International Journal of Food Science and Nutrition
www.foodsciencejournal.com
ISSN: 2455-4898
Received: 29-07-2026, Accepted: 28-08-2026, Published: 12-09-2026
Volume 11, Issue 3, 2026, Page No. 302-308

Comparative metabolomic profiling of volatile and non-volatile compounds in different fruit peels using GCMS/MS and LCMS/MS analysis

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DOI: https://doi.org/10.66856/ijfsn.2026.11.3.11165

Abstract

Agricultural byproducts such as fruit peels represent an underutilised source of high value bioactive compounds. The present study investigates the comprehensive volatile and non-volatile metabolomic profiling of four distinct fruit cultivars - pineapple, banana, mango, and sapota peels, utilising Gas Chromatography Tandem Mass Spectrometry (GCMS/MS) and Orbitrap High Resolution Liquid Chromatography Mass Spectrometry (Orbitrap HRLCMS). GCMS/MS characterisation of the volatile compounds revealed distinct variations: pineapple peels were dominated by organic acids (octanoic, nonanoic and heptanoic acids) and fatty acid esters such as hexadecenoic acid ethyl ester, banana and mango peels shared similar terpenes and alcohols including D-limonene, cyclohexanol, 1-methyl-4-(1-methylethyl)-, levomenthol, and dl-menthol, while mango peels specifically exhibited α-pinene, α-myrcene, and cis-13-octadecenoic acid. Similarly, the volatile profile of sapota peel was characterised by markers such as hydroperoxide, 1-ethylbutyl, 2-hydroxy-naphthalenecarboxaldehyde, lup-20(29)-en-3-ol, acetate, (3á)- and farnesyl bromide. Non-volatile profiling via Orbitrap HRLCMS identified organic acids and secondary metabolites, including gulonic acid, citric acid, 3-hydroxy-2H-pyran-2-one, and isocitrate in pineapple, dopamine, guanidinosuccinic acid, and ngamma nitro-L-arginine in banana, homomangiferin, (R)-mevalonic acid, and scutellarein 5,6,7,4'-tetramethyl ether in mango, and 5-keto-D-gluconate, lonchocarpenin, garcimangosone A and asparagoside B in sapota peels. The results represent that the specific fruit cultivar significantly modulates both qualitative and quantitative distribution of these bioactives. These findings establish a metabolomic framework for the targeted valorisation of these fruit wastes into value added functional foods and beverages.

Keywords: Fruit peels, agricultural byproducts, metabolomic profiling, volatile compounds

Introduction

In the agricultural food sector, food waste represents a prominent global challenge, as it ranks among the most produced residues worldwide, resulting in an estimated 1.3 billion tons of edible parts lost and disposed of globally each year (Gustavsson *et al*., 2011) [7]. The fruit processing sector produces a large amount of waste, usually between 25-30 percentage of the total weight of the product, depending on the fruit's shape and the processing technique (Kumar *et al*., 2020). Owing to their significant biodegradability and fermentability, these fruit wastes can pose a substantial environmental burden, leading to severe pollution problems such as the greenhouse effect, global warming, water and soil contamination, and risks to human health if not adequately managed. According to the circular economy concept, these fruit wastes could be valorised into commercially useful products as sustainable and renewable resources (Leong *et al*., 2022) [15].

Among the various forms of fruit waste, peels constitute approximately 15-60 per cent and are typically discarded (Rifna *et al*., 2021). In the case of banana, the peel alone constitutes 40 percentage of the edible fruit weight, resulting in an estimated 114 million metric tons of annual waste (Putra *et al*., 2022) [19]. Industrial mango processing similarly generates over 20 million tons of residue each year in the form of peels and kernels (Sharma *et al*., 2026) [24], while in some canning industries, pineapple non edible fractions might surpass 50 percentage of the raw fruit mass. Individual contributions from fruits like sapota are lower, with the peel accounting for 15-20 percentage of the residual (Abraham *et al*., 2023) [1]. However, these fruit peels contain significantly higher concentrations of antioxidants and minerals than in the fruit pulp serving as a natural source of antioxidants high in dietary fibre, carbohydrate, and pectin (Habiba *et al*., 2025) [8].

