Chapter 6

Identification and characterization of bioactive compounds from the potent extract of wild edible fruits

6.1 INTRODUCTION

The importance of wild fruits in the sustenance of humanity cannot be overstated, as they have provided crucial nutrients like minerals, vitamins, and bioactive compounds, among others [1]. Notably, alkaloids, flavonoids, tannins, and phenolic compounds are among the most important bioactive compounds found in wild fruits [2]. These compounds, collectively known as phytochemicals, are fundamental raw materials for drug production [3]. They possess the ability to scavenge free radicals and exhibit synergistic effects, contributing to their anti-inflammatory, antimicrobial, anti-mutagenic, anti-tumour, and neuroprotective properties [4,5]. Moreover, wild fruits contain an abundance of antioxidant compounds like phenolics, carotenoids, anthocyanins, and tocopherols [6]. The utilization of these fruits not only adds value but also aids in reducing environmental pollution [7].

The bioactive compounds derived from plant secondary metabolism hold significant therapeutic potential, particularly in terms of their antioxidant activities. Phenolics

and carotenoids, as the primary phytochemicals present in fruits and vegetables, have been closely associated with human health benefits [8]. Numerous epidemiological studies have consistently shown that diets rich in fruits and vegetables, as prime sources of natural antioxidants, are linked to a reduced risk of chronic diseases, including cancer, cardiovascular disease, and stroke [9,10]. To date, over 8,000 different phenolic compounds have been characterized, highlighting the vast diversity of natural antioxidants found in fruits and vegetables [11].

Despite being overlooked by the advancements of commercial agriculture, wild edible fruits have recently gained recognition as valuable sources of natural colorants and bioactive compounds. This new recognition has sparked an interest in exploring the potential of these compounds, particularly in wild fruits, for the development of functional foods that accommodate to the increasing demand for healthier options with additional health benefits [12]. Numerous scientific reports and studies have extensively documented the presence of abundant bioactive compounds in wild edible fruits, emphasizing their potential benefits in diverse areas such as anticancer, antimicrobial, antioxidant, antidiarrheal, analgesic, diabetic, and wound healing activities. Several workers have made noteworthy contribution in this field, including González-Aguilar et al., 2008 [13], Rafaela et al., 2013 [14], Singh et al., 2016 [7], Singh et al., 2016 [1], Li et al., 2016 [15], Bhutia et al., 2018 [16], Espirito Santo et al., 2020 [17], Sousa et al., 2021 [18], Bachheti et al., 2023 [19], and Vega et al., 2023 [20].

Furthermore, traditional medicinal practices have long relied on the utilization of wild fruits for treating various ailments, including cough, cold, fever, skin diseases, fertility disorders, and diabetes [5]. These fruits have been recognized for their therapeutic potential and have been incorporated into folk remedies to address specific health conditions. However, it is important to note that the existing knowledge regarding the presence and profiling of various bioactive constituents within these fruits remains limited. Therefore, an attempt has been made to fulfil the present objective by examining the presence of functional groups and analysing the bioactive compounds of wild edible fruits from Manipur.

6.2 MATERIALS AND METHODS

6.2.1 Experimental material

The present study aimed to investigate a total of fifteen samples of mature and healthy wild edible fruit species in order to determine the presence of functional groups. The selected fruit species included *Antidesma bunius* (L.) Spreng (F1), *Averrhoa carambola* L. (F2), *Dillenia indica* L. (F3), *Elaeocarpus floribundus* Bl. (F4), *Ficus cunia* Buch. -Ham.ex Roxb (F5), *Garcinia pedunculata* Roxb. (F6), *Garcinia xanthochymus* Hook.f. (F7), *Microcos paniculate* L. (F8), *Phylanthus emblica* L. (F9), *Psidium guajava* L. (F10), *Rhus semialata* Murr. (F11), *Solanum betaceum* Cav. (F12), *Spondius pinata* (L.f.) Kurz (F13), *Vangueria spinosa* (Roxb. ex-Link) Roxb (F14), and *Zizyphus mauritiana* Lamk (F15). However, for the analysis of the presence of bioactive compounds, a subset of seven fruits was selected out of the original fifteen, based on their antimicrobial activity. These selected fruits were *Antidesma bunius* (L.) Spreng, *Averrhoa carambola* L., *Elaeocarpus floribundus* Bl., *Garcinia pedunculata* Roxb., *Garcinia xanthochymus* Hook.f., *Phylanthus emblica* L., and *Spondius pinata* (L.f.) Kurz. These specific fruits were chosen for further examination of their bioactive compound content.

6.2.2 Fourier transform infrared spectroscopy (FT-IR)

FT-IR spectra of the samples were determined using Fourier transform infrared spectroscopy (The PerkinElmer Frontier™ MIR/FIR). 10 mg of sample was fitted with 100 mg of KBr pellet to prepare a translucent sample disc. This pellet was then loaded in FT-IR spectroscopy for the analysis with a resolution of 4 cm^{-1} and the functional groups were analysed within the range of 4000 – 400 cm^{-1}.

6.2.3 LC-MS (Liquid Chromatography-Mass Spectrometry)

6.2.3.1 Antimicrobial activity assay using disc diffusion method.

The antimicrobial activity of the fifteen fruit samples was assessed to determine the fruit samples suitable for LC-MS analysis, taking into consideration financial limitations.

The antimicrobial activity of the fruit extracts was evaluated using the disc diffusion method [21], a commonly employed in-vitro technique for evaluating the sensitivity of microorganisms to potentially antimicrobial compounds. The objective of this method is to determine the inhibitory effect of the fruit extracts (aqueous and ethanol) on microbial growth. The details of extraction process were explained in Chapter 5, section 5.2.4.1 and 5.2.4.2, while the ethanol extract was dissolved in DMSO (Dimethyl sulfoxide).

The study employed two gram-positive bacteria, namely *Staphylococcus aureus* (MTCC-3160) and *Listeria monocytogene* (KF894986), two gram-negative bacteria, namely *Klebsilla pneumonia* (MTCC-4030) and *Pseudomonas aeruginosa* (MTCC-7185); and one fungal strain, *Candida albicans* (MTCC-183). These microorganisms were obtained from IMTECH (Institute of Microbial Technology), located in Chandigarh. All strains were maintained on nutrient agar conical flasks. The antimicrobial activity was determined by measuring the diameter of the inhibition zone, which appears as a clear ring of free microbial growth around the disc. The average diameter of the inhibition zone for the plant extracts (aqueous and methanol) was measured and compared with the inhibition zone of the control (Gentamicin).

6.2.3.2 Analysis of aqueous extract by LC-MS

LC-MS analysis was outsourced to the esteemed Indian Institute of Technology, Bombay (IITB), but unfortunately, the specific methods followed by the outsourcing laboratory were not provided. As a result, certain details regarding the analytical procedures and instrument parameters are not available for reporting. However, efforts were made to ensure the validity and reliability of the analysis within this limitation.

The decision to outsource the LC-MS analysis was driven by the necessity for specialized expertise, access to cutting-edge equipment, and the constraints of laboratory facility in department and university. The central laboratory facility at IITB was chosen for outsourcing due to its reputable status, prioritization of researchers, and robust infrastructure.

In order to compensate for the absence of specific methods, meticulous measures were implemented to uphold scientific rigor. Detailed discussions were conducted with the laboratory personnel to communicate the specific requirements of the analysis. These discussions encompassed aspects such as sample preparation, LC instrument specifications, MS settings, and overall methodological considerations. The selection of the laboratory was based on their established proficiency and distinguished reputation in conducting LC-MS analyses. Moreover, it was ensured that the laboratory possessed state-of-the-art LC and MS instrumentation capable of meeting the analytical demands of the study. The communication with the laboratory officials was seamless, facilitating adherence to all necessary procedural formalities.

Although the absence of specific methods restricts the ability to provide detailed analytical procedures, the obtained results are presented and discussed to the best extent possible, considering the available information. Any potential implications or uncertainties resulting from the lack of provided methods are acknowledged and considered in the interpretation of the findings.

6.3 RESULTS

6.3.1 Analysis of crude sample by FT-IR

In the present study, FTIR spectroscopy was employed to analyse the functional groups present in fifteen wild edible fruits. Table 6.1 provides a summary of the identified functional groups, while Fig. 6.1 (a, b, c) visually represents the corresponding FTIR spectrum.

The FTIR analysis confirmed the presence of several functional groups in the studied fruit samples. The hydroxyl groups (O-H) were detected, indicating the presence of compounds such as alcohols and phenols. Ester groups (C=O) were also identified, suggesting the occurrence of esters in the fruits. Alkenes (C=C) were found, indicating the presence of unsaturated compounds. Additionally, alkyl halides (C-H) and aliphatic groups (R-O-R) were observed in most of the fruit samples. Furthermore, the FTIR spectrum exhibited the presence of a cyclohexane group, amines group (N-H), alkynes (C≡C-HC-H), and alkyl halides/glycogen (C-Br) in most of the fruit samples. Moreover, the presence of alkenes, nitrogen-containing compounds, and ether groups was specifically confirmed in one of the individual fruit samples.

Table 6.1 Details of FTIR spectrum of fifteen fruits (F1-F15)

Frequency range (cm^{-1})	Samples															Function group
	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10	F11	F12	F13	F14	F15	
3870-3550																O-H stretch alcohol
3500-3200	3418	3423	3418	3412	-	3418	3423	3413	3338	3399	-	3426	3413	3420	3398	O-H stretch vibration presence of alcohol, phenols
3300-2850	3011; 2960; 2853	2923; 2853	2928; 2853	2923; 2851	3011; 2924; 2852	2925	2925	2924; 2850	2923; 2852	3006; 2926; 2855	3005; 2925; 2854	2925; 2854	2925; 2853	2926	2923	O-H stretch vibration, carboxylic acids
2500-2300	-	-	-	2359	-	-	-	-	-	-	-	-	-	-	-	C-H stretch vibration, alkenes
2260-2100	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	C=C stretch vibration, alkynes
1990-1739	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Ester C=O stretch, lipids, triglycerides
1750-1700	1745	-	-	1732	1744	1736	1731	1735	1722	1745	1746	1743		1732	1726	Ester COOR
1700-1600	1630	1677	1637	1321	1627	1630	1629	1614	1624	1631		1632	1677; 1635	1639	1618	C=C stretch vibration, alkenes

Table 6.1 (Contd.) Details of FTIR spectrum of fifteen fruits (F1-F15)

Frequency range (cm^{-1})	Samples															Function group
	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10	F11	F12	F13	F14	F15	
1500-1475	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	N-O asymmetric stretch, nitro compounds
1470-1400	-	1452	-	1443	1458	1409	1404	1445	1455	-	1465	1424	-	1424	1418	C-C stretch vibration, aromatics
1400-1320	-	-	-	-	-	-	-	-	1343	-	-	-	-	-	-	N-Ostretch vibration, nitro compounds
1300-1290	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1238	C-C stretch vibration, alcohol, carboxylic acids, esters, ether
1275-1150	-	1259	-	1255	1236	1218	1214	-	1224	1238	1165	1252	1224	1259	-	C-H wag stretch vibration, alkyl halides
1160-1060	1070	1110	1060	-	1061	1064	-	-	1114	-	1098	-	1161	-	1065	R-O-R aliphatic
1055-1000	-	-	--	1054	-	-	1055	1054	1039	1055	-	-	1022	1053	-	Cyclohexane ring vibration

Table 6.1 (Contd.) Details of FTIR spectrum of fifteen fruits (F1-F15)

Frequency range (cm^{-1})	Samples															Function group
	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10	F11	F12	F13	F14	F15	
990-800	901; 842	-	-	832	-	-	893	816	918; 860; 800	-	-	819	861	-	818	N-H wag stretch vibration, primary & secondary amines
790-690	788	719	-	764	-	-	790	780	765; 663	-	722	780	763; 712	-	777	C (triple bond) C-HC-H bend stretch vibration, alkynes
680-510	677; 614; 567; 521	-	-	619	-	614	596	-	630	-	-	616	573; 524	629	634	C-Br stretch vibration, alkyl halides, glycogen
490-400	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Halogen compound

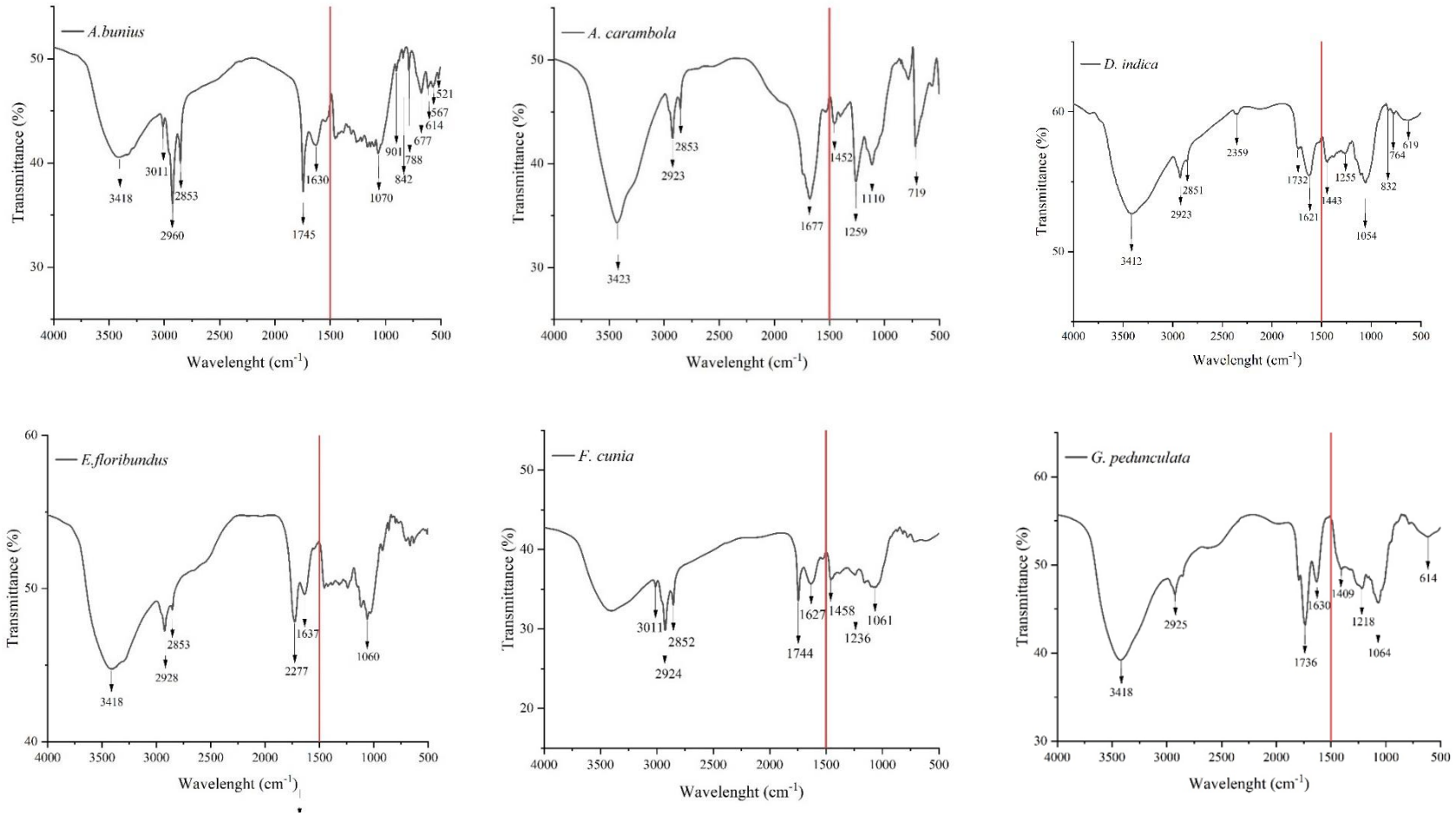

Fig. 6.1a Visual representation of FT-IR for fifteen wild edible fruits (generated using OriginPro)

