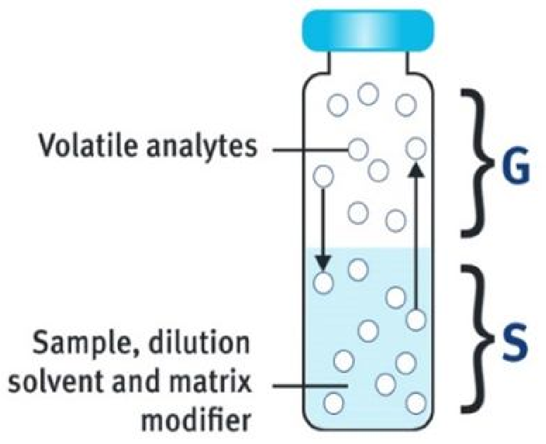


Figure 2: Phases of the headspace vial.

Typically, it is either a liquid or solid combined with a dilution solvent. After introducing the sample phase into the vial and sealing it, the volatile components migrate into the gas phase until equilibrium is achieved. The sample is then extracted from the headspace.

2.4 Inductively coupled plasma mass spectrometer (ICP-MS)

The determination of trace elements in sugarcane juice samples were carried out by using an ICP-MS (Thermo Scientific™ iCAP™ RQ). It is a single quadrupole mass spectrometer that detects trace elements by converting liquid samples into aerosol using a borosilicate glass nebulizer and quartz cyclonic spray chamber. The aerosol is ionized in a high-temperature plasma and the ions are filtered by their mass-to-charge ratio in the quadrupole mass analyzer, achieving a dynamic range greater than 9 orders of magnitude. The key components for analyzing the juice samples are: lithium (Li), beryllium (Be), boron (B), sodium (Na), magnesium (Mg), aluminium (Al), phosphorus (P), potassium (K), calcium (Ca), titanium (Ti), vanadium (Vn), chromium (Cr), manganese (Mn), iron (Fe), cobalt (Co), nickel (Ni), copper (Cu), zinc (Zn), arsenic (As), molybdenum (Mo), silver (Ag), cadmium (Cd), tin (Sn), antimony (Sb), cesium (Cs), barium (Br), mercury (Hg) and lead (Pb). ICP-MS combines an inductively coupled plasma (ICP) with mass spectrometry (MS) for elemental analysis by ionizing the sample. The ICP generates a high-temperature plasma, reaching up to 10,000°C, through which the pre-treated sample is introduced. This intense heat facilitates the ionization of elements, allowing them to be detected. The mass spectrometer then acts as the detector (de Souza *et al*., 2021).

2.5 Phytochemical screening

A phytochemical analysis of sugarcane juice of Co 86032 variety was conducted using standard procedures (Banu and Cathrine, 2015). The screening aimed to identify glycosides, alkaloids, phenols, tannins, saponins and carbohydrates. These compounds were identified based on the observed changes in color intensity or the development of precipitates during the tests. Various qualitative chemical tests were employed to detect the phytochemicals present in the sugarcane juice.

2.5.1 Alkaloids test

Dragendorff's test: When 1 ml of dragendorff's reagent was added to 2 ml of the extract, an orange-red precipitate appeared, suggesting the presence of alkaloids.

Hager's test: Treatment of 2 ml of the extract with a few drops of hager's reagent produced a yellow precipitate, confirming the presence of alkaloids.

2.5.2 Glycosides test

Keller-Killiani test: Mix 0.5 ml of a solution containing glacial acetic acid and 2-3 drops of ferric chloride with 2 ml of the extract. Next, gently add 1 ml of concentrated H_2SO_4 along the inner surface of the test tube. A deep blue color appearing at the boundary between the two layers suggests the presence of cardiac glycosides.

2.5.3 Phenols and tannins test

Ferric chloride test: A dark blue color developed when 2 ml of 5% neutral ferric chloride solution was mixed with 1 ml of the extract, signaling the presence of phenolic compounds and tannins.

Lead tetraacetate Test: The formation of a precipitate occurred when 1 ml of lead tetraacetate solution was added to 0.5 ml of the extract, indicating the presence of phenolic compounds and tannins.

2.5.4 Saponins test

One drop of sodium carbonate solution was added to 5 ml of the extract in a test tube. After vigorous shaking and letting it settle for 5 min, foam formation was noticed, indicating the presence of saponins.

2.5.5 Carbohydrates test

Molish test: Several drops of alcoholic α-naphthol solution were mixed with 2 ml of the extract. Concentrated H_2SO_4 was then carefully introduced along the sides of the test tube. A violet ring formed at the boundary between the two liquids, indicating the presence of carbohydrates.

Fehling's test: An equal amount of Fehling's solutions A and B was mixed with 2 ml of the extract and heated for 5 min. The appearance of a red or dark red precipitate confirmed the presence of carbohydrates.

2.6 Metabolite analysis

Metabolite identification was initially conducted by comparing results with the NIST 14 standard database, followed by validation using standards measured under identical conditions. Metabolites that remained unidentified were documented in the database for future identification. The gathered data was organized to examine the specific metabolites present in sugarcane juice sample (Zhang *et al*., 2020).