Characterisation is a prerequisite and crucial stage in determining the type of waste material, where the production and quality of value added products are determined by the waste material's composition (Zargar *et al*., 2023) [27]. While volatile aromatic compounds determine the sensory identity of the matrix through varietal aromas derived directly from the fruit and fermentative aromas produced by yeast metabolism, the minor components include polyphenols which influence the colour, mouthfeel, and health aspects (Chen *et al*., 2025) [6]. Consequently, this research examines a comparative analysis using Gas Chromatography Tandem Mass Spectrometry (GCMS/MS) and Orbitrap High Resolution Liquid Chromatography Mass Spectrometry (Orbitrap HRLCMS) for the identification of volatile and non-volatile compounds found in the primary and secondary metabolites of pineapple, banana, mango and sapota peels, thereby offering essential chemical characterisation for subsequent sustainable applications.

Materials and Methods

Fruit peels from banana (Poovan variety), mango (Neelam variety), sapota, and pineapple cultivars were collected from local fruit processing units and markets in the Thrissur district. The collected peels were thoroughly washed, chopped into fine pieces, and a 100g aliquot of each matrix are subjected to cold extraction using 250 ml of hexane for 24 h before filtration. This hexane extraction process was repeated thrice. The remaining residue was subsequently extracted three times using methanol. The resulting hexane and methanol fractions were concentrated using a rotary vacuum evaporator, and a 10 ppm working solution was prepared in methanol. Prior to chromatographic injection, the solutions were filtered through 0.22 μm PVDF syringe filters and transferred into autosampler vials.

Fig 1: Cold extraction of fruit peels

Fig 2: Peels extracted in hexane

Fig 3: Filtration in methanol

Fig 4: Hexane and methanol extract of fruit peels

GCMS/MS analysis: The GCMS spectra was obtained by using Thermo Scientific TSQ 8000 Evo equipped with TG-5 MS from Thermo Scientific. The control of the GCMS system and the data peak processing were controlled by means of Xcalibur software. For the separation of components helium gas was used as the carrier gas at a flow rate of 1ml/min. The temperature of the injector was maintained at 250°C. The sample of 1 µl was injected into the instrument with a split ratio of 1:20 where the temperature of the oven was 50°C for a hold time of 1min followed by a ramp of 20°C to reach 270°C which was held for 5 mins. The temperature of the oven was finally raised to 280°C at a rate of 5°C/min and maintained at 280 °C for 25mins. The conditions of the mass detector were a temperature of 290°C for the transfer line. The temperature of the ion source was 310°C, scan range of 35 - 500 m/z and dwell time of 0.2 sec. The comparison of the spectrum of components was carried out with the database of spectrum of known components stored in the NIST MS Search 2.0 library (Igwe *et al*., 2015) [9].

Orbitrap HRLCMS/MS analysis: The methanol extract of the sample was subjected to HRLCMS analysis. The Orbitrap High Resolution Liquid Chromatography Mass Spectrometry (O-HRLCMS) of sample were carried out in Sophisticated Analytical Instrument Facility (SAIF), in IIT Mumbai. Chemical finger prints of selected fruit peel extracts were prepared by Agilent high resolution liquid chromatography and mass spectrometry model- G6550A with TOF/ Q -TOF analyser. Dual AJS ESI was the ion source used. MS minimum and maximum range (m/z) was 60 and 1000 respectively. MS and MS/ MS scan rate (spectra/ rate) was 1.00. A gradient flow with water (solvent A) and acetonitrile (solvent B) was used as the solvent system and flow rate was maintained at 0.3 ml/min. The composition of the solvent system at various intervals were 95 per cent solvent A and 5 per cent solvent B for 1 min, 100 per cent solvent B for 25 minutes and 95 per cent solvent A, and 5 per cent solvent B for 30 minutes (Bajpai *et al*., 2016) [3].