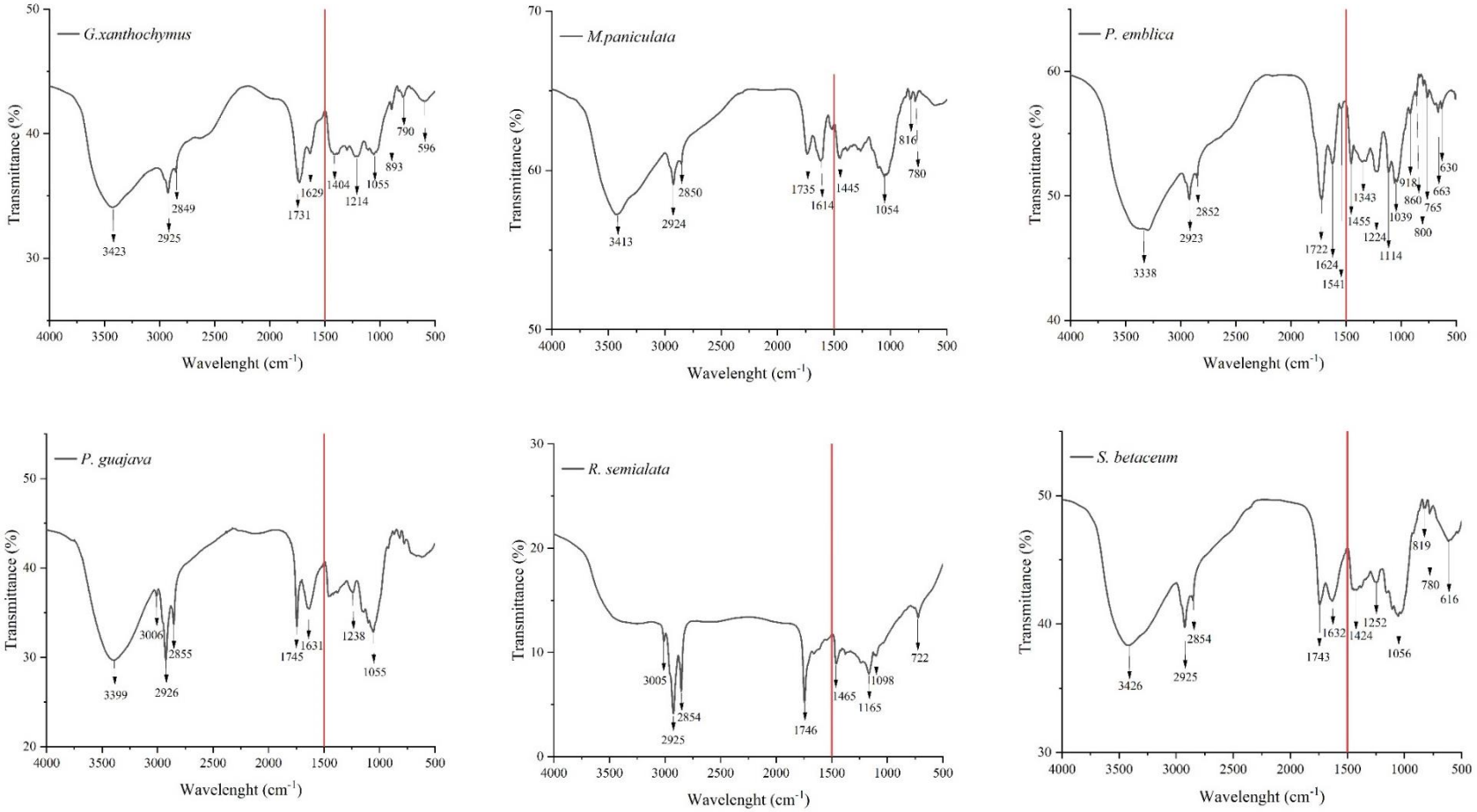

Fig. 6.1b Visual representation of FT-IR for fifteen wild edible fruits (generated using OriginPro)

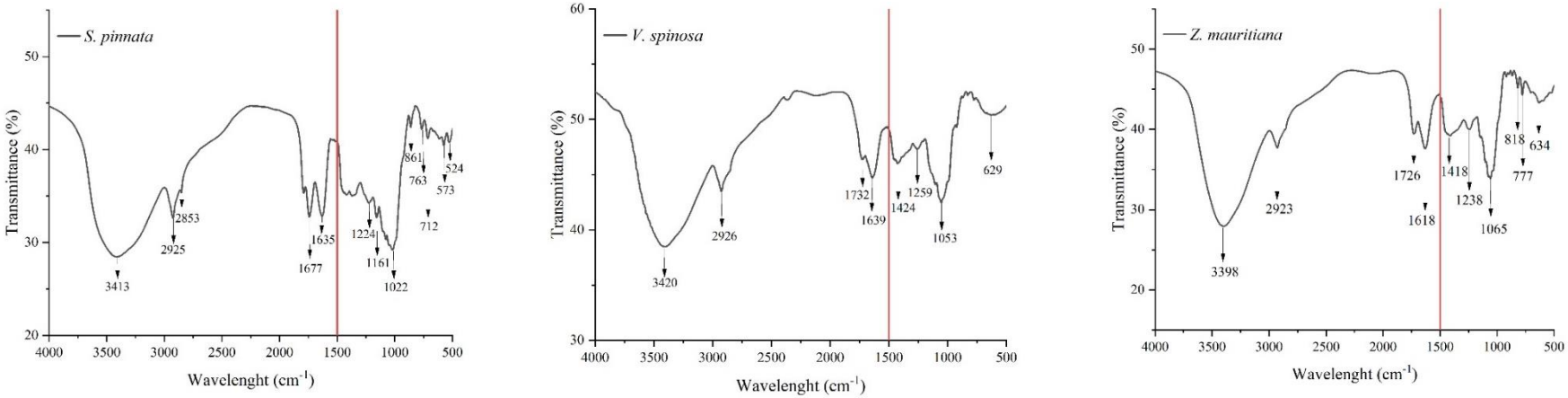

Fig. 6.1c Visual representation of FT-IR for fifteen wild edible fruits (generated using OriginPro)

6.3.2 Antimicrobial activity

The antimicrobial activity of the aqueous and ethanol extracts obtained from fifteen wild edible fruit samples was evaluated against two gram-positive bacteria, two gram-negative bacteria, and a fungal strain. Detailed information regarding the zones of inhibition is given in Table 6.2 and 6.3. The results indicate that the ethanol extract exhibited greater inhibitory effects compared to the aqueous extract against the tested microbial strains.

Among the fifteen fruit samples, eight of them exhibited antimicrobial activity upon aqueous extraction. These fruits are *A. bunius, A. carambola, P. emblica, D. indica, S. pinnata, G. pedunculata, G. xanthochymus,* and *E. floribundus*. However, none of the fruit samples demonstrated activity against C. albicans (as shown in Table 6.2). All eight fruit extracts displayed antimicrobial activity against *S. aureus*, with *P. emblica* exhibiting the highest inhibition zone of 14 mm. Only two fruit extracts, *G. xanthochymus* and *E. floribundus*, showed activity against *L. monocytogenes*. Concerning *K. pneumonia,* two fruits, namely *A. bunius* and *A. carambola,* did not exhibit antimicrobial activity, while the remaining six fruits showed activity, with *S. pinnata* displaying the maximum zone of inhibition at 12 mm. Five fruit samples, namely *A. carambola, E. floribundus, G. pedunculata, G. xanthochymus*, and *S. pinnata,* demonstrated activity against *P. aeruginosa*. When comparing the activity against all selected bacterial strains, *G. xanthochymus* and *E. floribundus* exhibited antimicrobial activity against them.

On the other hand, the ethanol extracts of all fruit samples exhibited antimicrobial responses against all the considered microbial strains including *C. albicans* (Table 6.3). Apart from *D. indica* and *P. emblica,* all other fruit samples showed antimicrobial activity against *S. aureus*, with inhibition zones ranging from 10 to 18 mm. Four fruits, namely *A. bunius, F. cunia, M. paniculata,* and *V. spinosa*, showed no activity against *L. monocytogenes*. Additionally, *F. cunia*, *M. paniculata,* and *Z. mauritiana* did not exhibit inhibition zones against *K. pneumonia*. Almost all ethanol

extracts of fruit samples showed inhibition zones ranging from 10 to 20 mm against *P. aeruginosa*, except for *F. cunia*. For *C. albicans*, inhibition zones were observed in the range of 8 to 12 mm, and this activity was exhibited by only eight fruit samples.

Table 6.2 Inhibition zone (mm) for aqueous extract (100mg/ml)

Name of the fruits	Gram positive	Gram negative		Fungus	
	S. aurius	*L. monocytogens*	*K. pneumonia*	*P. aeruginosa*	*C. albicans*
Antidesmus bunius	11	---	---	---	---
Averrhoa carambola	11	---	---	16	---
Dillenia indica	12	---	10	---	---
Elaeocarpus floribundus	10	8	10	10	---
Garcinia pedunculata	11	---	11	12	---
Garcinia xanthochymus	12	10	10	13	---
Phyllanthus emblica	14	---	10	---	---
Spondias pinnata	12	---	12	11	---
Gentamycin (3 µl)	18	25	30	20	11 - 13

Table 6.3 Inhibition zone (mm) for ethanol extract dissolved in DMSO (100 mg/ml)

Name of the fruits	Gram positive		Gram negative		Fungus
	S. aurius	*L. monocytogenes*	*K. pneumonia*	*P. aeruginosa*	*C. albicans*
Antidesmus bunius	17	---	13	14	---
Averrhoa carambola	16	17	18	17	8
Dillenia indica	---	14	16	16	---
Elaeocarpus floribundus	15	10	12	16	10
Ficus cunia	11	---	---	---	---
Garcinia pedunculata	20	10	20	20	12
Garcinia xanthochymus	12	21	15	19	12
Microcos paniculata	18	---	---	13	11
Phyllanthus emblica	---	14	19	27	10
Psidium guajuva	11	10	10	10	---
Rhys semialata	17	15	17	17	---
Solanum betaceum	11	10	11	10	---
Spondias pinnata	15	17	12	11	10
Vangueria spinosa	10	---	12	10	12
Ziziphus mauritiana	12	15	---	10	---
Gentamycin (3 µl)	14 - 24	18 - 28	23 - 27	12 - 20	13 - 15

6.3.3 LC-MS

The selection of seven wild edible fruits for Liquid Chromatography-Mass Spectrometer (LC-MS) analysis was based on their demonstrated microbial activity in the aqueous extract. LC-MS was utilized to identify and analyse the bioactive compounds present in the aqueous extracts of these fruits. The LC-MS chromatograms of positive and negative ions can be found in Fig. 6.2(a,b) and 6.3 (a,b), respectively. Tables 6.4 to 6.10 provide detailed information on the compounds analysed by LC-MS, including their relative peak retention time, molecular weight, molecular formula, and their respective percentile levels in the aqueous extracts of the fruit samples *A. bunius*, *A. carambola*, *E. floribundus*, *G. pedunculata*, *G. xanthochymus*, *P. emblica*, and *S. pinnata*. Among these fruits, *A. carambola* exhibited the highest number of identified compounds (103), followed by *S. pinnata* (83), *A. bunius* and *E. floribundus* (82), *G. pedunculata* and *G. xanthochymus* (77), and *P. emblica* (67).

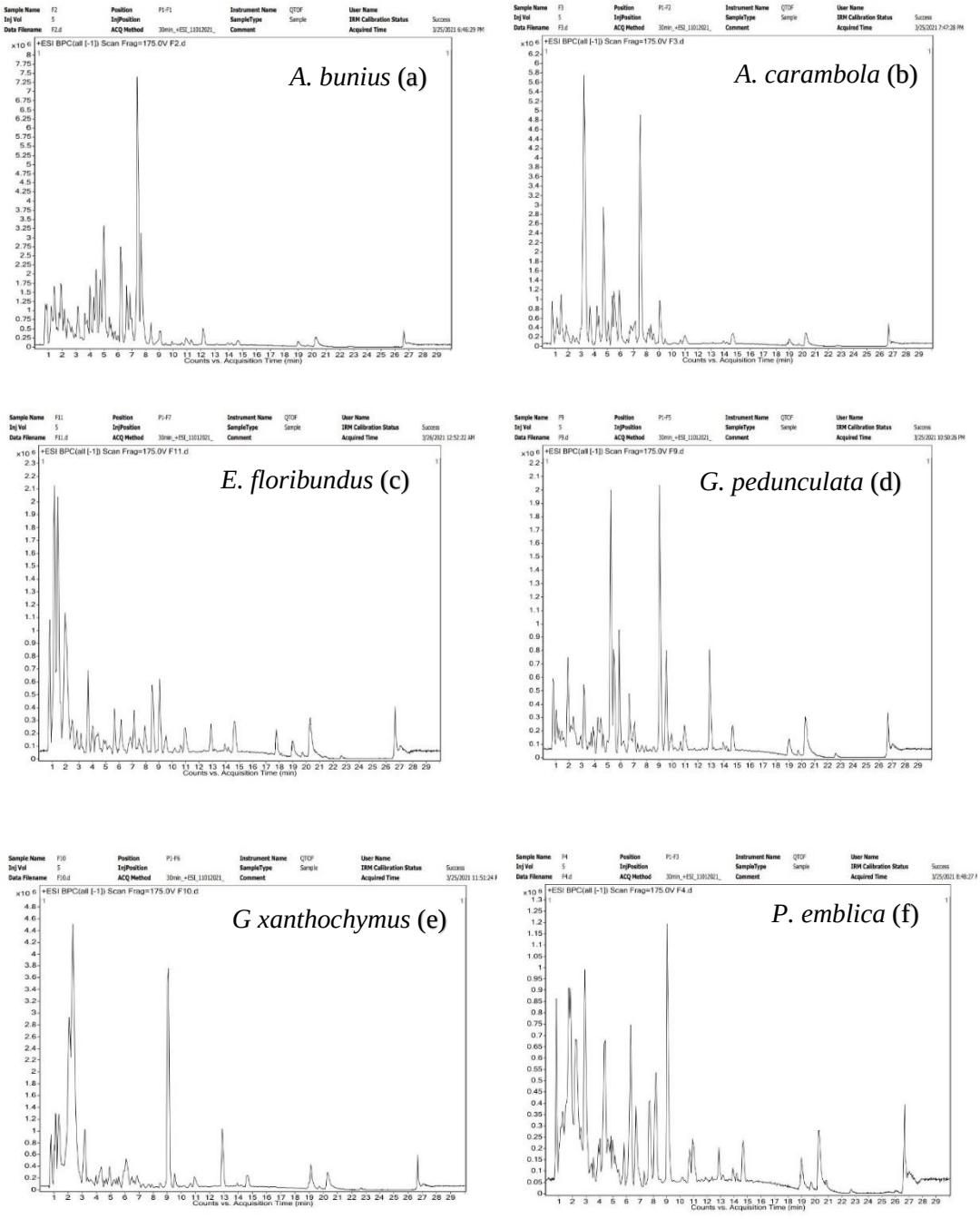

Fig. 6.2a LC-MS positive ion chromatograms of the aqueous extracts of the fruits sample *A. bunius* (a), *A. carambola* (b), *E. floribundus* (c), *G. pedunculata* (d), *G xanthochymus* (e), and *P. emblica* (f).

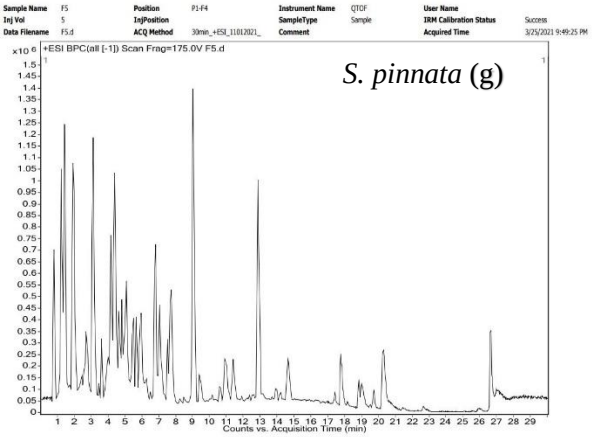

Fig. 6.2b LC-MS positive ion chromatograms of the aqueous extracts of the fruits sample *S. pinnata* (g).