2.6.1 Pathway and enrichment analysis

The KEGG database was used for pathway analysis. Identified compounds were mapped to KEGG pathways using KEGG Mapper.

2.6.2 Comparative analysis with *Arabidopsis thaliana*

The identified sugarcane metabolites were uploaded to MetaboAnalyst version 6.0 for comparative analysis with *Arabidopsis thaliana*. The hypergeometric test was used to determine the significance of pathway enrichment. To manage the false discovery rate (FDR), the Benjamini-Hochberg method was used for multiple testing corrections. Pathways were deemed significantly enriched, if they had an adjusted *p*-value (FDR) of less than 0.05.

3. Results

The results of volatile compounds profile in Co 86032 cane juice sample by head space technique of GC-MS analytical instrument revealed different volatile compounds in raw juice (Figure 3). The volatile compounds, *viz.,* (2,3-diphenylcyclopropyl) methyl phenyl sulfoxide (24.73%), octadecanoic acid (11.40%), pyridinium,1-(2-hydrazino-2-oxoethyl)-chloride (11.09 %), n-hexadecanoic acid (9.23%), oleic acid (8.27%) were present in more quantity with retention time of 39.86, 33.21, 6.09, 29.23, and 32.84 min, respectively (Figure 4). Some minor compounds present in the juice sample were spiro [2-cyclohexene-1,2'(1'H)-cyclopenta [de] nap hthacene]-9'-carboxmide (0.97%), (4,6-dimethyl - pyrimidin -2-yl)-(4-methyl-quinazolin-2-yl)-amine (0.91%), n-tridecan-1-ol (0.76%), dodecane,2-methyl- (0.55 %) (Table 2). The compounds identified belonged to various classes, including steroids, acids, phytosterols, alkaloids, ketones and esters. Also, among these compounds, (2,3-

diphenylcyclopropyl) methyl phenyl sulfoxide was the most abundant (24.73%) compound identified. Regardless of the relative amounts of organic volatile compounds in the raw juice samples, many of these compounds are known to exhibit pharmacological or other biological activities, as detailed in Table 3.

For instance, (2,3-diphenylcyclopropyl) methyl phenyl sulfoxide is a compound where the sulfur atom is bonded to both a phenyl group and a (2,3-diphenylcyclopropyl) methyl group. This sulfoxide is recognized as a metabolite in cancer metabolism and serves as a human metabolite. It belongs to the classes of sulfoxides, cyclopropanes, and benzenes. Stearic acid, also known as octadecanoic acid ($CH_3(CH_2)_{16}COOH$), is one of the most prevalent fatty acids. Found as a glycerol ester, it is present in most animal and plant fats. Stearic acid is notably more abundant in animal fat, comprising up to 30%, whereas it constitutes less than 5% of vegetable fat. It acts as a human metabolite and in lowering cholesterol levels. It is an excellent emollient meaning it works by softening and smoothing the skin.

Pyridinium, 1-(2-hydrazino-2-oxoethyl)-, chloride, commonly referred to as Girard's reagent, is utilized in a range of organic synthesis reactions. It has a lot of pharmacological properties in the manufacture of medicament for diabetic complications and aging-related diseases including kidney diseases, nerve damage, atherosclerosis, *etc*. The hydrazine group within this compound is known for its diverse bioactivities, suggesting that further research could uncover its potential as a therapeutic agent. n-hexadecanoic acid, a long chain fatty acid with 16-carbon backbone possesses antioxidant, nematicide, antiandrogenic, hypocholesterolemic, pesticide, hemolytic, and 5- alpha reductase inhibitor activities. Oleic acid is typically present as a glyceride, where it forms an ester with glycerol or with a long-chain alcohol. The compound is used as an excipient in pharmaceuticals, hindering the progression of adrenoleukodystrophy, a fatal disease that affects the brain and adrenal glands, responsible for hypotensive (blood pressure reducing), helps to boost the memory and is effective in treatment of skin papillomas.