Results

1. Volatile profiling of fruit peels via Gas Chromatography Tandem Mass Spectrometry (GCMS/MS)

The GCMS/MS analysis of pineapple, banana, mango and sapota peels exhibited distinct array of volatile compounds (VOCs) mainly esters, alcohols, organic acids, monoterpenes and phytosterols. These all imparts distinct aroma profiles to the peels. The major compounds identified in each fruit peels are shown in Table 1- 4

a. **Monoterpenes:** Monoterpenes act as the primary volatile compound across all the peel matrices. á-Pinene (RT - 4.83 min) and á-Myrcene (RT- 4.83 min) showed dominance in the volatile profile of mango peel which imparted floral aroma profiles. D-limonene was found across banana (RT-5.21 min), mango (RT-5.21 min) and sapota (RT-6.95 min) peels acting as an active aroma compound and natural antimicrobial agent. Sapota peel showed the presence of hydroperoxide,1-ethylbutyl (RT-5.61 min) as the key aroma compound. The levomenthol and cyclohexanol,1-methyl-4-(1-methylethyl)-, were also identified. These act as cooling/flavour modifying monoterpenes.

b. **Organic acids and wine esters:** Fatty acids and esters are the essential compounds required for fermentation. These were identified in all samples. Pineapple peel showed concentrated organic acid between octanoic acid, nonanoic acid and heptanoic acid (RT – 6.34 mins). Among all the four fruit peels, n-hexadecanoic acid (RT-11.23 -14.71 min) and hexadecenoic acid, ethyl ester (RT-11.38-11.40 min) were identified which provides a vital yeast sur*vivo*r factors, thus imparting fruity/floral wine ester profiles.

c. **Phytosterols and bioactive markers:** The identification of high boiling point triterpenoids and sterols at higher retention times. Pineapple peel exhibited accumulation of campesterol (RT-25.91 min), ergostanol (RT-26.14 min) and ç-Sitosterol (RT-28 min). Whereas, mango and sapota peels showed accumulation of bioactive pentacyclic triterpenoids, lupeol (RT- 32.63 -33.91min) and á-Amyrin (RT - 33.91-36.34 min) along with germanicol (RT -39.81 min) was found in the peels of sapota, which provides antiinflammatory and analgestic properties.

Table 1: Volatile compounds present in pineapple peel

Sl. No	Compounds	Retention time (RT) (mins)	Significance of compounds
1	Hydroperoxide, 1-methylpentyl	4.50	Aroma precursor
2	Octanoic acid	6.34	Taste and bouquets
3	Nonanoic acid	6.34	Waxy and cheesy like aroma
4	Heptanoic acid	6.34	Floral/fruity scents
5	Decanoic acid, 3-methyl-	7.72	Aroma fixative
6	Octane, 1-(ethenylthio)-	7.72	Aroma
7	l-(+)-Ascorbic acid 2,6-dihexadecanoate	11.23	Lipophilic antioxidant derivative
8	n-Hexadecanoic acid	11.23	Act as yeast nutrient
9	Hexadecanoic acid ethyl ester	11.38	Wine ester
10	Cis-vaccenic acid	12.24	Act as yeast nutrient
11	Hexanedioic acid, dioctyl ester	13.92	Structural base for aroma profile
12	Campesterol	25.91	Bioactive sterol
13	Ergostanol	26.14	Therapeutic marker
14	ç-Sitosterol	28.24	Antioxidant
15	Stigmast-4-en-3-one	32.48	Phytosteriod derivative