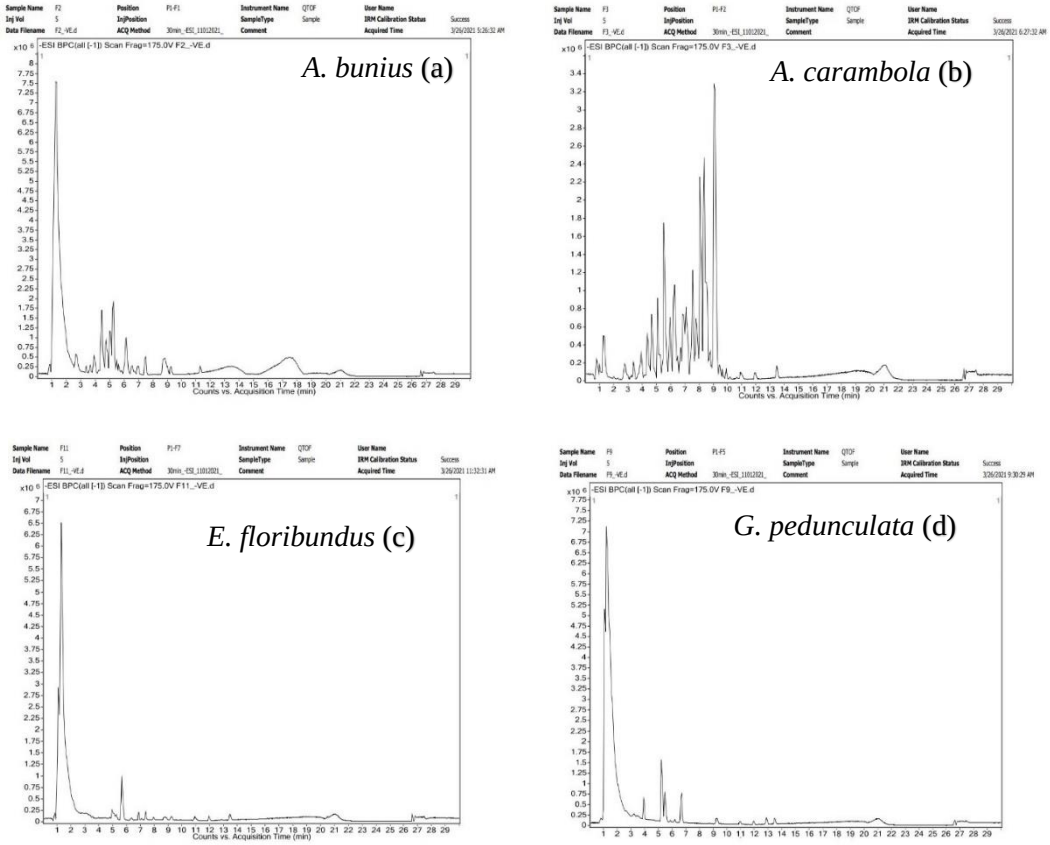

Fig. 6.3a LC-MS negative ion chromatograms of the aqueous extracts of the fruits sample where *A. bunius* (a), *A. carambola* (b), *E. floribundus* (c), *G. pedunculata* (d).

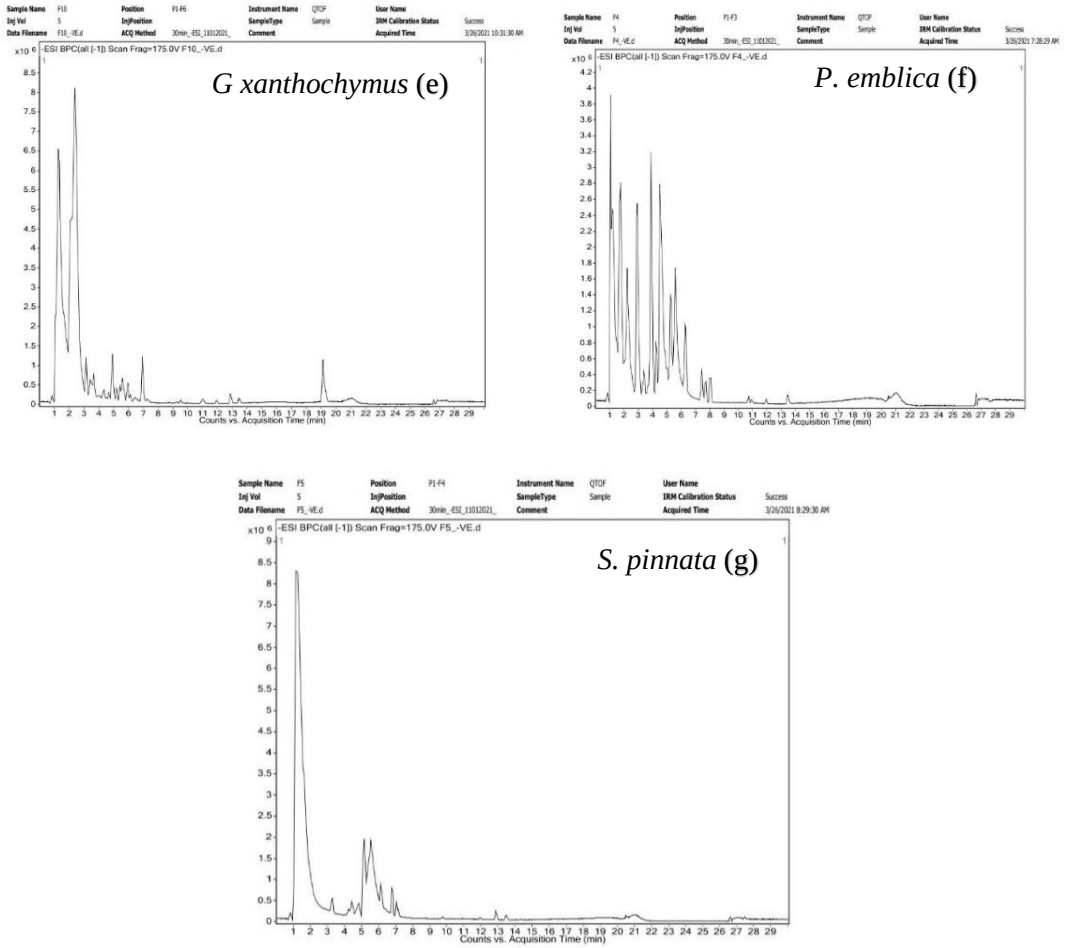

Fig. 6.3b LC-MS negative ion chromatograms of the aqueous extracts of the fruits sample where *G xanthochymus* (e), *P. emblica* (f), and *S. pinnata* (g)

The total percentile levels that each group of metabolites represents are shown in Table 6.11 Alcohols/polyols accounted for 0-6.08% in all seven fruit samples, except *G. xanthochymus* and *P. emblica*, which showed the absence of these compounds. Alkaloids and their derivatives were detected in all samples, with a contribution ranging from 3.91% to 40.47%, representing the highest among all metabolites. Amino acids/peptides contributed 0-11.28%, except for *G. xanthochymus*, which had no content of these compounds. Benzenoids and their derivatives ranged from 4.67% to 17.46%. Diazines were only detected in *G. xanthochymus* (2.81%), while esters were observed solely in *S. pinnata* (5.21%). Fatty acids/lipids ranged from 3.59% to 19.94%, flavonoids from 0.53% to 14.68%, nitrogenous compounds in *A. bunius* (4.11%) and *A. carambola* (3.59%), organic acids from 3.24% to 39.35%, phenolic

compounds from 1.55% to 17.62%, quinolines and derivatives from 0% to 2.71%, steroids from 0% to 3.58%, sugar content from 3.86% to 31.83%, tannins in three samples ranging from 0% to 15.04%, and terpenoids in all extracts except *P. emblica*, ranging from 0% to 12.02%. Other compounds accounted for 0-10.99% of the metabolites.

The metabolites present in *A. bunius* (Fig. 6.4a) showed the highest percentile level for alkaloids and their derivatives (18.16%), followed by organic acids (18.04%), and the lowest content was observed for flavonoids (1.47%). In *A. carambola* (Fig. 4a), alkaloids and their derivatives contributed the most (40.47%), while amino acids/peptides had the lowest content (0.7%). In *E. floribundus* (Fig. 6.4b), organic acids exhibited the highest percentile level (39.35%), while alcohols/polyols had the lowest content (0.63%). The extract of *G. pedunculata* (Fig. 6.4b) showed a high content of fatty acids/lipids (19.94%) and a low content of terpenoids (0.35%). *G. xanthochymus* (Fig. 6.4c) exhibited the highest content of organic acids (21.81%) and the lowest content of phenolic compounds (1.55%). *P. emblica* (Fig. 6.4c) had the highest content of phenolic compounds (17.62%) and the lowest content of steroids (2.48%). The aqueous extract of *S. pinnata* (Fig. 6.4d) showed a high content of organic acids (26.59%) and a low content of alcohols and polyols (1.36%). A bar graph depicting the percentile levels of metabolites present in the seven wild edible fruits is shown in Fig. 6.5.

The seven wild edible fruits demonstrate a wide range of biological activities such as antioxidant, antimicrobial, anti-inflammatory, anti-allergic, anti-tumour, anti-cancer, anticonvulsant, antihypertensive, among others. The identified bioactive compounds present in the seven wild edible fruits of Manipur are shown in Table 6.12.

Table 6.4 Metabolite and its relative percentile in aqueous extract of the fruit sample *A. bunius* as analysed by LC-MS

S.No.	R.Time	Metabolite (Alcohols/Polyols)	Molecular formula	Molecular weight	Area %	Total %
1	7.004	C16 Sphinganine	C16 H35 N O2	273.27	0.18	
2	7.296	3-Ketosphinganine	C18 H37 N O2	299.28	3.29	
3	10.933	(5alpha,8beta,9beta)-5,9-Epoxy-3,6-megastigmadien-8-ol	C13 H20 O2	208.15	0.48	6.08
4	5.276	Triethylene glycol diglycidyl ether	C12 H22 O6	262.14	2.13	
S.No.	R.Time	Metabolite (Alkaloids and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	5.414	1,4'-Bipiperidine-1'-carboxylic acid	C11 H20 N2 O2	212.15	0.44	
2	7.766	alpha-Eucaine	C19 H27 N O4	333.19	0.33	
3	7.688	Ankorine	C19 H29 N O4	335.21	3.96	
4	1.29	Borrerine	C16 H20 N2	240.16	0.08	
5	4.491	Caseadine	C20 H23 N O4	341.16	0.77	
6	6.936	Cassine	C18 H35 N O2	297.27	2.18	
7	6.008	Heteratisine	C22 H33 N O5	391.24	0.27	
8	1.682	Isolobinine	C18 H25 N O2	287.18	0.99	18.16
9	4.9	Lindheimerine	C22 H31 N O2	341.23	5.16	
10	2.894	Sinapoylputrescine	C15 H22 N2 O4	294.16	0.26	
11	6.615	Spirasine I	C22 H29 N O3	355.21	0.62	
12	2.87	Spiredine	C22 H27 N O3	353.2	0.36	
13	7.66	Tetrabenazine	C19 H27 N O3	317.2	0.32	
14	6.691	Tubulosine	C29 H37 N3 O3	475.28	1.61	
15	4.508	xi-Anomuricine	C19 H23 N O4	329.16	0.81	

Table 6.4 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *A. bunius* as analysed by LC-MS

S.No.	R.Time	Metabolite (Amino acids/Peptides)	Molecular formula	Molecular weight	Area %	Total %
1	1.916	Alanyl-Leucine	C9 H18 N2 O3	202.13	0.25	
2	1.784	N(alpha)-t-Butoxycarbonyl-L-leucine	C11 H21 N O4	231.15	1.42	
3	4.696	Isoleucyl-Phenylalanine	C15 H22 N2 O3	278.16	0.87	
4	3.96	Leucyl-Isoleucine	C12 H24 N2 O3	244.18	2.81	8.52
5	2.147	Leucyl-Valine	C11 H22 N2 O3	230.16	1.33	
6	1.218	L-isoleucyl-L-proline	C11 H20 N2 O3	228.15	1.38	
7	1.33	L-threo-3-Phenylserine	C9 H11 N O3	181.07	0.46	
S.No.	R.Time	Metabolite (Bezenoids and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	5.286	(±)-2-Methyl-3-(4-methylphenyl)propanal	C11 H14 O	162.1	0.48	
2	2.321	2-Hexylbenzothiazole	C13 H17 N S	219.11	1.37	
3	4.721	3-buten-2-one 1-(2,3,6-trimethyl phenyl)	C13 H16 O	188.12	0.89	
4	2.893	4,4-Disubstitutedcyclohexenone	C19 H25 N O5	347.17	0.41	5.38
5	14.627	Alpha-CEHC	C16 H22 O4	278.15	0.39	
6	5.23	Dihydroretrofractamide B	C22 H31 N O3	357.23	0.45	
7	5.52	Phrymarolin I	C24 H24 O11	488.13	0.66	
8	6.541	Pipercide	C22 H29 N O3	355.21	0.73	
S.No.	R.Time	Metabolite (Fatty acids/Lipids)	Molecular formula	Molecular weight	Area %	Total %
1	4.424	2-Phenylethyl 3-methylbutanoate	C13 H18 O2/206.13	206.13	2.5	
3	8.654	Corchorifatty acid F	C18 H32 O5/328.23	328.23	0.91	
4	4.404	Magnesium protoporphyrin	C34 H32 Mg N4 O4/584.22	548.22	3.67	7.68
5	6.133	N-acetyl-LTE4	C25 H39 N O6 S/481.25	481.25	0.6	

Table 6.4 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *A. bunius* as analysed by LC-MS

S.No.	R.Time	Metabolite (Flavonoids)	Molecular formula	Molecular weight	Area %	Total %
1	4.76	Diacetylfusarochromanone	C19 H24 N2 O6	376.16	1.03	1.47
2	5.642	Apigenin 7-glucoside	C21 H20 O10	432.1	0.44	
S.No.	R.Time	Metabolite (Nitrogenous compounds)	Molecular formula	Molecular weight	Area %	Total %
1	1.524	N,2,3-Trimethyl-2-(1-methylethyl)butanamide	C10 H21 N O	171.16	1.32	4.11
2	1.554	Pirbuterol	C12 H20 N2 O3	240.15	2.01	
3	3.695	Stilbamidine	C16 H16 N4	264.14	0.78	
S.No.	R.Time	Metabolite (Organic acids)	Molecular formula	Molecular weight	Area %	Total %
1	1.928	Benzocaine	C9 H11 N O2	165.08	2.77	18.04
2	3.345	Butoctamidehydrogen succinate	C16 H29 N O5	315.21	0.39	
3	3.667	Saxagliptin	C18 H25 N3 O2	315.2	0.74	
4	1.139	Isocitrate	C6 H8 O7	192.03	11.8	
5	2.527	D-Tartaric acid	C4 H6 O6	150.02	1.13	
6	4.632	Sinapoyltartronate	C14 H14 O9	326.06	0.72	
7	6.075	2-Hydroxy-6-oxo-6-(2-hydroxyphenoxy)-hexa-2,4- dienoate	C12 H10 O6	250.05	0.49	
S.No.	R.Time	Metabolite (Phenoic compounds)	Molecular formula	Molecular weight	Area %	Total %
1	3.484	Dihydrocapsaicin	C18 H29 N O3	307.21	0.35	5.19
2	12.178	Homocapsaicin	C19 H29 N O3	319.21	0.68	
3	4.406	Sarothralin	C31 H34 O8	534.23	3.39	
4	4.755	Chlorogenic acid	C16 H18 O9	354.1	0.77	

Table 6.4 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *A. bunius* as analysed by LC-MS