Table 2: GC-MS analysis of volatile compounds in Co 86032 variety

S.No.	Retention time (mins)	Area (%)	Height (%)	Name of the compound	Molecular formula	Molecular weight
1.	6.096	11.09	8.78	Pyridinium, 1-(2-hydrazino-2-oxoethyl)-, chloride	$C_7H_{10}ClN_3O$	187
2.	6.265	0.91	1.52	(4,6-Dimethyl-pyrimidin-2-yl)-(4-methyl-quinazolin-2-yl)-amine	$C_{15}H_{15}N_5$	265
3.	15.750	1.37	1.24	4,4,4-Trichlorobutyramide	$C_4H_6Cl_3NO$	189
4.	26.437	1.55	2.05	Heptasiloxane, hexadecamethyl	$C_{16}H_{48}O_6Si_7$	532
5.	27.563	0.76	1.03	n-Tridecan-1-ol	$C_{13}H_{28}O$	200
6.	28.357	1.40	1.55	Pentadecanal	$C_{15}H_{30}O$	226
7.	28.490	1.35	1.27	Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	270
8.	29.230	9.23	7.17	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	256
9.	29.430	0.63	0.97	2,6-Dihydroxybenzoic acid, 3TMS derivative	$C_{16}H_{30}O_4Si_3$	370
10.	29.637	1.02	1.97	3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasilaxane	$C_{18}H_{52}O_7Si_7$	576
11.	31.560	0.97	1.05	Spiro[2-cyclohexene-1,2'(1'H)-cyclopenta[de]naphth acene]-9'-carboxmide	$C_{30}H_{31}NO_{10}$	565
12.	31.652	1.25	1.70	Cyclohexadecane	$C_{16}H_{32}$	224
13.	31.941	0.55	0.97	Dodecane, 2-methyl	$C_{13}H_{28}$	184
14.	32.588	2.56	2.59	Heptasiloxane, hexadecamethyl	$C_{16}H_{48}O_6Si_7$	532
15.	32.751	3.65	4.58	Oleic Acid	$C_{18}H_{34}O_2$	282
16.	32.847	8.27	6.19	Oleic Acid	$C_{18}H_{34}O_2$	282
17.	33.219	11.40	9.52	Octadecanoic acid	$C_{18}H_{36}O_2$	284
18.	34.033	1.29	1.29	Nonadecane, 9-methyl	$C_{20}H_{42}$	282
19.	35.984	3.02	3.49	Heptasiloxane, hexadecamethyl	$C_{16}H_{48}O_6Si_7$	532
20.	38.607	1.68	1.47	Eicosanoic acid, 2-phenyl-1,3-dioxan-5-yl ester	$C_{30}H_{50}O_4$	474
21.	39.216	3.26	3.97	Heptasiloxane, hexadecamethyl	$C_{16}H_{48}O_6Si_7$	532
22.	39.864	24.73	26.43	(2,3-Diphenylcyclopropyl)methyl phenyl sulfoxide,trans	$C_{22}H_{20}OS$	332
23.	42.030	4.13	4.27	Heptasiloxane, hexadecamethyl	$C_{16}H_{48}O_6Si_7$	532
24.	44.388	1.06	1.31	2-Thiopheneacetic acid, 2-tridecyl ester	$C_{19}H_{32}O_2S$	324
25.	44.517	2.86	3.64	Heptasiloxane, hexadecamethyl	$C_{16}H_{48}O_6Si_7$	532

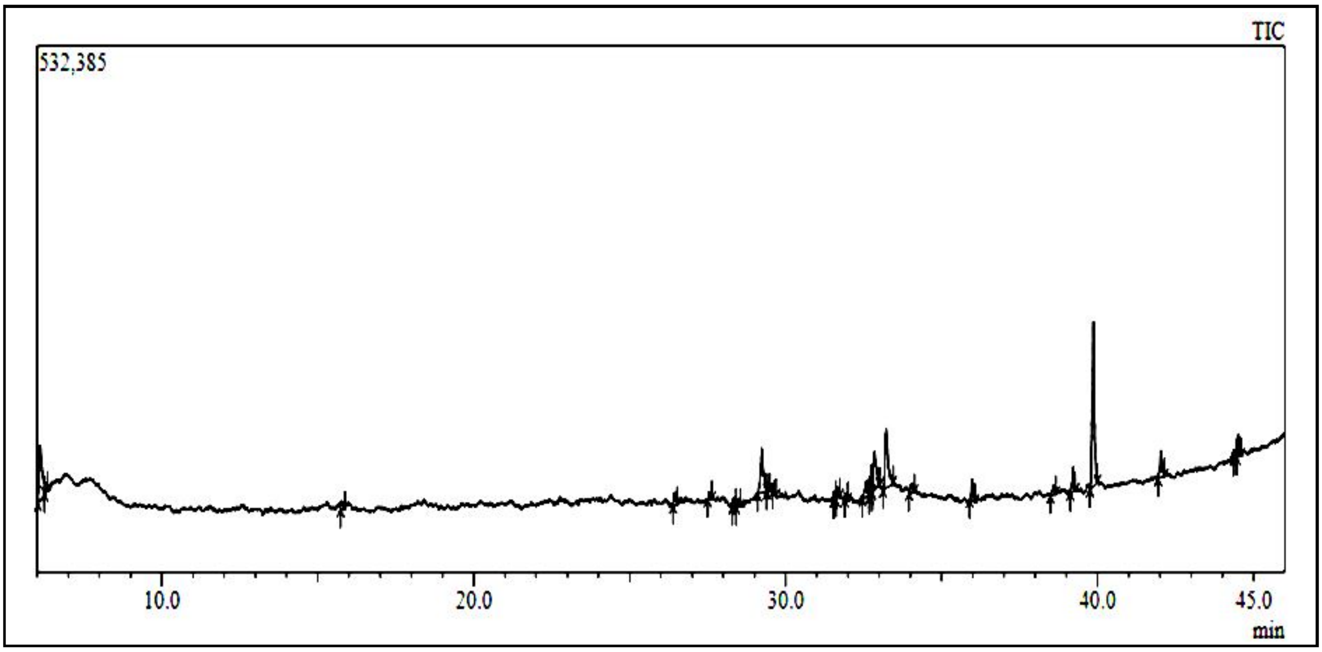
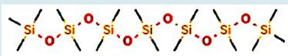
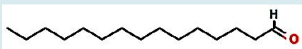
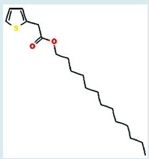
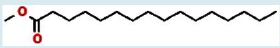
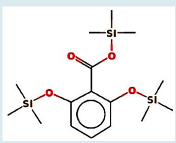
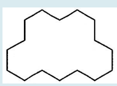


Figure 3: GC-MS chromatogram of variety Co 86032 juice sample.