Table 2: Volatile compounds present in banana peel

Sl. No	Compounds	Retention time (RT) (mins)	Significance of compounds
1	D-limonene	5.21	Active aroma volatile and natural antimicrobial
2	Cyclohexanol, 1-methyl-4-(1-methylethyl)-	6.41	Flavour modifier
3	Levomenthol	6.41	Imparts flavour profile
4	*dl*-Menthol	6.41	Enhances flavour
5	l-(+)-Ascorbic acid 2,6-dihexadecanoate	11.25	Antioxidant ester
6	n-Hexadecanoic acid	11.25	Yeast sur*vivo*r factor
7	Pentadecanoic acid	11.25	Antimicrobial lipid
8	Hexadecanoic acid, ethyl ester	11.40	Wine ester
9	9,12-Octadecadienoic acid (Z,Z)-	12.34	Helps in yeast activity
10	Ethyl 9,12,15-octadecatrienoate	12.49	Aroma fixative
11	Ethanol, 2-(9-octadecenyloxy)-, (Z)-	24.77	Fluid stability in wine
12	9,19-Cycloergost-24(28)-en-3-ol, 4,14- dimethyl-, acetate, (3β,4α,5α)	33.57	Act as an anti-inflammatory and antimicrobial

Table 3: Volatile compounds present in mango peel

Sl. No	Compounds	Retention time (RT) (mins)	Significance of compounds
1	á-Pinene	4.83	Primary volatile aroma
2	á-Myrcene	4.83	Aroma
3	D-Limonene	5.21	Active aroma volatile
4	Cyclohexanol, 1-methyl-4-(1-methylethyl)-	6.41	Act as flavour modifier
5	n-Hexadecanoic acid	11.23	Yeast sur*vivo*r factor
6	Hexadecanoic acid, ethyl ester	11.39	Wine ester
7	cis-13-Octadecenoic acid	12.38	Act as yeast nutrient
8	Ethanol, 2-(9-octadecenyloxy)-, (Z)-	17.65	Helps to stabilises must
9	17.alfa.,21á-28,30-Bisnorhopane	23.42	Act as maturity biomarker
10	ç-Sitosterol	33.52	Antioxidant
11	Lupeol	33.91	Bioactive molecule
12	à-Amyrin	33.91	Act as an analgestic and antiinflammatory

Table 4: Volatile compounds present in sapota peel

Sl. No	Compounds	Retention time (RT) (mins)	Significance of compounds
1	Hydroperoxide, 1-ethylbutyl	5.61	Aroma precursor
2	D-limonene	6.95	Active aroma volatile
3	Levomenthol	9.08	Imparts flavour profile
4	1-Naphthalenecarboxaldehyde, 2-hydroxy-	12.99	Aroma fixative
5	n-Hexadecanoic acid	14.71	Yeast sur*vivo*r factor
6	1-(+)-Ascorbic acid 2,6-dihexadecanoate	14.71	Antioxidant ester
7	Lup-20(29)-en-3-ol, acetate, (3á)-	28.37	Antioxidant properties
8	Farnesyl bromide	28.37	Aroma
9	Lupeol	32.63	Bioactive molecule
10	á-Amyrin	36.34	Act as therapeutic compound
11	12-Oleanen-3-yl acetate, (3à)-,	36.34	Act as functional phytochemical
12	Germanicol	39.81	Act as an anti-inflammatory and anticancerous

2. **Non-volatile profiling of fruit peels using Orbitrap High Resolution Liquid Chromatography Mass Spectrometry (OHRLCMS)**

OHRLCMS analysis revealed a complete comprehensive non-volatile profiling of fruit peels (pineapple, banana, mango and sapota) and showed distinct array of organic acids, polyphenols, catecholamines, triterpenoids and lipids. The Table 5-9, shows the non-volatile compounds present in the four fruit peels.

a. **Organic acids and metabolites:** The main compound responsible for fruit's tissue acidity and respiration is gluonic acid (RT-1.01-1.04 min), citric acid (RT- 1.09-1.27 min) and 2,4-dihydroxy-butanoic acid (RT-1.24-1.47 min), which identified across all fruit peels. While, sapota peel exhibited 5-keto-D-gluconate (RT-1.05 min), shows the active pentose phosphate pathway (PPP) activity during maturation.