S.No.	R.Time	Metabolite (Steroids)	Molecular formula	Molecular weight	Area %	Total %
1	4.016	17beta-Nitro-5alpha-androstane	C19 H31 N O2	305.23	0.55	3.58
2	12.157	17-Hydroxy-3-oxo-17alpha-pregna-1,4-diene-21- carboxylic acid, gamma- lactone	C22 H28 O3	340.21	0.62	
3	5.029	6"-O-Malonylwistin	C26 H26 O13	546.14	0.29	
4	15.865	Norethindrone acetate	C22 H28 O3	340.21	1.93	
5	1.731	Triamcinolonehexacetonide	C30 H41 F O7	532.28	0.19	
S.No.	R.Time	Metabolite (Sugars)	Molecular formula	Molecular weight	Area %	Total %
1	4.414	3-Oxo-alpha-ionol 9-[apiosyl-(1->6)-glucoside]	C24 H38 O11	502.24	2.14	12.27
2	5.523	Swertiamarin	C16 H22 O10	372.12	0.52	
3	4.756	1-(3-Methyl-2-butenoyl)-6-apiosylglucose	C16 H26 O11	394.15	1.04	
4	4.898	15-Hydroxymarasmen-3-one	C15 H20 O4	264.14	0.98	
5	5.396	3-(4-Hydroxy-3-methoxyphenyl)-1,2-propanediol 2-O-(galloyl- glucoside)	C23 H28 O13	512.15	0.98	
6	2.194	Cymorcin diglucoside	C22 H34 O12	490.21	0.55	
7	2.912	D-Erythroascorbic acid 1'-a-D-glucoside	C11 H16 O10	308.07	1.03	
8	7.479	Foeniculoside VII	C16 H28 O8	348.18	1.07	
9	5.656	Genistein 8-C-glucoside	C21 H20 O10	432.11	0.7	
10	6.877	Glucosyl 6-hydroxy-2,6-dimethyl-2E,7-octadienoate	C16 H26 O8	346.16	0.61	
11	5.016	Kaempferol 3-rhamnoside 7-xyloside	C26 H28 O14	564.15	2.26	
12	4.274	Lepidimoic acid	C12 H18 O10	322.09	0.39	

Table 6.4 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *A. bunius* as analysed by LC-MS

S.No.	R.Time	Metabolite (Terpenoids)	Molecular formula	Molecular weight	Area %	Total %
1	6.181	(2S,2"S,3S,3"R,4S)-3,4',5,7-Tetrahydroxyflavan (2->7,4->8)-3,4',5,7-tetrahydroxyflavan	C30 H24 O10	544.14	0.9	
2	1.829	11-Copaen-4-ol	C15 H24 O	220.18	1.58	
3	4.865	2-Oxo-5,11(13)-eudesmadien-12,8-olide	C15 H18 O3	246.12	0.44	
4	6.18	8'-Hydroxyabscisate	C15 H20 O5	280.13	0.96	7.13
5	6.246	Ceanothenic acid	C29 H42 O4	454.31	1.11	
6	6.22	Glycinoeclepin C	C29 H38 O8	514.26	0.43	
7	4.275	Gossyrubilone	C20 H25 N O4	343.18	0.88	
8	2.257	Scutigeral	C23 H32 O4	372.24	0.47	
9	6.129	Teresantalol	C10 H16 O	152.12	0.36	

Table 6.5 Metabolite and its relative percentile in aqueous extract of the fruit sample *A. carambola* as analysed by LC-MS

S.No.	R.Time	Metabolite (Alcohols)	Molecular formula	Molecular weight	Area %	Total %
1	3.34	5-Methoxytryptophol	C11 H13 N O2	191.09	0.94	
2	7.54	(all-E)-3,5,7-Tridecatriene-9,11-diyn-1-ol	C13 H14 O	186.1	1.39	2.33
S.No.	R.Time	Metabolite (Alkaloids and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	1.60	Aziridyl benzoquinone	C16 H22 N2 O6	338.15	0.36	
2	8.16	2,3-Dihydro-6-methyl-5-propanoyl-1H-pyrrolizine	C11 H15 N O	177.11	1.42	4.47
3	4.43	Trichotomine	C30 H20 N4 O6	532.14	2.69	
S.No.	R.Time	Metabolite (Amino acid/Peptide)	Molecular formula	Molecular weight	Area %	Total %
1	1.21	L-isoleucyl-L-proline	C11 H20 N2 O3	228.15	0.70	0.70

Table 6.5 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *A. carambola* as analysed by LC-MS

S.No.	R.Time	Metabolite (Benzenoids and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	1.40	2-Octyl-4-propylthiazole	C14 H25 N S	239.17	0.65	
2	5.11	2-(3-Phenylpropyl)tetrahydrofuran	C13 H18 O	190.13	0.27	
3	5.95	1,2-Dihydro-1,1,6-trimethylnaphthalene	C13 H16	172.12	0.63	
4	7.53	2,4,6-Trimethyl-4-phenyl-1,3-dioxane	C13 H18 O2	206.13	3.60	
5	7.54	2-(2-Methylpropoxy) naphthalene	C14 H16 O	200.12	1.51	
6	7.55	Levosimendan	C14 H12 N6 O	280.11	0.33	
7	7.59	1,2-Dihydro-1,1,6-trimethylnaphthalene	C13 H16	172.12	1.21	
8	7.80	Edulan I	C13 H20 O	192.15	1.03	
9	8.87	Heterophylol	C26 H32 O4	408.24	0.35	17.46
10	10.92	(5alpha,8beta,9beta)-5,9-Epoxy-3,6-megastigmadien-8-ol	C13 H20 O2	208.15	0.67	
11	14.65	Alpha-CEHC	C16 H22 O4	278.15	0.96	
12	4.72	Diacetylfusarochromanone	C19 H24 N2 O6	376.16	0.85	
13	7.55	3,4-Dihydro-2,2,5,7,8-pentamethyl-2H-1-benzopyran-6-ol	C14 H20 O2	220.15	1.27	
14	7.79	Isoscopoletin	C10 H8 O4	192.04	1.85	
15	7.84	Pyruvophenone	C9 H8 O2	148.05	1.33	
16	20.86	3,5-Dichloro-4-hydroxy-2-methoxy-6-methylbenzoic acid	C9 H8 Cl2 O4	249.98	0.94	

Table 6.5 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *A. carambola* as analysed by LC-MS

S.No.	R.Time	Metabolite (Fatty acids/Lipids)	Molecular formula	Molecular weight	Area %	Total %
1	3.22	2-amino-8-oxo-9,10-epoxy-decanoic acid	C10 H17 N O4	215.12	0.52	
2	4.72	2-Phenylethyl 3-methylbutanoate	C13 H18 O2	206.13	1.27	
3	4.79	Furfuryl octanoate	C13 H20 O3	224.14	0.32	
4	5.41	2-Phenylethyl 3-methylbutanoate	C13 H18 O2	206.13	2.21	15.55
5	7.45	11-Hydroxy-9-tridecenoic acid	C13 H24 O3	228.17	0.56	
6	7.52	3-Methylbutyl 2-furanbutanoate	C13 H20 O3	224.14	8.79	
7	3.86	(±)-Glycerol 1,2-diacetate	C13 H20 O3	176.07	1.02	
8	5.55	3-hydroxy-sebacic acid	C13 H20 O3	218.12	0.87	
S.No.	R.Time	Metabolite (Flavonoids)	Molecular formula	Molecular weight	Area %	Total %
1	1.19	Gambiriin B1	C30 H26 O11	562.15	0.89	
2	4.42	Procyanidin B7	C30 H26 O12	578.14	0.80	
3	5.54	Catechin	C15 H14 O6	290.08	0.66	
4	5.68	Calendoflaside	C28 H32 O15	608.17	0.74	
5	6.79	Kinetin	C10 H9 N5 O	215.08	1.06	
6	8.10	Glucoliquiritin apioside	C32 H40 O18	712.23	1.51	14.68
7	5.10	Biorobin	C27 H30 O15	594.16	1.02	
8	5.75	Albanol A	C34 H26 O8	562.16	0.44	
9	6.86	Apimaysin	C27 H28 O13	560.15	2.78	
10	7.57	Glycyphyllin	C21 H24 O9	420.14	0.53	
11	5.54	Daidzein 4',7-diglucoside	C27 H30 O14	578.16	4.23	

Table 6.5 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *A. carambola* as analysed by LC-MS

S.No.	R.Time	Metabolite (Nitrogenous compounds)	Molecular formula	Molecular weight	Area %	Total %
1	1.48	N,2,3-Trimethyl-2-(1-methylethyl) butanamide	C10 H21 N O	171.16	1.20	3.59
2	3.67	Ampalex	C14 H15 N3 O	241.12	1.87	
3	4.14	Fenitropan	C13 H15 N O6	281.09	0.52	
S.No.	R.Time	Metabolite (Nucleotides/Nucleosides)	Molecular formula	Molecular weight	Area %	Total %
1	1.04	5-Methylcytidine	C10 H15 N3 O5	257.1	1.34	2.82
2	1.70	8-Hydroxyadenine	C5 H5 N5 O	151.05	0.39	
3	4.21	Gemcitabine	C9 H11 F2 N3 O4	263.08	0.70	
4	6.36	Famciclovir	C14 H19 N5 O4	321.14	0.40	

Table 6.5 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *A. carambola* as analysed by LC-MS

S.No.	R.Time	Metabolite (Organic acids)	Molecular formula	Molecular weight	Area %	Total %
1	1.44	Methyl o-methoxyhippuric acid	C11 H13 N O4	223.08	1.76	
2	2.00	Benzocaine	C9 H11 N O2	165.09	0.74	
3	4.35	4-Hydroxyphenylacetylglutamine	C13 H15 N O6	281.09	1.26	
4	6.06	Hexyl 2-furoate	C11 H16 O3	196.11	0.58	
5	6.51	(3S,4S)-3-hydroxytetradecane-1,3,4-tricarboxylic acid	C17 H30 O7	346.2	0.74	
6	6.95	2-Carboxy-4-dodecanolide	C13 H22 O4	242.15	0.33	15.75
7	7.95	(x)-1-Nonen-3-yl acetate	C11 H20 O2	184.15	0.43	
8	0.76	2,4-Dichloro-3-oxoadipate	C6 H6 Cl2 O5	227.96	0.51	
9	1.28	Isocitrate	C6 H8 O7	192.03	1.83	
10	6.24	Benzoyl meso-tartaric acid	C11 H10 O7	254.04	3.37	
11	6.79	N-Benzoylaspartic acid	C11 H11 N O5	237.06	1.32	
12	8.63	5-Methyltetrahydropteroylpentag lutamate	C40 H53 N11 O18	974.34	2.88	

Table 6.5 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *A. carambola* as analysed by LC-MS

S.No.	R.Time	Metabolite (Phenolic compounds)	Molecular formula	Molecular weight	Area %	Total %
1	3.00	NH2Mec	C10 H9 N O2	175.06	0.61	
2	4.13	Scopoletin	C10 H8 O4	192.04	0.94	
3	7.37	Dihydrocapsaicin	C18 H29 N O3	307.21	0.33	
4	9.46	3-tert-Butyl-5-methylcatechol	C11 H16 O2	180.11	0.39	
5	14.20	Venlafaxine	C17 H27 N O2	277.2	0.27	6.65
6	2.77	2,4-Dihydroxyacetophenone 5-sulfate	C8 H8 O6 S	232	0.63	
7	4.64	(-)-Epicatechin	C15 H14 O6	290.08	2.68	
8	5.75	5-(3',5'-Dihydroxyphenyl)-gamma-valerolactone	C11 H12 O4	208.07	0.79	
S.No.	R.Time	Metabolite (Steroids)	Molecular formula	Molecular weight	Area %	Total %
1	6.91	beta-Solamarine	C45 H73 N O15	867.5	0.89	
2	7.94	Physalin E	C28 H32 O11	544.21	0.30	2.29
3	8.58	Physalin O	C28 H32 O10	528.2	0.62	
4	7.56	Physapubenolide	C30 H40 O8	528.27	0.48	

Table 6.5 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *A. carambola* as analysed by LC-MS

S.No.	R.Time	Metabolite (Sugars)	Molecular formula	Molecular weight	Area %	Total %
1	1.57	N-Acetyl-beta-D-glucosaminylamine	C8 H16 N2 O5	220.11	0.20	
2	1.64	N-(1-Deoxy-1-fructosyl)threonine	C10 H19 N O8	281.11	1.10	
3	2.22	Lotaustralin	C11 H19 N O6	261.12	0.39	
4	4.42	Apiosylglucosyl 4-hydroxybenzoate	C18 H24 O12	432.13	0.89	
5	5.12	Kaempferol 4'-glucoside 7-rhamnoside	C27 H30 O15	594.16	1.54	
6	5.55	7-Dehydrologanin tetraacetate	C25 H32 O14	556.18	3.13	
7	5.92	15-Hydroxymarasmen-3-one	C15 H20 O4	264.13	0.43	
8	6.92	Garcimangosone D	C19 H20 O9	392.11	0.76	
9	7.36	15-Hydroxymarasmen-3-one	C15 H20 O4	264.13	0.21	
10	9.09	Sesamolinol 4'-O-b-D-glucosyl (1->6)-O-b-D- glucoside	C32 H40 O17	696.24	1.94	20.75
11	4.93	3-Methyl-3-butenyl apiosyl-(1->6)-glucoside	C16 H28 O10	380.17	0.38	
12	7.09	(+)-Pinoresinol 4-O-[beta-D-Glucopyranosyl-(1->2)-[beta-D-glucopyranosyl-(1->6)]-beta-D-glucopyranoside]	C38 H52 O21	884.3	1.59	
13	8.14	Maltohexaose	C36 H62 O31	990.34	2.41	
14	8.63	(8R,8'R)-Secoisolariciresinol 9,9'-bis-[4-carboxy-3-hydroxy-3- methylbutanoyl-(->6)- glucoside]	C44 H62 O24	974.34	4.07	
15	7.19	Lyoniresinol 9'-sulfate	C22 H28 O11 S	500.14	1.71	

Table 6.5 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *A. carambola* as analysed by LC-MS

S.No.	R.Time	Metabolite (Terpenoids)	Molecular formula	Molecular weight	Area %	Total %
1	5.99	2-Oxo-5,11(13)-eudesmadien-12,8-olide	C15 H18 O3	246.12	1.27	
2	7.17	Oleuropein	C25 H32 O13	540.18	1.91	
3	7.17	alpha-Rotunol	C15 H22 O2	234.16	0.78	
4	7.28	Lippioside I	C25 H30 O13	538.17	0.51	
5	8.09	Ligustroside	C25 H32 O12	524.19	0.65	
6	5.03	(10S)-Juvenile hormone III diol phosphate	C16 H29 O7 P	364.17	0.54	
7	5.83	3b,8b-Dihydroxy-6b-(3-chloro-2-hydroxy-2- methylbutanoyloxy)-7(11)-eremophilen-12,8-olide	C20 H29 Cl O7	416.16	1.37	12.02
8	5.90	11,13-Dihydrotaraxinic acid glucosyl ester	C21 H30 O9	426.19	0.68	
9	7.09	Vulgarin	C15 H20 O4	264.19	1.41	
10	7.09	10-Acetoxyligustroside	C27 H34 O14	582.2	2.23	
11	7.95	Brusatol	C26 H32 O11	520.2	0.68	

Table 6.6 Metabolite and its relative percentile in aqueous extract of the fruit sample *E. floribundus* as analysed by LC-MS