Table 3: Biological activity of the compounds identified in Co 86032 variety

S.No.	Compound	Structure	Biological/pharmacological activities	Reference
1.	Heptasiloxane, hexadecamethyl		Antibacterial and antimicrobial	Hassan, 2016.
2.	n-Tridecan-1-ol		Anaphylactic, antitumor, myo-neuro-stimulant, narcotic, nauseant, nematicide, and neurodepressant	Preethi *et al.*, 2014
3.	Pentadecanal		Antimicrobial agent, Inherited human peroxisomal disorders	Velumani and Selvi, 2019
4.	2-Thiopheneacetic acid, 2-tridecyl ester		Antimicrobial activity	Meena and Santhi, 2018
5.	Hexadecanoic acid, methyl ester		Anti-oxidant, anti-inflammatory, 5-alpha-reductase inhibitor, hemolytic, pesticide, decrease blood cholesterol nematicide and anti-androgenic	Tyagi and Agarwal, 2017
6.	n-Hexadecanoic acid		Anti-inflammatory, anticancer, antispasmodic and antiviral	Dia and Jacoeb, 2020
7.	2,6-Dihydroxybenzoic acid, 3TMS derivative		Hydroxylation of liver enzymnes during phase I metabolism, antipyretic, anti-rheumatism, analgesic and antimicrobial activity	Juurlink *et al.*, 2014
8.	Cyclohexadecane		Insecticidal, antioxidant and anticancer	Habib and Karim, 2016

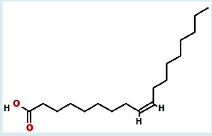
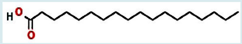
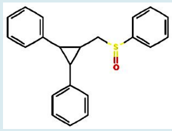
9.	Oleic Acid		Antioxidant, antiandrogenic antibacterial, cancer preventive, anti-inflammatory, 5-alpha reductase inhibitor, insectifuge dermatitigenic hypocholeste-rolemic, and anemiagenic	Farag *et al*., 2021
10.	Octadecanoic acid		Antifungal, antitumor activity and antibacterial	Hsouna *et al*., 2011
11.	(2,3-Diphenylcyclopropyl) methyl phenyl sulfoxide,trans		Antibacterial and antifungal	Bayrak *et al*., 2009

Table 4: Identification of multi elements in Co 86032 variety by ICP-MS

S.No.	Elements	Sample- Co 86032 (ppm)	S.No.	Elements	Sample- Co 86032 (ppm)
1.	7Li (Lithium)	Nil	15.	59Co (Cobalt)	0.0006
2.	9Be (Beryllium)	Nil	16.	60Ni (Nickel)	0.0259
3.	11B (Boron)	0.0684	17.	63Cu (Copper)	0.0251
4.	23Na (Sodium)	7.4472	18.	66Zn (Zinc)	0.6311
5.	24Mg (Magnesium)	192.202	19.	75As (Arsenic)	Nil
6.	27Al (Aluminium)	Nil	20.	95Mo (Molybdenum)	0.0012
7.	31P (Phosphorus)	106.8956	21.	107Ag (Silver)	Nil
8.	39K (Potassium)	1786.897	22.	111Cd (Cadmium)	0.0011
9.	44Ca (Calcium)	190.3079	23.	118Sn (Tin)	Nil
10.	48Ti (Titanium)	0.2134	24.	121Sb (Antimony)	Nil
11.	51V (Vanadium)	Nil	25.	133Cs (Cesium)	Nil
12.	52Cr (Chromium)	Nil	26.	137Ba (Barium)	0.0909
13.	55Mn (Manganese)	0.3851	27.	202Hg (Mercury)	Nil
14.	57Fe (Iron)	21.6403	28.	208Pb (Lead)	Nil