b. **Phenolics, catecholamines and bioactive flavonoids:** Bioactive biomarkers are responsible for the characterisation of each fruit peel profile. Banana peel has shown water soluble catecholamines dopamine (RT - 2.76min) and flavonoid rutin (RT-7.13 min). Mango peel was dominated by xanthone C-glycoside , homomangiferin (RT-6.10 min) which act as a major antioxidant marker, furthermore mulberrofuran P (RT-6.38min) and salicylic acid (RT - 4.15 min). Whereas in sapota peel lonchocarpenin (RT-4.58min) a prenylated phenolics and germangosone A (RT- 5.49min) were identified. Pineapple peel showed the presence of polyphenol cinchonain Ib (RT- 6.40min).

c. **Lipids and triterpenoids:** Lipids and triterpenoids provides the protection of exocarp. Monomenthyl succinate (RT-15.08-15.13 min) was seen across banana and sapota peels. Sapota peels contained triterpenoid saponins - asparagoside B (RT-17.00 min) and ganodermatiol (RT-21.09 min) and mainly lipophilic antioxidant γ-Tocopherol (17.45 min).

Table 5: Non-volatile compounds present in pineapple peel

Sl. No	Compounds	Retention time (RT)(mins)	Significance of compounds
1	Gulonic acid	1.03	Biosynthesis of L-ascorbic acid
2	Citric acid	1.09	Major organic acid
3	3-Hydroxy-2H-pyran-2-one	1.15	Aroma volatile
4	Isocitrate	1.45	Intermediate in kreb's cycle
5	2,4-dihydroxy-butanoic acid	1.47	Primary respiration and fruit acidity
6	a,b-dihydroxy-isobutyric acid	1.67	Organic acids
7	2-Deoxy-D-ribose	4.24	Monosaccharide sugar

8	Trimethyloxazole	4.39	Flavour compound
9	LysoPE(18:3(6Z,9Z,12Z)/0:0)	5.98	Polar lipid
10	2'-Deoxycytidine	6.15	Plant nucleoside
11	Cinchonain Ib	6.40	Polyphenol

Table 6: Non-volatile compounds present in banana peel

Sl. No	Compounds	Retention time (RT) (mins)	Significance of compounds
1	Citric acid	1.27	Major organic acid
2	Guanidinosuccinic acid	2.03	Organic/amino acid derivative
3	Dopamine	2.76	Antioxidant and substrate for polyphenol oxidase
4	Ngamma nitro-L-arginine	3.34	Amino acid derivative
5	dYCD/2'-Deoxycytidine	6.18	Plant nucleotide
6	Rutin	7.13	Antioxidant flavonoid
7	Monomenthyl succinate	15.08	Protects peel's cuticle layer
8	5-Hydroxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone	18.36	Natural antioxidant

Table 7: Non-volatile compounds present in mango peel

Sl. No	Compounds	Retention time (RT) (mins)	Significance of compounds
1	Gulonic acid	1.04	Biosynthesis of L-ascorbic acid
2	2,4-dihydroxy-butanoic acid	1.24	Primary respiration and fruit acidity
3	Scutellarein 5,6,7,4'-tetramethyl ether	1.25	Polyphenols
4	(R)-Mevalonic acid	2.49	Imparts bright colour to skins
5	a,b-dihydroxy-isobutyric acid	2.61	Organic acids
6	(E)-1-[4-Hydroxy-3-(3-methyl-1,3- butadienyl)phenyl]-2-(3,5-dihydroxyphenyl)ethylene	3.30	Antioxidants
7	Salicyclic acid	4.15	Give defense responses
8	Trehalose 6-phosphate	4.68	Carbohydrate molecule
9	Tripteroside	5.69	Polyphenols
10	Apigenin 4'-[feruloyl-(->2)- glucuronyl-(1->2)-glucuronide]	5.79	Flavonoid compound
11	Homomangiferin	6.10	Antioxidant
12	Mulberrofuran P	6.38	Act as stilbenoid
13	dCYD / 2'-Deoxycytidine	6.17	Plant nucleoside
14	Chryso-obtusin glucoside	6.49	Polyphenols
15	Resorcinol	6.99	Polyphenolic lipids
16	D-glycero-D-manno-Heptose 7- phosphate	7.44	Sugar phosphate
17	(E)-Resveratrol 3-glucoside 4'- sulfate	22.24	Glycosylated antioxidant