S.No.	R.Time	Metabolite (Alcohols/Polyols)	Molecular formula	Molecular weight	Area %	Total %
1	5.42	5-O-Feruloylquinic acid	C17 H20 O9	368.11	0.17	
2	10.93	2,2,6,7-Tetramethylbicyclo[4.3.0]nona-1(9),4-diene-7,8-diol	C13 H20 O2	208.15	0.46	0.63
S.No.	R.Time	Metabolite (Alkaloids)	Molecular formula	Molecular weight	Area %	Total %
1	1.63	Echitovenine	C23 H28 N2 O4	396.2	0.38	
2	2.52	Koenigicine	C20 H21 N O3	323.16	0.84	
3	4.67	(1xi,3xi)-1,2,3,4-Tetrahydro-1-methyl-beta- carboline-3-carboxylic acid	C13 H14 N2 O2	230.1	0.54	3.56
4	5.02	Lindheimerine	C22 H31 N O2	341.23	0.91	
5	5.12	Cuauchichicine	C22 H33 N O2	343.25	0.60	
6	6.49	Beiwutine	C33 H45 N O12	647.28	0.29	
S.No.	R.Time	Metabolite (Amino acids/Peptides)	Molecular formula	Molecular weight	Area %	Total %
1	1.17	L-isoleucyl-L-proline	C11 H20 N2 O3	228.15	1.26	
2	1.50	Prolyl-Arginine	C11 H21 N5 O3	271.16	7.96	
3	2.29	N-Methacrylylglycine methyl ester	C7 H11 N O3	157.07	0.62	11.28
4	4.34	Leucyl-Isoleucine	C12 H24 N2 O3	244.18	0.66	
5	4.95	Isoleucyl-Phenylalanine	C15 H22 N2 O3	278.16	0.77	

Table 6.6 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *E. floribundus* as analysed by LC-MS

S.No.	R.Time	Metabolite (Bezenoids and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	0.82	8-Hydroxy-2-chlorodibenzofuran	C12 H7 Cl O2	218.01	1.99	
2	1.02	3-Methoxy-4,5-methylenedioxybenzoic acid	C9 H8 O5	196.04	1.71	
3	1.96	Benzocaine	C9 H11 N O2	165.08	2.15	
4	4.34	Ibutilide	C20 H36 N2 O3 S	384.25	0.64	
5	5.44	Dihydroretrofractamide B	C22 H31 N O3	357.23	0.40	
6	6.88	Methyl 3-(2,3-dihydroxy-3-methylbutyl)-4- hydroxybenzoate	C13 H18 O5	254.11	0.66	12.02
7	8.36	2-Phenylethyl propanoate	C11 H14 O2	178.1	0.37	
8	10.92	(5alpha,8beta,9beta)-5,9-Epoxy-3,6-megastigmadien-8-ol	C13 H20 O2	208.15	0.99	
9	1.46	Cromolyn	C23 H16 O11	468.08	1.40	
10	2.38	2,6-dihydroxybenzoic acid	C7 H6 O4	154.03	0.67	
11	20.83	3,5-Dichloro-4-hydroxy-2-methoxy-6-methylbenzoic acid	C9 H8 Cl2 O4	249.98	1.05	

Table 6.6 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *E. floribundus* as analysed by LC-MS

S.No.	R.Time	Metabolite (Fatty acids/Lipids)	Molecular formula	Molecular weight	Area %	Total %
1	3.33	Furanojaponin	C20 H28 O3	316.2	0.60	
2	7.59	2-Oxo-5,11(13)-eudesmadien-12,8-olide	C15 H18 O3	246.12	0.63	
3	7.60	TG(8:0/8:0/8:0)	C27 H50 O6	470.36	0.41	
4	7.89	Blumenol C O-[apiosyl-(1->6)-glucoside]	C24 H40 O11	504.26	0.95	
5	9.62	C16 Sphinganine	C16 H35 N O2	273.27	0.66	4.47
6	10.20	Furfuryl octanoate	C13 H20 O3	224.14	0.41	
7	8.70	Corchorifatty acid F	C18 H32 O5	328.23	0.41	
8	9.25	9,10-Dihydroxy-12,13-epoxyoctadecanoate	C18 H34 O5	330.24	0.41	
S.No.	R.Time	Metabolite (Flavonoids)	Molecular formula	Molecular weight	Area %	Total %
1	5.68	Gossypetin	C15 H10 O8	318.04	1.13	
2	5.71	Myricitrin	C21 H20 O12	464.1	3.13	4.42
3	6.35	Cynaroside	C21 H20 O11	448.1	0.16	
S.No.	R.Time	Metabolite (Nucleotides/Nucleosides)	Molecular formula	Molecular weight	Area %	Total %
1	1.17	5-Methylcytidine	C10 H15 N3 O5	257.1	2.36	
2	1.25	2'-Deoxyadenosine	C10 H13 N5 O3	521.1	1.24	
3	1.58	Pirbuterol	C12 H20 N2 O3	240.15	1.41	6.98
4	2.90	Dihydrozeatin riboside	C15 H23 N5 O5	353.17	0.57	
5	3.20	Entecavir	C12 H15 N5 O3	277.12	0.69	
6	4.47	Nifedipine	C17 H18 N2 O6	346.12	0.71	

Table 6.6 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *E. floribundus* as analysed by LC-MS

S.No.	R.Time	Metabolite (Organic acids)	Molecular formula	Molecular weight	Area %	Total %
1	1.84	N-Jasmonoylisoleucine	C18 H29 N O4/323.21	323.21	0.71	
2	2.16	N1,N10-Diferuloylspermidine	C27 H35 N3 O6/497.25	497.25	0.70	
3	10.70	N-(5-Methyl-3-oxohexyl)alanine	C10 H19 N O3/201.14	201.14	0.33	
4	1.23	Oxalosuccinic acid	C6 H6 O7/190.01	190.01	0.20	
5	1.39	Isocitrate	C6 H8 O7/192.03	192.03	36.05	39.85
6	1.90	Homoisocitrate	C7 H10 O7/206.04	206.04	0.68	
7	4.98	S-(PGA1)-glutathione	C30 H49 N3 O10 S/643.32	643.32	0.38	
8	5.31	11-o-Galloylbergenin	C21 H20 O13	480.09	0.56	
9	6.02	2-Hydroxy-6-oxo-6-(2-hydroxyphenoxy)-hexa-2,4- dienoate	C12 H10 O6/250.05	250.05	0.22	
S.No.	R.Time	Metabolite (Phenolic compounds)	Molecular formula	Molecular weight	Area %	Total %
1	1.52	4-(3,5-Diphenylcyclohexyl) phenol	C24 H24 O	328.19	1.31	1.68
2	7.36	Dihydrocapsaicin	C18 H29 N O3	307.21	0.37	
S.No.	R.Time	Metabolite (Quinolines and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	2.22	Neoacrimarine A	C40 H43 N O9	681.29	0.25	0.83
2	2.80	Indacaterol	C24 H28 N2 O3	392.21	0.57	

Table 6.6 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *E. floribundus* as analysed by LC-MS

S.No.	R.Time	Metabolite (Sugars)	Molecular formula	Molecular weight	Area %	Total %
1	1.17	Epithienamycin E	C13 H16 N2 O8 S2	392.03	5.87	
2	1.58	Niazicin A	C17 H23 N O7 S	385.12	1.73	
3	1.97	N-(1-Deoxy-1-fructosyl)phenylalanine	C15 H21 N O7	327.13	3.74	
4	2.79	(S)-Nerolidol 3-O-[a-L-Rhamnopyranosyl-(1->4)-a-L-rhamnopyranosyl-(1->2)-b-D-glucopyranoside]	C33 H56 O14	676.37	0.36	
5	5.97	11,13-Dihydrotaraxinic acid glucosyl ester	C21 H30 O9	426.19	0.47	31.83
6	7.12	Glucosyl (2E,6E,10x)-10,11-dihydroxy-2,6- farnesadienoate	C21 H36 O9	432.23	0.76	
7	1.10	D-Glucarate	C6 H10 O8	210.04	7.43	
8	1.11	D-Erythroascorbic acid 1'-a-D-glucoside	C11 H16 O10	308.07	10.02	
9	2.56	Lepidimoic acid	C12 H18 O10	322.09	0.39	
10	4.54	Asperuloside	C18 H22 O11	414.12	0.22	
11	6.36	Benzyl beta-primeveroside	C18 H26 O10	402.15	0.54	
12	6.91	Phenylethyl primeveroside	C19 H28 O10	416.17	0.29	

Table 6.6 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *E. floribundus* as analysed by LC-MS

S.No.	R.Time	Metabolite (Terpenoids)	Molecular formula	Molecular weight	Area %	Total %
1	1.40	Cincassiol B	C20 H32 O8	400.21	0.79	
2	2.51	Trilobolide	C27 H38 O10	522.24	0.52	
3	6.27	Ceanothenic acid	C29 H42 O4	454.32	1.08	2.87
4	7.99	Glycosyl-4,4'-diaponeurosporenoate	C36 H50 O7	594.36	0.30	
5	4.45	3,4-Hexahydroxydiphenoylarabinose	C19 H16 O13	452.06	0.18	
S.No.	R.Time	Metabolite (Others)	Molecular formula	Molecular weight	Area %	Total %
1	1.96	Ketotifen	C19 H19 N O S	309.12	4.62	
2	3.06	Rhodoxanthin	C40 H50 O2	562.39	0.36	
3	4.33	Benzoylagmatine	C12 H18 N4 O	234.15	0.49	
4	4.46	(3S,2'S)-4-Ketomyxol 2'-α-L-fucoside	C46 H64 O8	744.46	0.34	
5	4.89	11beta,17,21-Trihydroxy-2alpha-methylpregn-4-ene-3,20-dione 21-acetate	C24 H34 O6	418.23	0.48	
6	5.23	Hexyl 2-furoate	C11 H16 O3	196.11	0.41	10.99
7	8.87	Heterophylol	C26 H32 O4	408.24	0.36	
8	10.70	Buspirone	C21 H31 N5 O2	385.25	0.47	
9	1.10	SC-58125	C17 H12 F4 N2 O2 S	384.05	2.05	
10	7.90	Clocortolone pivalate	C27 H36 Cl F O5	494.23	0.40	
11	1.27	Sulfaphenazole	C15 H14 N4 O2 S	314.09	1.01	

Table 6.7 Metabolite and its relative percentile in aqueous extract of the fruit sample *G. pedunculata* as analysed by LC-MS

S.No.	R.Time	Metabolite (Alcohols)	Molecular formula	Molecular weight	Area %	Total %
1	0.83	2,2-Dichloro-1,1-ethanediol	C2 H4 Cl2 O2	129.96	0.31	0.53
2	10.95	2,2,6,7-Tetramethylbicyclo[4.3.0]nona-1(9),4-diene-7,8-diol	C13 H20 O2	208.15	0.22	
S.No.	R.Time	Metabolite (Alkaloids)	Molecular formula	Molecular weight	Area %	Total %
1	4.677	(±)-Nicotine	C10 H14 N2	162.12	0.50	3.56
2	4.905	Elaeocarpidine	C17 H21 N3	267.17	0.42	
3	8.144	Anhalonidine	C12 H17 N O3	223.12	0.42	
4	5.23	Nigellimine N-oxide	C12 H13 N O3	219.09	2.22	
S.No.	R.Time	Metabolite (Amino acids/Peptides)	Molecular formula	Molecular weight	Area %	Total %
1	1.254	L-isoleucyl-L-proline	C11 H20 N2 O3	228.15	1.91	5.63
2	1.311	L-threo-3-Phenylserine	C9 H11 N O3	181.07	1.35	
3	1.313	N,N-Dihydroxy-L-tyrosine	C9 H11 N O5	213.06	1.04	
4	2.826	Glutamyl-glutamate	C10 H15 N2 O7	275.09	0.61	
5	3.031	N5-(4-Methoxybenzyl) glutamine	C13 H18 N2 O4	266.13	0.34	
6	7.491	N-(5-Methyl-3-oxohexyl) alanine	C10 H19 N O3	201.14	0.39	

Table 6.7 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *G. pedunculata* as analysed by LC-MS

S.No.	R.Time	Metabolite (Benzenoids and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	0.793	4-chloro-3-hydroxy-N-(propylcarbamoyl)benzenesulfonamide	C10 H13 Cl N2 O4 S	292.03	0.97	
2	1.409	Methyl n-formylanthranilate	C9 H9 N O3	179.06	1.08	
3	1.471	3-Hydroxyhippuric acid	C9 H9 N O4	195.05	0.64	
4	1.931	Benzocaine	C9 H11 N O2	165.08	1.99	
5	2.315	2-Phenyl-1,3-propanediyl monocarbamate	C10 H13 N O3	195.09	1.89	
6	4.544	Pheneturide	C11 H14 N2 O2	206.11	1.05	
7	5.929	Talinolol	C20 H33 N3 O3	363.25	2.94	
8	8.245	2-Phenylethyl propanoate	C11 H14 O2	178.1	0.39	
9	10.109	Sulfadimidine	C12 H14 N4 O2 S	278.09	0.38	16.49
10	10.968	(5alpha,8beta,9beta)-5,9-Epoxy-3,6-megastigmadien-8-ol	C13 H20 O2	208.15	1.42	
11	11.297	6,6-Dimethoxy-2,5,5-trimethyl-2-hexene	C11 H22 O2	186.16	0.48	
12	11.375	Butyl 2-aminobenzoate	C11 H15 N O2	193.11	0.39	
13	14.603	Alpha-CEHC	C16 H22 O4	278.15	1.21	
14	14.676	3-Butylidene-7-hydroxyphthalide	C12 H12 O3	204.08	0.56	
15	0.85	4-Hydroxy-2,2',4',6'-tetrachlorobiphenyl	C12 H6 Cl4 O	305.92	0.33	
16	2.86	2,6-dihydroxybenzoic acid	C7 H6 O4	154.03	0.29	
17	20.70	3,5-Dichloro-4-hydroxy-2-methoxy-6-methylbenzoic acid	C9 H8 Cl2 O4	249.98	0.46	

Table 6.7 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *G. pedunculata* as analysed by LC-MS

S.No.	R.Time	Metabolite (Fatty acids/Lipids)	Molecular formula	Molecular weight	Area %	Total %
1	1.598	S-Acetyldihydrolipoamide	C10 H19 N O2 S2	249.08	0.69	
2	9.565	C16 Sphinganine	C16 H35 N O2	273.27	3.50	
3	9.953	Isovaltrate	C22 H30 O8	422.19	0.72	
4	5.33	Veranisatin C	C16 H20 O10	372.11	0.23	
5	9.23	9,10-Dihydroxy-12,13-epoxyoctadecanoate	C18 H34 O5	330.24	0.36	6.63
6	8.608	Valtratum	C22 H30 O8	422.2	0.48	
7	1.27	4'-Methylisoscutellarein 8-(2"-sulfoglucoside)	C22 H22 O14 S	542.08	0.27	
8	7.99	7,11-Bisdeacetylvaltrate 7-(3-methylpentanoate) 11-(3- hydroxy-3-methylbutanoate)	C26 H38 O9	494.25	0.38	
S.No.	R.Time	Metabolite (Flavonoids)	Molecular formula	Molecular weight	Area %	Total %
1	5.578	Apigenin 7-glucoside	C21 H20 O10	432.1	0.49	
2	1.23	Tectorigenin 4'-sulfate	C16 H12 O9 S	380.02	1.75	3.24
3	5.51	Daidzein 4',7-diglucoside	C27 H30 O14	578.16	1.00	
S.No.	R.Time	Metabolite (Nucleotides)	Molecular formula	Molecular weight	Area %	Total %
1	1.349	Pirbuterol	C12 H20 N2 O3	240.15	0.67	
2	1.66	6-Amino-9H-purine-9-propanoic acid	C8 H9 N5 O2	207.07	0.80	4.25
3	2.519	Penciclovir	C10 H15 N5 O3	253.12	0.64	
4	4.313	Isopentenyladenine	C10 H13 N5	203.12	2.15	

Table 6.7 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *G. pedunculata* as analysed by LC-MS