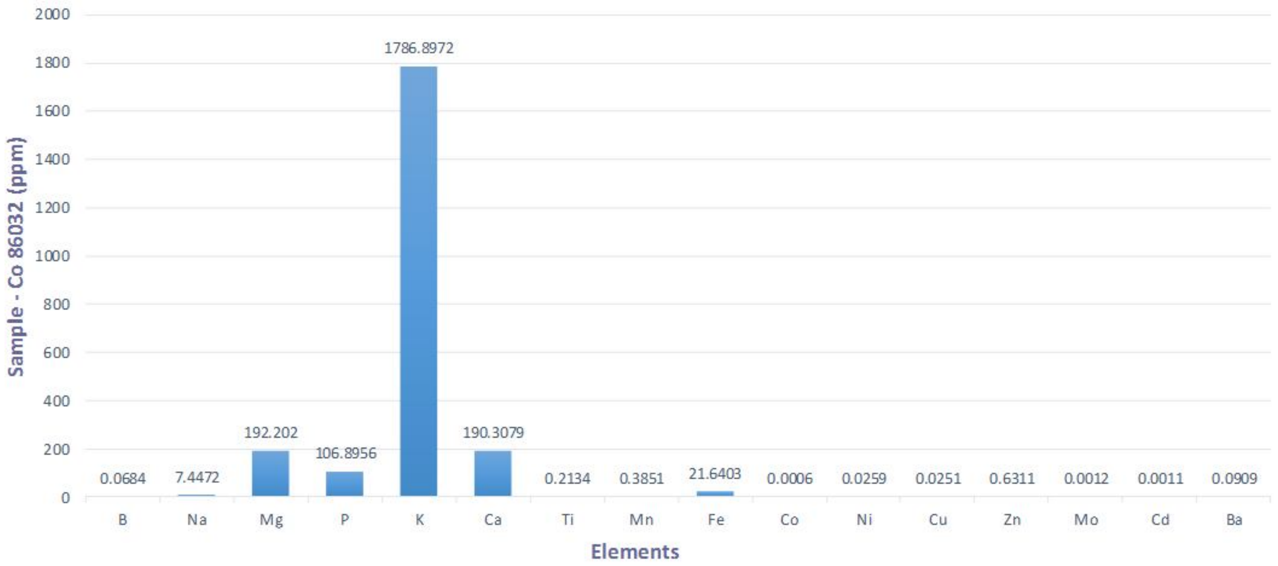


Figure 5: Identification of multi elements in Co 86032 variety by ICP-MS.

Multi-element analysis of Co 86032 variety using ICP-MS revealed the presence of 16 key elements, including boron, sodium, magnesium, phosphorus, potassium, calcium, titanium, manganese, iron, cobalt, nickel, copper, zinc, molybdenum, cadmium, and barium. The cane juice was notably rich in potassium, magnesium, calcium, phosphorus and iron, with concentrations of 1786.9, 192.2, 190.3, 106.9 and 21.6 ppm, respectively (Table 4 and Figure 5). The results indicated that potassium was present in the highest amount, followed by magnesium and calcium.

Phytochemical analysis of sugarcane juice has identified various compounds, including alkaloids, glycosides, phenols, saponins, tannins, and carbohydrates (Table 5). These compounds are recognized for their therapeutic effects against pathogens that cause diseases. As a result, sugarcane juice could be a valuable source for developing new pharmacological agents that promote health.

In this study, the metabolomic profile of the Co86032 sugarcane variety was created using a non-targeted metabolic profile analysis *via* GC-MS. Metabolites were separated and identified, revealing six specific fatty acids along with their KEGG ID (Table 6). The combined enrichment and pathway analysis of the sugarcane juice GC-MS data reveals significant enrichment of pathways related to the biosynthesis of unsaturated fatty acids, fatty acid biosynthesis, and cutin, suberine, and wax biosynthesis. The enrichment analysis revealed that the "biosynthesis of unsaturated fatty acids," "fatty acid biosynthesis," and "cutin, suberine, and wax biosynthesis" pathways were significantly enriched in the dataset.

Table 5: Qualitative assessment of phytochemical constituents in Co 86032 variety

S.No.	Phytochemical constituents	Presence (+) / Absence (-)
1.	Alkaloids	+
2.	Carbohydrates	+
3.	Saponins	+
4.	Glycosides	+
5.	Tannins	+
6.	Phenols	+

Table 6: Specific metabolites identified in juice sample of Co 86032 variety

S.No.	Retention time	Compound name	KEGG ID
1.	27.563	Tridecanol	C14509
2.	28.357	Pentadecanal	C01948
3.	28.490	Hexadecanoic acid, methyl ester	C16995
4.	29.230	Palmitic acid	C00249
5.	32.751	Oleic acid	C00712
6.	33.219	Stearic acid	C01530

Table 7: Metabolic pathway of metabolites obtained from Co 86032 variety using GC-MS

Pathway	Total	Expected	Hits	Raw p	Holm adjusted	FDR	Impact
Biosynthesis of unsaturated fatty acids	22	0.044	3	2.74E-06	0.00024964	0.00024964	0
Fatty acids biosynthesis	56	0.112	3	4.94E-05	0.0044441	0.0022467	0.01123
Cutin, suberine, and wax biosynthesis	18	0.036	2	0.00040537	0.036077	0.012296	0.125
Fatty acid elongation	23	0.046	1	0.045328	1	1	0
Fatty acid degradation	37	0.074	1	0.072237	1	1	0

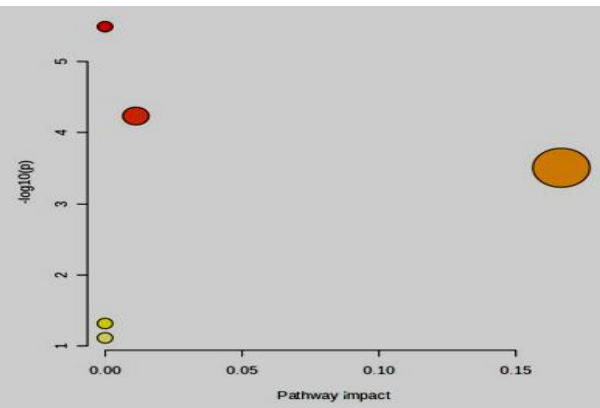


Figure 6: Metabolic pathway of specific metabolites obtained from Co 86032 variety.