Table 9: Non-volatile compounds present in sapota peel

Sl. No	Compounds	Retention time (RT) (mins)	Significance of compounds
1	Gulonic acid	1.01	Biosynthesis of L-ascorbic acid
2	5-Keto-D-gluconate	1.05	Act as sugar oxidation intermediate
3	2,4 -dihydroxy-butanoic acid	1.29	Primary respiration and fruit acidity
4	a,b-dihydroxy-isobutyric acid	2.90	Organic acids
5	Lonchocarpenin	4.58	Polyphenols
6	Garcimangosone A	5.49	Flavonoid glycoside
7	dYCD/2'-Deoxycytidine	6.18	Cellular nucleioside
8	1-[(5-Amino-5-carboxypentyl)amino]-1-deoxyfructose	7.21	Sugar amino acid conjugate
9	(E)-3-hexadecenoic acid	15.02	Unsaturated fatty acid
10	Monomethyl succinate	15.13	Protects peel's cuticle layer
11	Asparagoside B	17.00	Triterpenoid saponin
12	γ-Tocopherol	17.45	Vitamin E
13	Monoolein	19.69	Monoglyceride lipid
14	Ganodermatriol	21.09	Triterpenoid derivative

Disscussion

1. **Volatile compounds identified in fruit peels via GCMS/MS analysis**

a. **Pineapple peels:** The volatile profile of pineapple peels was dominated by medium chain organic acids (octanoic, nonanoic and heptanoic acids). These imparts cheesy, waxy and floral/fruity notes. During the process of fermentation, these fatty acids act as substrate for volatile ethyl esters. The presence of hexadecenoic acid ethyl ester reveals the lipid fraction responsible for fruity notes. These outcomes aligns with Baretto *et al.* (2013) highlighted the identification of esters (35 per cent), ketones (26 per cent) and alcohols (18 per cent) as the dominated volatile fractions in the pineapple byproduct. Similarly, Ravichandran *et al.* (2020) [20] revealed by using headspace extraction studies, esters like ethyl acetate (40 per cent) in raw peels, octanoic acid ester (11.3-16.1 per cent) in core residues were seen. The identification of aliphatic acids in the study confirmed acidic profile for fermentation.

b. Banana peels: The Poovan variety of banana peel was dominated by monoterpenes and liophilic molecules. D-limonene was found as primary active aroma volatile, which also acts as antimicrobial agent. Pentadecanoic and n-hexadecanoic acids were also seen. In contrast, key findings of Ji and Srzednicki (2013) [11] and Silveria and Morcelli (2022) revealed the presence of isoamyl acetate, isoamyl butyrate and 2-pentanol which are synthesised by alcohol acyltransferase pathyways. The presence of terpenoids and long chain lipids in the study reveals defense mechanisms in the peels of Poovan variety. The identification of sterols such as 9,19-cycloergost-24(28)-en-3-ol, 4,14-dimethyl-, acetate shows the therapeutic qualities of the peel.

c. Mango peel: The Neelam variety in the study exhibited high concentrations of volatile monoterpenes (á-Pinene and á-Myrcene) and pentacyclic triterpenoids (lupeol and à-Amyrin). Indian mango cultivars imparts green and fruity notes. This results aligns with the findings of Zhang *et al*. (2025) [28] revealed the 3-carene, β-Ocimene, 3-carene and terpinolene were the dominant terpenoids in mangoes. as dominant aroma profiles in mango peels. Tamura *et al*. (2001) [26] observed high levels of hexanal,(E) -2-hexenal and γ-terpinene in green Thai mangoes. The identification of palmitic acid and its derivatives and lipids in the study concluded the defensive mechanism of exocarp as reported by Albrahim *et al*. (2025) [2].

d. Sapota peels: The major aroma compound in the sapota peel was hydroperoxide, 1-ethylbutyl along with D-limonene, levomenthol and farnesyl bromide. These helps to generate sweet, active aroma profiles of sapota. This aligned with the results of Sampath *et al*. (2025) [22], where it was reported that hydroxyketones and lactones are responsible for carbohydrate degradation and post harvest softening of the peels. The presence of monoterpenes and phytochemicals 12-oleanen-3-yl acetate and germanicol imparts a dual role in the generation of aroma and antimicrobial defense.