S.No.	R.Time	Metabolite (Organic acids)	Molecular formula	Molecular weight	Area %	Total %
1	6.894	AK-toxin I	C23 H27 N O6	413.19	0.42	
2	1.09	D-4-Hydroxy-2-oxoglutarate	C5 H6 O6	162.02	8.31	
3	1.09	Oxalosuccinic acid	C6 H6 O7	190.01	9.33	
4	2.48	cis,cis-2,4-Dihydroxy-5-methyl-6-oxo-2,4- hexadienoate	C7 H8 O5	172.04	0.36	19.94
5	6.69	Nonate	C9 H16 O4	188.1	0.92	
6	2.16	4-Hydroxy-4-methyl-2-oxoadipate	C7 H10 O6	190.05	0.60	
S.No.	R.Time	Metabolite (Phenolic compounds)	Molecular formula	Molecular weight	Area %	Total %
1	1.119	(+)-Chebulic acid	C14 H12 O11	356.04	1.52	
2	3.533	4-Hydroxybenzyl isothiocyanate rhamnoside	C14 H17 N O5 S	311.09	0.68	
3	7.417	Dihydrocapsaicin	C18 H29 N O3	307.21	0.45	
4	8.98	Heterophylol	C26 H32 O4	408.24	0.51	5.47
5	13.961	Nordihydrocapsaicin	C17 H27 N O3	293.2	0.59	
6	3.02	2-O-Galloylgalactaric acid	C13 H14 O12	362.05	0.33	
7	3.93	Caffeic acid 3-glucoside	C15 H18 O9	342.1	0.79	
8	14.256	Venlafaxine	C17 H27 N O2	277.2	0.61	
S.No.	R.Time	Metabolite (Quinolines)	Molecular formula	Molecular weight	Area %	Total %
1	7.101	8-Propanoylneosolaniol	C22 H30 O9	438.19	0.61	0.61

Table 6.7 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *G. pedunculata* as analysed by LC-MS

S.No.	R.Time	Metabolite (Sugars)	Molecular formula	Molecular weight	Area %	Total %
1	1.931	2-O-Galloylgalactaric acid	C13 H14 O12	362.05	1.01	7.88
2	1.997	N-(1-Deoxy-1-fructosyl) phenylalanine	C15 H21 N O7	327.13	0.62	
3	5.203	Kaempferol 4'-glucoside 7-rhamnoside	C27 H30 O15	594.16	1.00	
4	5.483	7-Dehydrologanin tetraacetate	C25 H32 O14	556.18	3.41	
5	1.09	Digalacturonate	C12 H18 O13	370.07	1.22	
6	6.28	Osmundalin	C12 H18 O8	290.1	0.25	
7	1.46	D-Galacturonolactone	C6 H8 O6	176.03	0.27	
8	4.36	1-O-Feruloylglucose	C16 H20 O9	356.11	0.11	
S.No.	R.Time	Metabolite (Steroids)	Molecular formula	Molecular weight	Area %	Total %
1	6.24	Physalin I	C29 H34 O11	558.21	0.31	3.05
2	12.88	Fluticasone propionate	C25 H31 F3 O5 S	500.18	2.74	
S.No.	R.Time	Metabolite (Tannins)	Molecular formula	Molecular weight	Area %	Total %
1	9.412	Tigloylgomicin H	C28 H36 O8	500.24	0.41	0.41
S.No.	R.Time	Metabolite (Terpenoids)	Molecular formula	Molecular weight	Area %	Total %
1	10.89	Ganoderic acid Mc	C36 H54 O9	630.38	0.35	0.35
S.No.	R.Time	Metabolite (Others)	Molecular formula	Molecular weight	Area %	Total %
1	2.097	Altretamine	C9 H18 N6	210.16	0.85	5.71
2	2.219	Acetylagmatine	C7 H16 N4 O	172.13	0.52	
3	3.175	Methyldopa	C10 H13 N O4	211.08	2.17	
4	10.666	Buspirone	C21 H31 N5 O2	385.24	0.52	
5	19.16	N-Hexadecanoylpyrrolidine	C20 H39 N O	309.3	0.80	
6	0.819	(+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone	C9 H12 O2 S	184.06	0.85	

Table 6.8 Metabolite and its relative percentile in aqueous extract of the fruit sample *G. xanthochymus* as analysed by LC-MS

S.No.	R.Time	Metabolite (Alkaloids)	Molecular formula	Molecular weight	Area %	Total %
1	1.091	Pandamarilactam 3x	C13 H17 N O3	235.12	1.98	
2	3.384	Leonurine	C14 H21 N3 O5	311.15	0.54	
3	4.862	Elaeocarpidine	C17 H21 N3	267.17	0.20	3.19
4	5.25	Icacine	C22 H31 N O6	405.21	0.25	
5	9.78	Protoveratrine A	C41 H63 N O14	793.43	0.21	
S.No.	R.Time	Metabolite (Benzene and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	0.771	8-Hydroxy-2-chlorodibenzofuran	C12 H7 Cl O2	218.01	1.11	
2	0.793	4-chloro-3-hydroxy-N-(propylcarbamoyl)benzenesulfonamide	C10 H13 Cl N2 O4 S	292.03	0.20	
3	1.74	Theaflagallin	C20 H16 O9	400.09	0.89	
4	4.069	3-Phenoxypropionic acid	C9 H10 O3	166.06	0.43	
5	10.922	(5alpha,8beta,9beta)-5,9-Epoxy-3,6-megastigmadien-8-ol	C13 H20 O2	208.15	0.54	4.67
6	14.637	Alpha-CEHC	C16 H22 O4	278.15	0.75	
7	7.24	Norathyriol	C13 H8 O6	260.03	0.34	
8	21.186	3,5-Dichloro-4-hydroxy-2-methoxy-6-methylbenzoic acid	C9 H8 Cl2 O4	249.98	0.42	

Table 6.8 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *G. xanthochymus* as analysed by LC-MS

S.No.	R.Time	Metabolite (Diazines)	Molecular formula	Molecular weight	Area %	Total %
1	1.343	5-Acetylamino-6-formylamino-3-methyluracil	C8 H10 N4 O4	226.07	2.56	2.81
2	10.683	Buspirone	C21 H31 N5 O2	385.24	0.25	
S.No.	R.Time	Metabolite (Fatty acids/Prenol Lipids)	Molecular formula	Molecular weight	Area %	Total %
1	5.168	Anopterine	C31 H43 N O7	541.31	0.47	4.18
2	5.59	N-acetyl-LTE4	C25 H39 N O6 S	481.25	0.52	
3	5.775	Glucosylgalactosyl hydroxylysine	C18 H34 N2 O13	486.21	0.35	
4	19.127	dolichyl beta-D-glucosyl phosphate	C31 H55 O9 P	602.36	0.79	
5	4.938	1-Deacetylvaltrate 11-(3-hydroxy-3-methylbutanoate)	C25 H36 O9	480.24	1.76	
6	5.992	Glaucarubol 15-O-beta-D-glucopyranoside	C26 H38 O13	558.23	0.30	
S.No.	R.Time	Metabolite (Flavonoids)	Molecular formula	Molecular weight	Area %	Total %
1	2.868	Pachyrrhizone	C20 H14 O7	366.08	0.21	3.61
2	5.021	Kaempferol 3-rhamnoside 7-xyloside	C26 H28 O14	564.15	0.22	
3	6.52	Myricetin 3-arabinoside	C20 H18 O12	450.08	0.58	
4	7.318	3,3',5,5'-Tetrahydroxy-6,7-methyleneoxy-4'- methoxyflavone 3-glucuronide	C23 H20 O15	536.08	0.22	
5	1.392	Dihydromorelloflavone	C30 H22 O11	558.11	1.73	
6	2.082	Shoyuflavone B	C19 H14 O10	402.06	0.40	
7	6.233	3,4',5,6-Tetrahydroxy-3',7-dimethoxyflavone 3- glucuronide	C23 H22 O14	522.1	0.27	

Table 6.8 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *G. xanthochymus* as analysed by LC-MS

S.No.	R.Time	Metabolite (Nucleotides)	Molecular formula	Molecular weight	Area %	Total %
1	1.135	XMP	C10 H13 N4 O9 P	364.04	0.95	
2	1.219	Ribosylzeatin phosphate	C15 H22 N5 O8 P	431.12	0.48	
3	1.346	Guanosine	C10 H13 N5 O5	283.09	0.90	
4	3.062	Succinoadenosine	C14 H17 N5 O8	383.11	1.25	
5	4.514	3-Butylpyridine	C9 H13 N	135.11	0.41	14.02
6	6.486	Agmatine	C5 H14 N4	130.12	0.18	
7	3.049	Clitidine 5'-phosphate	C11 H15 N2 O9 P	350.05	0.52	
8	3.275	5'-Methylthioadenosine	C11 H15 N5 O3 S	297.09	1.86	
9	1.988	5'-Butyrylphosphouridine	C13 H19 N2 O10 P	394.08	7.47	
S.No.	R.Time	Metabolite (Organic acids)	Molecular formula	Molecular weight	Area %	Total %
1	1.18	N-(1-Deoxy-1-fructosyl) proline	C11 H19 N O7	277.12	1.49	
2	1.29	2-O-Caffeoyltartronic acid	C12 H10 O8	282.04	2.86	
3	3.991	Mumefural	C12 H12 O9	300.05	0.34	
4	6.247	Valganciclovir	C14 H22 N6 O5	354.16	0.28	
5	9.858	N-(5-Methyl-3-oxohexyl) alanine	C10 H19 N O3	201.14	0.18	
6	0.78	2,4-Dichloro-3-oxoadipate	C6 H6 Cl2 O5	227.96	0.27	
7	1.163	L-Ascorbic acid-2-glucoside	C12 H18 O11	338.09	4.04	21.81
8	1.163	Isocitrate	C6 H8 O7	192.03	8.27	
9	1.326	Monoglyceride citrate	C9 H14 O9	266.06	2.07	
10	3.91	Starch acetate	C12 H18 O9	306.1	0.40	
11	3.981	3-oxoglutaric acid	C5 H6 O5	146.02	0.52	
12	5.643	2-O-(Z-p-Hydroxycinnamoyl)-(x)- glyceric acid	C12 H12 O6	252.06	0.62	
13	4.714	2,4'-Diphenyldiamine	C12 H12 N2	184.1	0.44	

Table 6.8 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *G. xanthochymus* as analysed by LC-MS

S.No.	R.Time	Metabolite (Phenolic compounds)	Molecular formula	Molecular weight	Area %	Total %
1	7.324	Dihydrocapsaicin	C18 H29 N O3	307.21	0.43	
2	13.967	Nordihydrocapsaicin	C17 H27 N O3	293.2	0.29	
3	14.194	Venlafaxine	C17 H27 N O2	277.2	0.21	1.55
4	3.48	5-Hydroxydantrolene	C14 H10 N4 O6	330.06	0.44	
5	13.467	Dinoseb	C10 H12 N2 O5	240.07	0.18	
S.No.	R.Time	Metabolite (Quinolines and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	1.572	Neoacrimarine J	C28 H23 N O9	517.13	0.68	
2	2.538	Neoacrimarine I	C29 H25 N O9	531.14	1.89	2.71
3	4.222	Kynurenic acid	C10 H7 N O3	189.04	0.15	
S.No.	R.Time	Metabolite (Sugars and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	1.993	1-Methyl 2-galloylgalactarate	C14 H16 O12	376.06	0.71	
2	2.282	3-O-(3,6-Anhydro-alpha-D-galactopyranosyl)-D- galactose 4-O-sulfate	C12 H20 O13 S	404.06	1.13	
3	2.735	Aldobiouronic acid D3	C11 H18 O11	326.09	0.70	4.81
4	4.354	cyclo-Dopa 5-O-glucoside	C15 H19 N O9	357.1	0.69	
5	1.163	D-Erythroascorbic acid 1'-a-D-glucoside	C11 H16 O10	308.07	0.80	
6	4.35	Cichoriin	C15 H16 O9	340.08	0.33	
7	5.381	7-Hydroxy-2-methyl-4-oxo-4H-1-benzopyran-5- carboxylic acid 7-glucoside	C17 H18 O10	382.09	0.44	

Table 6.8 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *G. xanthochymus* as analysed by LC-MS

S.No.	R.Time	Metabolite (Terpenoids)	Molecular formula	Molecular weight	Area %	Total %
1	5.655	Gibberellin A112	C20 H28 O5	348.19	0.68	
2	6.171	Teresantalol	C10 H16 O	152.12	0.81	
3	5.533	Catheduline E2	C38 H40 N2 O11	700.26	0.86	
4	5.642	Cinnzeylanol	C20 H32 O7	384.22	0.29	6.25
5	5.673	Trichilin A	C35 H46 O13	674.28	0.86	
6	6.941	Resiniferonol	C20 H28 O6	364.19	1.34	
7	10.982	Lucidenic acid D1	C27 H34 O7	470.23	0.21	
8	19.126	(+)-Isoxanthochymol	C38 H50 O6	602.36	1.20	
S.No.	R.Time	Metabolite (Others)	Molecular formula	Molecular weight	Area %	Total %
1	1.034	Fosamine	C3 H8 N O4 P	153.02	0.64	
2	8.95	Heterophylol	C26 H32 O4	408.24	0.27	
3	19.01	N-Hexadecanoylpyrrolidine	C20 H39 N O	309.3	0.30	3.52
4	4.067	Hexahydro-2',4-dimethylspiro[1,3-dithiolo[4,5- c]furan-2,3'(2'H)-furan]	C10 H16 O2 S2	232.06	2.31	

Table 6.9 Metabolite and its relative percentile in aqueous extract of the fruit sample *P. emblica* as analysed by LC-MS

S.No.	R.Time	Metabolite (Alkaloids)	Molecular formula	Molecular weight	Area %	Total %
1	3.42	Bremazocine	C20 H29 N O2	315.21	0.39	
2	4.38	(1xi,3xi)-1,2,3,4-Tetrahydro-1-methyl-beta- carboline-3-carboxylic acid	C13 H14 N2 O2	230.1	2.55	
3	4.93	Lindheimerine	C22 H31 N O2	341.23	0.61	
4	5.37	Cuauchichicine	C22 H33 N O2	343.25	0.67	8.42
5	7.78	Flazine	C17 H12 N2 O4	308.08	2.08	
6	9.19	Dehydroxymethylflazine	C16 H10 N2 O3	278.07	1.19	
7	9.95	Anhalonidine	C12 H17 N O3	223.12	0.38	
8	4.95	Chebulagic acid	C41 H30 O27	952.09	0.56	
S.No.	R.Time	Metabolite (Amino acids/Peptidess)	Molecular formula	Molecular weight	Area %	Total %
1	1.40	Alanyl-Leucine	C9 H18 N2 O3	202.13	0.74	
2	2.58	Leucyl-Valine	C11 H22 N2 O3	230.16	1.17	2.94
3	5.60	Leucyl-leucyl-norleucine	C18 H35 N3 O4	357.26	0.43	
4	4.78	Phenylalanyl-glutamate	C14 H18 N2 O5	294.12	0.60	

Table 6.9 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *P. emblica* as analysed by LC-MS

S.No.	R.Time	Metabolite (Benzenoids and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	0.81	4-chloro-3-hydroxy-N-(propylcarbamoyl)benzenesulf onamide	C10 H13 Cl N2 O4 S	292.03	0.79	
2	1.22	2-O-Galloyl-1,4-galactarolactone	C13 H12 O11	344.04	1.78	
3	1.96	Benzocaine	C9 H11 N O2	165.08	1.38	
4	2.57	2-Hexylbenzothiazole	C13 H17 N S	219.11	0.26	
5	3.45	3,4-Dihydro-7-methoxy-2-methylene-3-oxo-2H-1,4-benzoxazine-5- carboxylic acid	C11 H9 N O5	235.05	0.61	
6	4.45	Salicylanilide	C13 H11 N O2	213.08	1.31	
7	4.51	Pheneturide	C11 H14 N2 O2	206.11	1.05	14.77
8	5.45	Methadyl Acetate	C23 H31 N O2	353.23	0.38	
9	10.04	Sulfadimidine	C12 H14 N4 O2 S	278.08	0.26	
10	1.46	2-O-Galloyl-1,4-galactarolactone	C13 H12 O11	344.04	1.50	
11	4.33	Amlaic acid	C27 H24 O19	652.09	0.63	
12	10.79	Granisetron	C18 H24 N4 O	312.19	0.47	
13	10.94	(5alpha,8beta,9beta)-5,9-Epoxy-3,6-megastigmadien-8-ol	C13 H20 O2	208.15	1.08	
14	14.62	Alpha-CEHC	C16 H22 O4	278.15	1.02	
15	8.20	7-Hydroxy-2-methyl-4-oxo-4H-1-benzopyran-5-acetic acid	C12 H10 O5	234.05	2.26	