Unsaturated fatty acids, crucial for health, must be obtained from the diet and offer numerous benefits, including reduced cardiovascular risk and anti-inflammatory effects. Fatty acid biosynthesis is essential for energy storage and maintaining cellular membranes, highlighting the importance of a balanced intake of dietary fats. Meanwhile, cutin, suberin, and waxes, though not directly consumable, play vital roles in plant protection and can indirectly impact the nutritional quality of plant-based foods. Understanding these biochemical pathways enhances dietary choices and promotes overall health. These findings suggest that these pathways play a critical role in the metabolic processes of sugarcane juice (Table 7 and Figure 6). In contrast, the pathways related to "fatty acid elongation" and "fatty acid degradation" did not show significant enrichment.

4. Discussion

The studies reviewed a comprehensive overview of the diverse phytochemical and volatile profiles of sugarcane juice and its derivatives, highlighting their potential health benefits and industrial applications. Earlier studies on various crops were conducted to identify their components and assess their bioactivity (Tiwari *et al*., 2023; Bamne *et al*., 2023; Banu *et al*., 2024; Singh *et al*., 2024; Shenbagavalli *et al*., 2024). Identification of forty volatile compounds from 6 chinese sugarcane varieties using an optimized HS-SPME method coupled with GC-MS. The daheixiong variety exhibited the highest concentration of volatile compounds, with ethyl alcohol, limonene, hexanol, 2-heptanol, and acetic acid being the most abundant, indicating its rich aromatic profile (Yang *et al*., 2014).

Sharma *et al*. (2015) found sucrose as the dominant compound (30.64%) in Mungo 254 (*S. barberi*) juice, along with significant amounts of 2-3-deoxy-d-mannoic lactone, furancarboxaldehyde 5-hydroxymethyl, and 9-octadecenoic acid. These compounds have various biological activities, supporting the juice's potential as a functional food. Singh *et al*. (2015) reviewed the health benefits of sugarcane components, noting the presence of fatty acids, phytosterols, flavonoids, and phenolic acids. They emphasized the traditional use of sugarcane juice in India for treating ailments and called for further investigation into its medicinal applications.

Del Rio *et al*. (2015) highlighted the potential of sugarcane bagasse and straw extracts as sources of valuable phytochemicals, including n-aldehydes, n-fatty alcohols, sterols, and tocopherols. This underscores the importance of utilizing agricultural byproducts for sustainable and economic value. Mineral elements like Ca, Fe, Na, Cu, P, Zn, Mn and K has been earlier reported in sugarcane juice (de Souza *et al*., 2015; Takahashi *et al.,* 2016). Rajendran *et al*. (2017) identified major phytochemicals in sugarcane juice, such as 5-hydroxymethylfurfural and cyclopropyl 4-methoxyphenyl ketone. Their findings suggest that sugarcane juice has potential for functional and pharmaceutical applications. They also explored the impact of additives like ginger and lemon, which exhibited various biological activities and enhanced the juice's shelf-life.

Ali *et al.* (2019) found that molasses, compared to sugarcane juice, had higher antioxidant activity and total phenolic content. Both extracts exhibited antihyperglycemic effects, indicating potential health benefits and applications in functional foods. Pino *et al.* (2019) characterized 96 volatile compounds in sugarcane wine, with major constituents like 3-methylbutan-1-ol and ethyl octanoate, highlighting its potential in the beverage industry. Souza *et al*. (2019) developed an optimized ICP-OES method to test 14 sugarcane juice samples from markets and identified different elements like calcium, copper, iron, potassium, and magnesium.

Chen *et al.* (2020) identified numerous phenolic and volatile compounds during sugarcane fermentation, suggesting its potential as an alternative to wine due to its unique characteristics as an alcoholic fermented beverage. Ge *et al.* (2021) identified 111 volatile compounds in sugarcane juice, emphasizing the role of various heterocyclic compounds and precursors in developing its characteristic aroma. Shanmuganathan *et al.* (2024) examined sirukamboor badila canes, identifying 50 flavor compounds and 17 essential elements using GC-MS and ICP-OES, respectively, underscoring their unique flavors and nutritional significance. These findings suggest the potential for expanded cultivation and highlight the canes ecological adaptability and sensory appeal. By comparing the metabolites identified in the sugarcane juice sample against plant-specific pathway databases, you can uncover the metabolic pathways that are potentially involved, providing valuable insights into the biochemical composition and potential health benefits of sugarcane juice (Rajagopalan *et al*., 2022).

Collectively, these studies illustrate the multifaceted nature of sugarcane as a source of beneficial phytochemicals. The presence of bioactive compounds across different parts of the sugarcane plant and its derivatives suggests extensive potential in food, beverage, pharmaceutical, and nutraceutical applications. Future research should focus on isolating and characterizing these compounds to better understand their mechanisms of action and therapeutic efficacy. Additionally, exploring the sustainable use of sugarcane byproducts could contribute to the development of eco-friendly nutraceuticals and pharmaceuticals, enhancing the overall value chain of sugarcane.