2. Non-volatile compounds identified in fruit peels using OHRLCMS

a. Pineapple peels: The major non volatile compound found in the fruit peel was primary organic acids, including gulonic, citric, 2,4-dihydroxy-butanoic and a,b-dihydroxy-isobutyric acid. Gulonic acid acts as an intermediate L-ascorbic acid biosynthesis. The secondary metabolites found in the study by Jatav *et al*. (2022) [10], Polaki *et al*. (2024) [18] and Mala *et al*. (2024) [16] emphasised on ferulic acid, syringic acid, gallic acid and caffeic acid along with flavonoids (quercetin and kaempferol) are also connected to the cell wall. The current study shows rich organic acids profile with lipids like LysoPE(18:3(6Z,9Z,12Z)/0:0) and polyphenols like cinchonain Ib.

b. Banana peels: The Poovan variety of banana peel was dominated by the water soluble catecholamines dopamine. This was followed by amino acid precursors (guanidinosuccinic acid and Ngamma nitro-L-arginine) and rutin. Chandraju *et al*. (2011) [5] reported that carbohydrates are responsible for the downstream secondary pathways. To bridge this, Khalangre *et al*. (2025) [12] observed that amino acids such as L-phenylalanine, L-tyrosine were responsible for the structural dopamine biosynthesis (32.09mg/kg DE). The presence of dopamine and rutin in the current study validates the metabolic pathway that aids in antioxidant defense and nutritional value to the peel.

c. Mango peel: The dominant non-volatile compound present in the Neelam variety is homomangeiferin. Bioactive compounds such as (R) -mevalonic acid, cutellarein 5,6,7,4'-tetramethyl ether, salicylic acid, mulberrofuran P, and (E)-resveratrol 3-glucoside 4'-sulfate are also seen. Key findings from the study conducted by Schieber *et al*.(2003) [23], Peng *et al*. (2019) [17] and Kucuk *et al*. (2024) reported high levels of mangiferin, quercetin glycosides, catechin, gallic acid and ellagic acid. These compounds acts as free radical scavengers. The high concentrations of methylated homomangiferin in the current study points the downstream methyltransferase activity which aids in lipophilicity, membrane permeability and cuticle protection.

d. Sapota peel: The sapota peels were dominated by 2,4-dihydroxy-butanoic acid, 5-keto-D-gluconate, prenylated/glycosylated flavonoids lonchocarpenin, garcimangosone A and lipophilic vitamins *γ*-tocopherol. 5-keto-D-gluconate aids in carbohydrate processing via PPP pathways. Monomethyl succinate and triterpenoid saponins asparagoside B and ganodetmatriol aids in barrier mechanism against pathogens. These results confirm that sapota peels are rich source of bioactive compounds.

Conclusion

Fruit peels are considered as agricultural waste and are thrown out without proper utilisation, contributing to environmental burdens and resource loss. However, the current study demonstrates a comprehensive characterisation of tropical fruit peels (pineapple, banana, mango and sapota). These are rich in array of distinct volatile organic compounds and non-volatile compounds. GCMS/MS and LCMS/MS analysis, found the dominant compound responsible for the aroma and flavour profiles of each peels. Bioactive compounds present in peels act as a significant therapeutic and antioxidant compounds. This metabolomic profiling confirms that peel residues hold potential for effective upcycling and value addition, furthermore, it can be used as functional food ingredient, nutraceutical formulations or in pharmaceutical applications.

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