Table 6.9 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *P. emblica* as analysed by LC-MS

S.No.	R.Time	Metabolite (Fatty acids/Lipids)	Molecular formula	Molecular weight	Area %	Total %
1	1.22	Mesaconic acid	C5 H6 O4	130.03	2.18	3.59
2	10.21	3-Hydroxynonyl acetate	C11 H22 O3	202.16	0.42	
3	6.28	Teresantalol	C10 H16 O	152.12	0.65	
4	8.50	Arlatin	C15 H22 O4	266.15	0.34	
S.No.	R.Time	Metabolite (Flavonoids)	Molecular formula	Molecular weight	Area %	Total %
1	5.83	Quercetin	C15 H10 O7	302.04	0.71	4.80
2	4.75	Shoyuflavone C	C19 H14 O11	418.05	0.31	
3	5.50	Shoyuflavone B	C19 H14 O10	402.06	0.54	
4	6.36	Cynaroside	C21 H20 O11	448.1	2.34	
5	7.57	Tectoridin	C22 H22 O11	462.12	0.90	

Table 6.9 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *P. emblica* as analysed by LC-MS

S.No.	R.Time	Metabolite (Organic acids)	Molecular formula	Molecular weight	Area %	Total %
1	3.72	Butoctamide hydrogen succinate	C16 H29 N O5	315.21	0.43	
2	6.74	(3Z)-4-(2-Carboxyphenyl)-2-oxobut-3-enoate	C11 H8 O5	220.04	1.27	
3	6.75	Cordeauxione	C14 H12 O7	292.06	0.59	5.96
4	7.05	Hydroxyvernolide	C19 H22 O8	378.13	0.45	
5	9.35	N-(5-Methyl-3-oxohexyl)alanine	C10 H19 N O3	201.14	0.36	
6	1.14	Isocitrate	C6 H8 O7	192.03	2.26	
7	4.46	3,4-Dihydroxyphenylglycol O- sulfate	C8 H10 O7 S	250.01	0.59	
S.No.	R.Time	Metabolite (Phenolic compounds)	Molecular formula	Molecular weight	Area %	Total %
1	1.09	Cis-Caffeoyl tartaric acid	C13 H12 O9	312.05	1.73	
2	1.69	4-(3,5-Diphenylcyclohexyl)phenol	C24 H24 O	328.19	0.56	
3	14.27	Venlafaxine	C17 H27 N O2	277.2	0.43	
4	1.14	2-O-Galloylgalactaric acid	C13 H14 O12	362.05	5.69	17.62
5	1.44	(+)-Chebulic acid	C14 H12 O11	356.04	0.92	
6	1.69	Gallic acid	C7 H6 O5	170.02	3.47	
7	5.59	Ellagic acid	C14 H6 O8	302.01	4.39	
8	3.03	Dihydrocapsaicin	C18 H29 N O3	307.21	0.43	

Table 6.9 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *P. emblica* as analysed by LC-MS

S.No.	R.Time	Metabolite (Steroids)	Molecular formula	Molecular weight	Area %	Total %
1	4.16	17beta-Nitro-5alpha-androstane	C19 H31 N O2	305.23	0.30	2.48
2	2.94	6-(Dibromomethylene)-17beta- hydroxy-androst-4-en-3-one propionate	C23 H30 Br2 O3	512.05	2.18	
S.No.	R.Time	Metabolite (Sugars)	Molecular formula	Molecular weight	Area %	Total %
1	1.06	D-Glucarate	C6 H10 O8	210.04	2.80	3.86
2	3.41	2,6-Digalloylglucose	C20 H20 O14	484.09	1.06	
S.No.	R.Time	Metabolite (Tannins)	Molecular formula	Molecular weight	Area %	Total %
1	4.25	Putranjivain A	C46 H36 O31	1084.13	1.32	15.04
2	4.53	Punicacortein B	C27 H22 O18	634.08	4.66	
3	4.69	Sanguiin H11	C41 H28 O27	952.09	3.73	
4	4.84	1-O,2-O,6-O-Trigalloyl-beta-D-glucose	C27 H24 O18	636.1	1.12	
5	5.12	Tercatain	C34 H26 O22	786.1	1.23	
6	5.25	Isoterchebin	C34 H26 O22	954.1	2.98	
S.No.	R.Time	Metabolite (Others)	Molecular formula	Molecular weight	Area %	Total %
1	1.76	Rofecoxib	C17 H14 O4 S	314.06	1.32	6.34
2	1.96	Ketotifen	C19 H19 N O S	309.12	1.12	
3	4.38	3-Butylpyridine	C9 H13 N	135.11	1.82	
4	4.45	Nifedipine	C17 H18 N2 O6	346.12	1.01	
5	8.04	N-Benzoyl-D-arginine	C13 H18 N4 O3	278.14	0.59	
6	18.98	N-Hexadecanoylpyrrolidine	C20 H39 N O	309.3	0.47	

Table 6.10 Metabolite and its relative percentile in aqueous extract of the fruit sample *S. pinnata* as analysed by LC-MS

S.No.	R.Time	Metabolite (Alcohol)	Molecular formula	Molecular weight	Area %	Total %
1	4.44	5-Methoxytryptophol	C11 H13 N O2	191.1	1.36	1.36
S.No.	R.Time	Metabolite (Alkaloids)	Molecular formula	Molecular weight	Area %	Total %
1	3.39	(±)-Pandamarine	C18 H25 N3 O2	315.2	0.13	
2	3.49	Diamorphine (Heroin)	C21 H23 N O5	369.16	0.46	
3	3.76	Sinapoylputrescine	C15 H22 N2 O4	294.16	0.52	
4	4.39	(1xi,3xi)-1,2,3,4-Tetrahydro-1-methyl-beta- carboline-3-carboxylic acid	C13 H14 N2 O2	230.1	2.37	7.08
5	4.87	Lindheimerine	C22 H31 N O2	341.23	0.95	
6	7.76	Flazine	C17 H12 N2 O4	308.08	2.65	
S.No.	R.Time	Metabolite (Amino acids/Peptides)	Molecular formula	Molecular weight	Area %	Total %
1	1.26	L-isoleucyl-L-proline	C11 H20 N2 O3	228.15	2.23	
2	1.81	N-Glycosyl-L-asparagine	C10 H18 N2 O8	294.11	0.28	
3	3.15	L-Tryptophan	C11 H12 N2 O2	204.09	1.16	
4	4.05	Leucyl-Isoleucine	C12 H24 N2 O3	244.18	1.08	7.29
5	4.93	Isoleucyl-Phenylalanine	C15 H22 N2 O3	278.16	0.73	
6	5.98	N2-Malonyl-D-tryptophan	C14 H14 N2 O5	290.09	0.89	
7	4.89	N-Ethylmaleimide-S-glutathione	C16 H22 N4 O8 S	430.12	0.92	

Table 6.10 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *S. pinnata* as analysed by LC-MS

S.No.	R.Time	Metabolite (Benzenoids and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	1.46	Benzocaine	C9 H11 N O2	165.08	1.08	
2	2.44	2-Hexylbenzothiazole	C13 H17 N S	219.11	0.49	
3	3.28	Benzoyl meso-tartaric acid	C11 H10 O7	254.04	0.51	
4	4.50	Troglitazone	C11 H10 O7	441.16	0.76	
5	4.71	Salicylanilide	C11 H10 O7	213.08	1.10	5.55
6	11.27	(5alpha,8beta,9beta)-5,9-Epoxy-3,6-megastigmadien-8-ol	C11 H10 O7	208.15	0.41	
7	14.62	Alpha-CEHC	C11 H10 O7	278.15	0.96	
8	3.73	2,6-Digalloylglucose	C11 H10 O7	484.09	0.24	
S.No.	R.Time	Metabolite (Ester)	Molecular formula	Molecular weight	Area %	Total %
1	0.80	(+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone	C9 H12 O2 S	184.06	0.82	
2	3.01	alpha-Terpinyl cinnamate	C19 H24 O2	284.18	0.67	5.21
3	4.17	m-Coumaric acid	C9 H8 O3	164.05	0.68	
4	12.87	Triamcinolone diacetate	C25 H31 F O8	478.2	3.03	
S.No.	R.Time	Metabolite (Fatty acids/Prenol lipids)	Molecular formula	Molecular weight	Area %	Total %
1	3.62	2-Oxo-5,11(13)-eudesmadien-12,8-olide	C15 H18 O3	246.12	0.46	
2	5.88	Glucosylgalactosyl hydroxylysine	C18 H34 N2 O13	486.21	1.34	
3	6.00	(all-E)-3,5,7-Tridecatriene-9,11-diyn-1-ol	C13 H14 O	186.1	0.39	4.23
4	6.04	N-acetyl-LTE4	C25 H39 N O6 S	481.25	1.25	
5	8.44	Menthyl ethylene glycol carbonate	C13 H24 O4	244.17	0.33	
6	10.19	3-Hydroxynonyl acetate	C11 H22 O3	202.16	0.46	

Table 6.10 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *S. pinnata* as analysed by LC-MS

S.No.	R.Time	Metabolite (Flavonoids)	Molecular formula	Molecular weight	Area %	Total %
1	4.96	Kaempferol 3-rhamnoside 7-xyloside	C26 H28 O14	564.15	2.42	
2	6.84	3-O-Methylquercetin	C16 H12 O7	316.06	2.73	
3	6.85	Rhamnetin 3-sophoroside	C28 H32 O17	640.16	1.04	
4	7.22	(+)-Sophorol	C16 H12 O6	300.06	0.82	9.55
5	1.20	Tectorigenin 4'-sulfate	C16 H12 O9 S	380.02	1.38	
6	4.68	Shoyuflavone C	C19 H14 O11	418.06	0.85	
7	6.03	Natsudaidain 3-glucoside	C27 H32 O14	580.18	0.31	
S.No.	R.Time	Metabolite (Nucleotides/Nucleosides)	Molecular formula	Molecular weight	Area %	Total %
1	1.33	Pirbuterol	C12 H20 N2 O3	240.15	3.04	
2	4.39	3-Butylpyridine	C9 H13 N	135.11	1.86	6.57
3	6.16	XMP	C10 H13 N4 O9 P	364.05	1.21	
4	6.40	dIMP	C10 H13 N4 O7 P	332.05	0.47	
S.No.	R.Time	Metabolite (Organic acids)	Molecular formula	Molecular weight	Area %	Total %
1	1.38	Medicanine	C7 H13 N O3	159.09	0.60	
2	12.96	Phenylbutyrylglutamine	C15 H20 N2 O4	292.14	0.59	
3	1.07	D-4-Hydroxy-2-oxoglutarate	C5 H6 O6	162.02	4.17	
4	1.11	Oxalosuccinic acid	C6 H6 O7	190.01	16.40	24.87
5	4.48	2'-(E)-Feruloyl-3-(arabinosylxylose)	C20 H26 O12	458.14	0.74	
6	5.17	2-Caffeoylisocitrate	C15 H14 O10	354.06	1.15	
7	6.79	Rhamnetin 3-laminaribioside	C28 H32 O17	640.17	1.21	

Table 6.10 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *S. pinnata* as analysed by LC-MS

S.No.	R.Time	Metabolite (Phenolic compounds)	Molecular formula	Molecular weight	Area %	Total %
1	2.34	Venlafaxine	C17 H27 N O2	277.2	0.37	9.26
2	7.39	Dihydrocapsaicin	C18 H29 N O3	307.21	0.40	
3	8.90	Heterophylol	C26 H32 O4	408.24	0.57	
4	9.44	3-tert-Butyl-5-methylcatechol	C11 H16 O2	180.11	0.54	
5	13.93	Nordihydrocapsaicin	C17 H27 N O3	293.2	0.43	
6	5.58	Ellagic acid	C14 H6 O8	302.01	4.73	
7	1.66	Gallic acid	C7 H6 O5	170.02	1.73	
S.No.	R.Time	Metabolite (Quinolines and derivatives)	Molecular formula	Molecular weight	Area %	Total %
1	4.23	Sparfloxacin	C19 H22 F2 N4 O3	392.17	1.04	2.13
2	7.04	Protoaphin aglucone	C30 H28 O11	564.17	0.37	
3	6.07	Haematopodin	C13 H12 N2 O3	244.08	0.72	
S.No.	R.Time	Metabolite (Sugars)	Molecular formula	Molecular weight	Area %	Total %
1	1.33	Miserotoxin	C9 H17 N O8	267.1	0.89	4.07
2	3.63	15-Hydroxymarasmen-3-one	C15 H20 O4	264.14	0.89	
3	5.41	3-(4-Hydroxy-3-methoxyphenyl)-1,2-propanediol 2-O-(galloyl- glucoside)	C23 H28 O13	512.15	1.29	
4	4.07	Dihydroferulic acid 4-O-glucuronide	C16 H20 O10	372.11	0.30	
5	4.39	5-Hydroxy-6-methoxycoumarin 7-glucoside	C16 H18 O10	370.09	0.40	
6	4.84	Lucuminic acid	C19 H26 O12	444.13	0.30	

Table 6.10 (Contd.) Metabolite and its relative percentile in aqueous extract of the fruit sample *S. pinnata* as analysed by LC-MS

S.No.	R.Time	Metabolite (Tannins)	Molecular formula	Molecular weight	Area %	Total %
1	3.41	Punicacortein B	C27 H22 O18	634.08	1.14	5.17
2	5.09	Sanguiin H11	C41 H28 O27	952.09	3.75	
3	5.38	2-O-Galloylpunicalin	C41 H26 O26	934.07	0.29	
S.No.	R.Time	Metabolite (Terpenoids)	Molecular formula	Molecular weight	Area %	Total %
1	5.07	Cuauchichicine	C22 H33 N O2	343.25	0.96	1.81
2	17.78	Ganoderic acid F	C32 H42 O9	570.28	0.86	
S.No.	R.Time	Metabolite (Others)	Molecular formula	Molecular weight	Area %	Total %
1	2.73	2-Descarboxy-cyclo-dopa	C8 H9 N O2	151.06	0.43	8.70
2	3.12	Indoleacrylic acid	C11 H9 N O2	187.06	1.95	
3	4.11	1,4-Dihydroxynaphthalene	C10 H8 O2	160.05	0.90	
4	4.44	DHAP(10:0)	C13 H25 O7 P	324.13	0.94	
5	5.67	Scopoletin	C10 H8 O4	192.04	1.28	
6	7.54	2-(2-Methylpropoxy) naphthalene	C14 H16 O	200.12	0.51	
7	10.70	Buspirone	C21 H31 N5 O2	385.24	0.56	
8	4.33	5-(3-Hydroxy-4-acetoxybut-1-ynyl)-2,2'- bithiophene	C14 H12 O3 S2	292.02	0.41	
9	5.95	Mephobarbital	C13 H14 N2 O3	246.1	1.02	
10	6.86	CMP-N-glycoloylneuraminate	C20 H31 N4 O17 P	630.13	0.32	
11	7.08	Chlorohyssopifolin A	C19 H24 Cl2 O7	434.09	0.38	

Table 6.11 Percentile level of metabolites present in the seven wild edible fruits of Manipur.