5. Conclusion

Co 86032 is the most popular sugarcane variety in tropical India. Sugarcane juice, known for its nutritional value, is a notable source of diverse hydrophilic components with substantial biological activities. Based on the results from phytocomponents screening, GC-MS and ICP-MS along with enrichment and pathway analysis of sugarcane juice, it is evident that, in addition to being a source of sugar (carbon), the juice contains different compounds and mineral elements. These compounds have demonstrated significant pharmacological effects, underscoring their beneficial presence in sugarcane juice. These findings suggest the potential medical value of the sugarcane plant, warranting further investigation to optimize its use in exploring medicinal applications.

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Conflict of interest

The authors declare no conflicts of interest relevant to this article.

References

Ali, S. E.; El Gedaily, R. A.; Mocan, A.; Farag, M. A. and El-Seedi, H. R. (2019). Profiling metabolites and biological activities of sugarcane (*Saccharum officinarum* Linn.) juice and its product molasses *via* multiplex metabolomics approach. Molecules, **24**(5):934.

Bamne, F.; Shaikh, N.; Momin, M.; Khan, T. and Ali, A. (2023). Phytochemical analysis, antioxidant and DNA nicking protection assay of some selected medicinal plants. Ann. Phytomed., **12**(2):406-413.

Banu, K. S. and Cathrine, L. (2015). General techniques involved in phytochemical analysis. International Journal of Advanced Research in Chemical Science, **2**(4):25-32.

Banu, Z.; Poduri, R. R. and Bhattamisra, S. K. (2024). A comprehensive review on phytochemistry, health benefits, and therapeutic potential of *Elaeocarpus angustifolius* Blume. Ann. Phytomed., 13 (1):370-383.

Bayrak, H.; Demirbas, A.; Karaoglu, S. A. and Demirbas N. (2009). Synthesis of some new 1,2,3-triazole, their Mannich and Schiff bases and evaluation of their antimicrobial activities. Eur. J. Med. Chem., 44:1057-1066.

Carvalho, M. J.; Oliveira, A. L.; Pedrosa, S. S.; Pintado, M. and Madureira, A. R. (2021). Potential of sugarcane extracts as cosmetic and skincare ingredients. Industrial Crops and Products, 169:113625.

Chen, G. L.; Zheng, F. J.; Lin, B.; Lao, S. B.; He, J.; Huang, Z. and Verma, K. K. (2020). Phenolic and volatile compounds in the production of sugarcane vinegar. ACS omega, 5(47):30587-30595.

de Souza, M. J.; Barciela-Alonso, M. C.; Aboal-Somoza, M. and Bermejo-Barrera, P. (2021). Determination of the trace element contents of fruit juice samples by ICP OES and ICP-MS. Braz. J. Anal. Chem., 9:49-61.

del Río, J. C.; Marques, G.; Lino, A. G.; Lima, C. F.; Colodette, J. L. and Gutiérrez, A. (2015). Lipophilic phytochemicals from sugarcane bagasse and straw. Industrial Crops and Products, 77:992-1000.

Dia, S. P. S. and Jacoeb, A. M. (2020). Identification of active compounds from lindur root plants (*Bruguiera gymnorrhiza*) as α-glucosidase inhibitors. In IOP Conference Series: Earth and Environmental Science, 404(1):012062

FAOSTAT. (2022). Food and agriculture data. https://www.fao.org/faostat/en/#home

Farag, S. M.; Essa, E. E.; Alharbi, S. A.; Alfarraj, S. and El-Hassan, G. A. (2021). Agro-waste derived compounds (flax and black seed peels): Toxicological effect against the West Nile virus vector, *Culex pipiens* L. with special reference to GC-MS analysis. Saudi Journal of Biological Sciences, 28(9):5261-5267.

Ge, Y.; K. Li, C.; Xie, Y.; Xu, C.; Shi, Hang, F. and Doherty, W.O.(2021). Formation of volatile and aroma compounds during the dehydration of membrane-clarified sugarcane juice to non-centrifugal sugar. Foods, 10(7):1561.

Habib, M. R. and Karim, M. R. (2016). Chemical characterization and insecticidal activity of *Calotropis gigantea* L. flower extract against *Tribolium castaneum* (Herbst). Asian Pacific Journal of Tropical Disease, 6(12):996-999.

Hassan, S. W. M. (2016). Antibacterial, anticoagulant and anti-inflammatory activities of marine *Bacillus cereus* S1. Journal of Pure and Applied Microbiology, 10(4):2593-2606.

Hewawansa, U. H. A. J.; Houghton, M. J.; Barber, E.; Costa, R. J. S.; Kitchen, B. and Williamson, G. (2024). Flavonoids and phenolic acids from sugarcane: Distribution in the plant, changes during processing, and potential benefits to industry and health. Comprehensive Reviews in Food Science and Food Safety, 23:13307.

Hsouna, A. B.; Trigui, M.; Mansour, R. B.; Jarraya, R. M.; Damak, M. and Jaoua, S. (2011). Chemical composition, cytotoxicity effect and antimicrobial activity of *Ceratonia siliqua* essential oil with preservative effects against Listeria inoculated in minced beef meat. International journal of food microbiology, 148(1):66-72.

Jamir, L.; Kumar, V.; Kaur, J.; Kumar, S. and Singh, H. (2021). Composition, valorization and therapeutical potential of molasses: Acritical review. Environmental Technology Reviews, 10(1):131-142.

Juurlink, B. H.; Azouz, H. J.; Aldalati, A. M.; AlTinawi, B. M. and Ganguly, P. (2014). Hydroxybenzoic acid isomers and the cardiovascular system. Nutrition journal, 13:1-10.

Meena, B. and Santhi, G. (2018). Phytochemical screening and in vitro hepatoprotective activity of *Ipomoea obscura*. World Journal of Pharmaceutical Research, 7(3):1623-1636.

Organisation for Economic Co-operation and Development & Food and Agriculture Organization of the United Nations. (2021). OECD–FAO agricultural outlook 2021-2030: Sugar.

Pino, J.A.; J.C. Perez. and E. Roncal. (2019). Analysis of the volatile compounds in sugarcane juice wine using solid-phase microextraction techniques coupled with gas chromatography-mass. Revista CENIC Ciencias Químicas, 50(1):001-009.

Preethi, P.; Soorianathasundaram, K. and Subramanian, K. S. (2014). Aroma volatile compounds of mango cultivars neelum and banganapalli. Biochemical and Cellular Archives, 14(2):421-425.

Rajagopalan, V. R.; Manickam, S. and Muthurajan, R. (2022). A comparative metabolomic analysis reveals the nutritional and therapeutic potential of grains of the traditional rice variety Mappillai Samba. Plants, 11(4):543.

Rajendran, P.; R. Bharathidasan. and K. Sureshkumar. (2017). GC-MS analysis of phyto-components in raw and treated sugarcane juice. International Journal of Current Microbiology and Applied Sciences 6 (7):51-61.

Shanmuganathan, M.; Gayathry, G.; Maheshwari, P. and Vellaikumar, S. (2024). Identification of flavor producing compounds and multi elements from chewing cane (*Saccharum officinarum* L. cv. Badila). Sugar Tech., 26(1):87-94.

Sharma, M. D.; Indra Rautela, I. R.; Nishesh Sharma, N. S.; Manoj Gahlot, M. G. and Koshy, E. P. (2015). GC-MS analysis of phytocomponents in juice sample of Indian cane: *Saccharum barberi*. International Journal of Pharmaceutical Sciences and Research, 6(12):5147-5153.

Shenbagavalli, S.; Prabhu, T.; Shalini, K.; Rajangam, J.; Rubika, R. and Dhanushkodi, V. (2024). Phytochemical analysis and identification of different metabolites profiling in oil extracted from ginger (*Zingiber officinale* Rosc.) using gas chromatography and mass spectroscopy technique. Ann. Phytomed., 13(1):1193-1198.

Singh, A.; Lal, U.; Mukhtar, H.; Singh, P.; Shah, G. and Dhawan, R. (2015). Phytochemical profile of sugarcane and its potential health aspects. Pharmacognosy Reviews, 9(17):45-54.

Singh, M.; Khan, M. I.; Badruddeen, J. A.; Ahmad, M.; Fatima, G.; Siddiqui, Z. and Islam, A. (2024). GC-MS analysis of bioactive compounds, standardization, and assessment of antimicrobial efficacy of himalayan *Juniperus communis* L. stems. Ann. Phytomed., 13(1):815-824.

Souza, S.O.; Costa, S.S.L.; Brum, B.C.T.; Santos, S.H.; Garcia, C.A.B. and Araujo, R.G.O. (2019). Determination of nutrients in sugarcane juice using slurry sampling and detection by ICP OES. Food Chemistry 273:57-63.

Takahashi, M.; Ishmael, M.; Asikin, Y.; Hirose, N.; Mizu, M.; Shikanai, T. and Wada, K. (2016). Composition, taste, aroma, and antioxidant activity of solidified noncentrifugal brown sugars prepared from whole stalk and separated pith of sugarcane (*Saccharum officinarum* L.). Journal of Food Science, 81(11):C2647-C2655.

Tiwari, P.; Srivastava, R. and Mishra, M. K. (2023). Pharmacognostic investigation and biological evaluation of *Allium sativum* L. Ann. Phytomed., 12(1):1-7.

Tyagi, T. and Agarwal, M. (2017). Phytochemical screening and GC-MS analysis of bioactive constituents in the ethanolic extract of *Pistia stratiotes* L. and *Eichhornia crassipes* (Mart.) solms. Journal of Pharmacognosy and phytochemistry, **6**(1):195-206.

Velumani, A. and Selvi, V. S. (2019). Gas chromatography and mass spectroscopic analysis of bioactive constituents in *Mangifera indica* leaves extract. Journal of Advanced Scientific Research, **10**(04):96-100.

Yang, H. F.; Wang, S. L.; Yu, S. J.; Zeng, X. A. and Wen Sun, D. (2014). Characterization and semiquantitative analysis of volatile compounds in six varieties of sugarcane juice. International Journal of Food Engineering, **10**(4):821-828.

Zhang, L.; Yu, Y. and Yu, R. (2020). Analysis of metabolites and metabolic pathways in three maize (*Zea mays* L.) varieties from the same origin using GC-MS. Scientific Reports, **10**(1):17990.

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