S.No.	Metabolites	*A. bunius*	*A. carambola*	*E. floribundus*	*G. pedunculata*	*G. xanthochymus*	*P. emblica*	*S. pinnata*
1	Alcohols/Polyols	6.08	2.33	0.63	1.37	0.00	0.00	1.36
2	Alkaloids and derivatives	18.16	40.47	3.56	3.56	3.19	8.42	7.08
3	Amino acids/Peptides	8.52	0.70	11.28	4.25	0.00	2.94	7.29
4	Benzenoids and derivatives	5.38	17.46	12.02	16.49	4.67	14.77	5.55
5	Diazines	0.00	0.00	0.00	0.00	2.81	0.00	0.00
6	Ester	0.00	0.00	0.00	0.00	0.00	0.00	5.21
7	Fatty acids/Lipids	7.68	15.55	4.47	19.94	4.18	3.59	4.23
8	Flavonoids	1.47	14.68	4.42	0.53	3.61	4.80	9.55
9	Nitrogenous compounds	4.11	3.59	0.00	0.00	0.00	0.00	0.00
10	Nucleotides/Nucleosides	0.00	2.82	6.98	5.63	14.02	0.00	6.57
11	Organic acids	18.04	15.75	39.35	3.24	21.81	5.96	24.87
12	Others	0.00	0.65	10.99	5.71	3.52	6.34	8.70
13	Phenolic compounds	5.19	6.65	1.68	7.88	1.55	17.62	9.26
14	Quinolines and derivatives	0.00	0.00	0.83	0.61	2.71	0.00	2.13
15	Steroids	3.58	2.29	0.00	3.05	0.00	2.48	0.00
16	Sugars	12.27	20.75	31.83	5.47	4.81	3.86	4.07
17	Tannins	0.00	0.00	0.00	0.41	0.00	15.04	5.17
18	Terpenoids	7.13	12.02	2.87	0.35	6.25	0.00	1.81

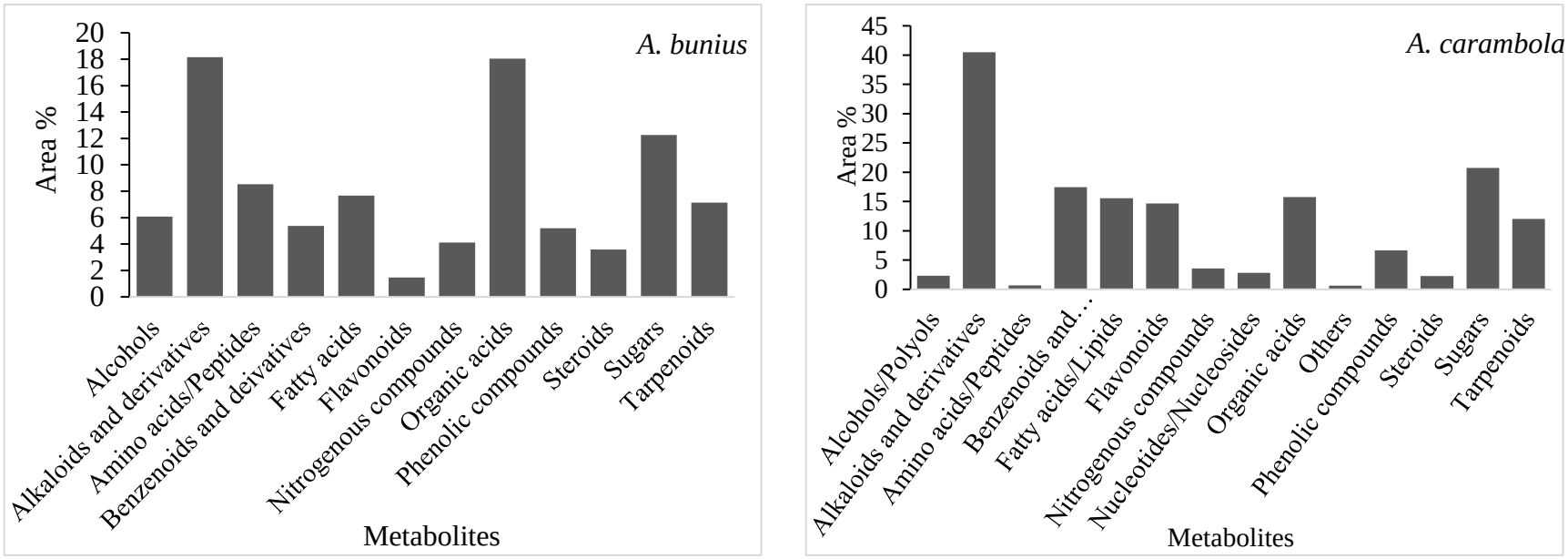

Fig. 6.4a Percentile level of metabolite classes in wild edible fruits, *A. bunius* and *A. carambola* analysed by LC-MS

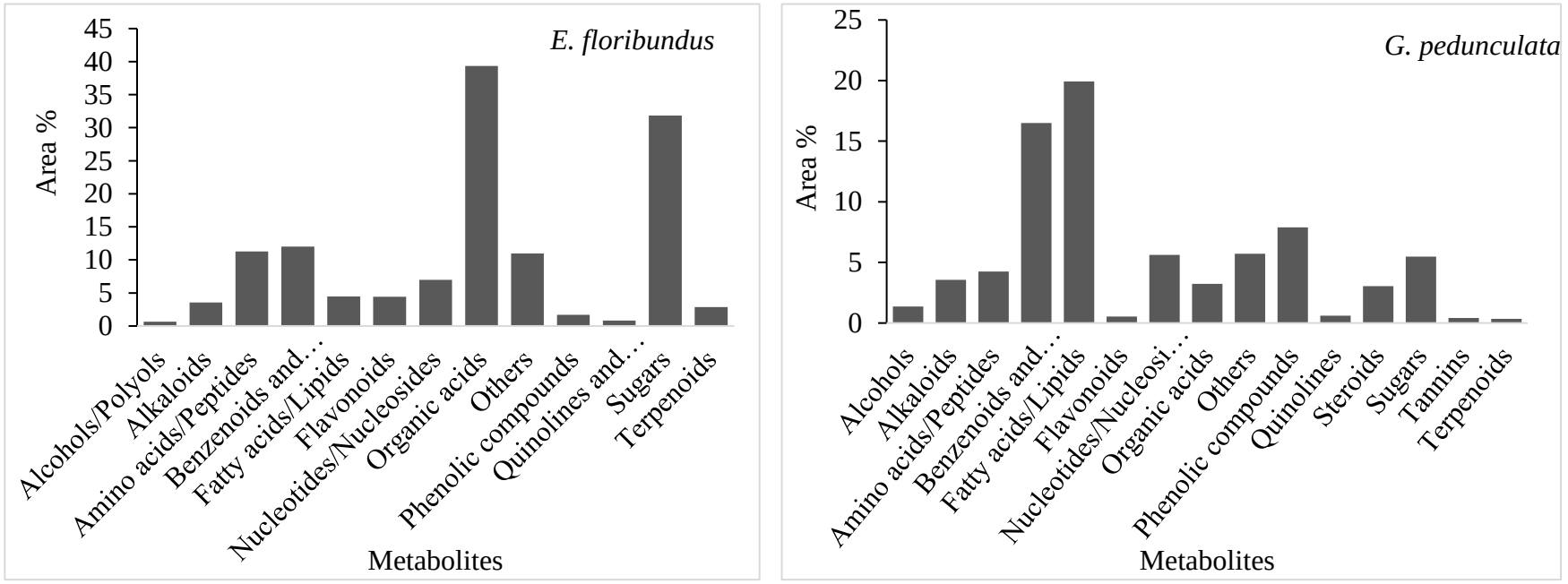

Fig. 6.4b Percentile level of metabolite classes in seven wild edible fruits analysed by LC-MS: (a) *E. floribundus* (b) *G. pedunculata*

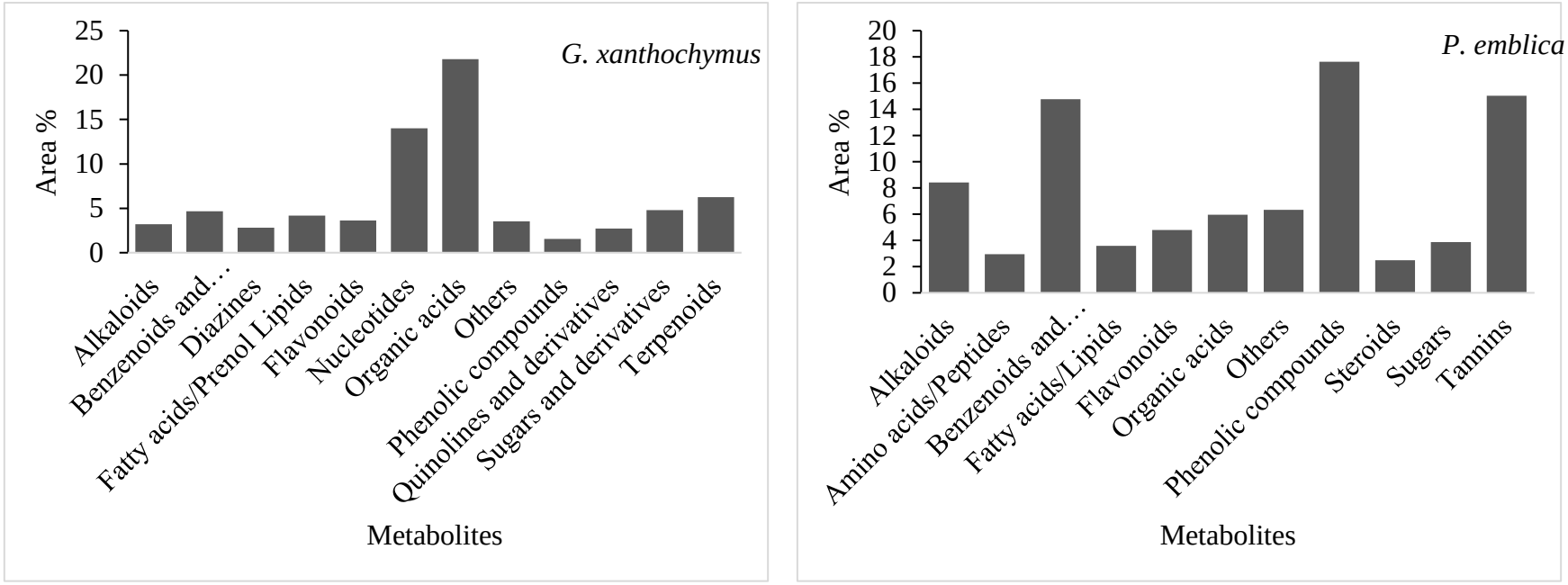

Fig. 6.4c Percentile level of metabolite classes in wild edible fruits, *G. xanthochymus* and *P. emblica* analysed by LC-MS

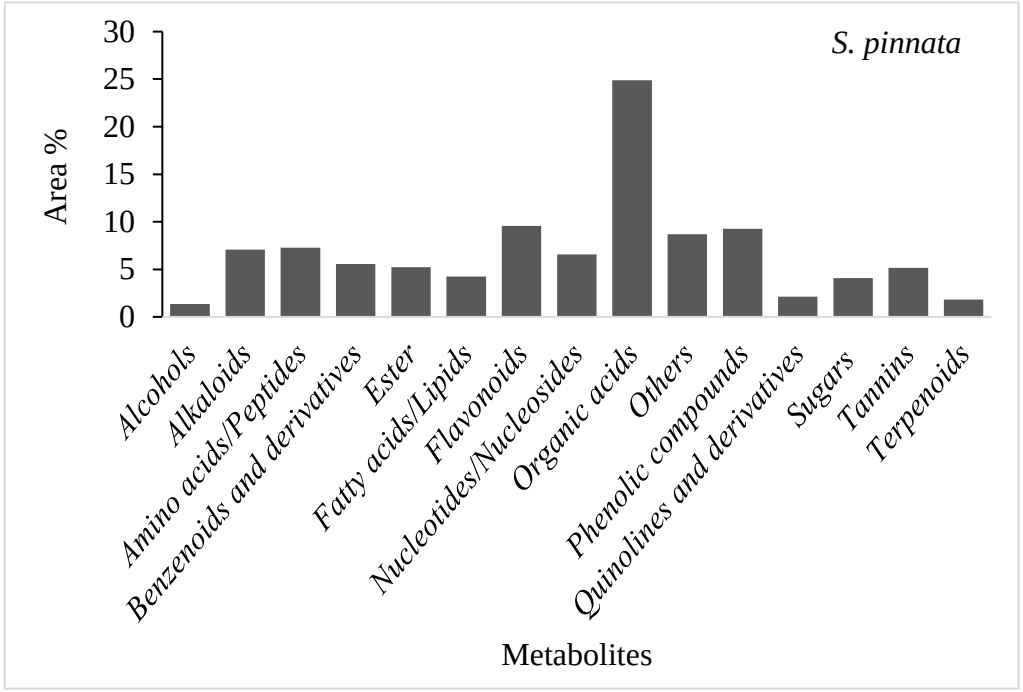

Fig. 6.4d Percentile level of metabolite classes in *S. pinnata* analysed by LC-MS

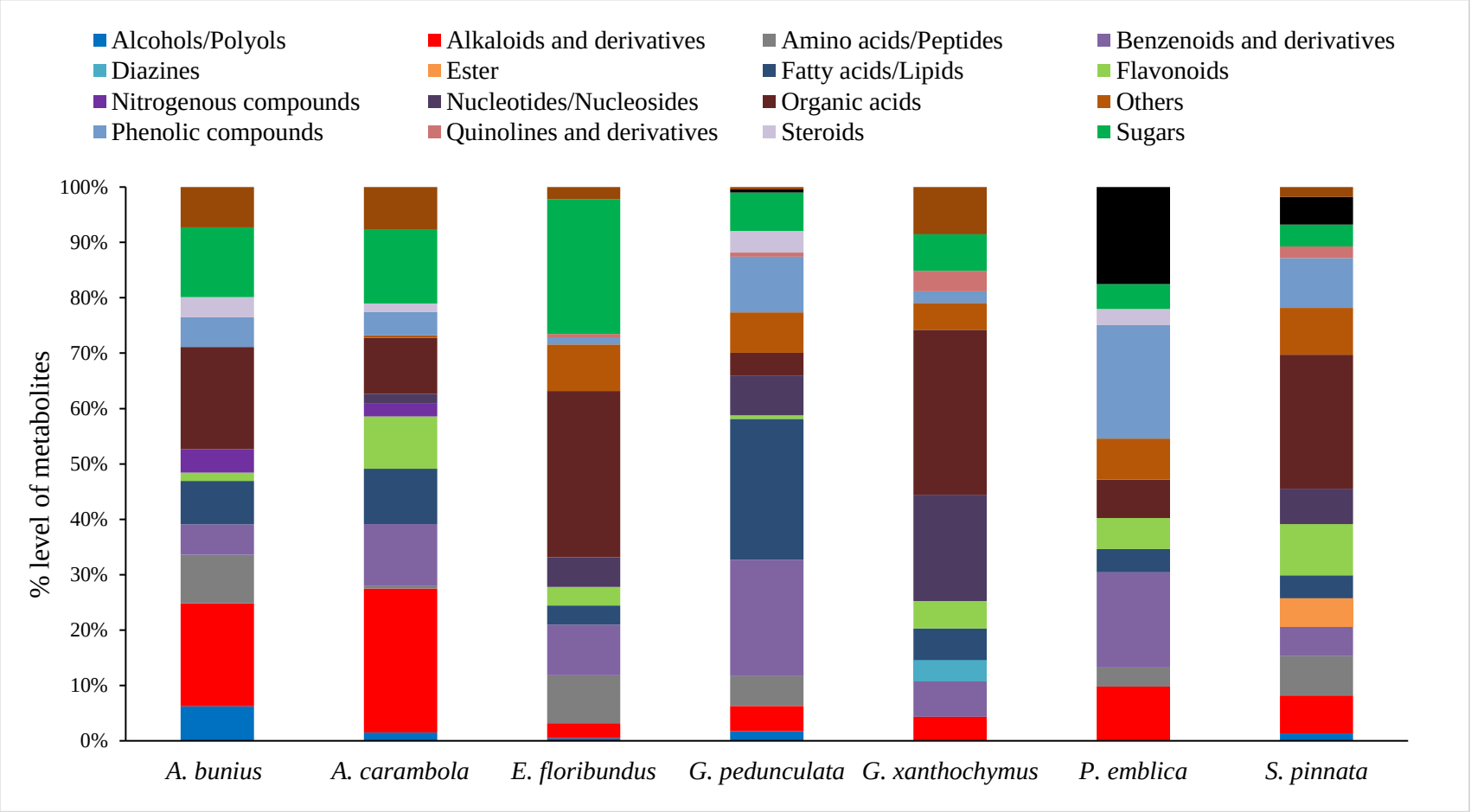

Fig. 6.5 Percentile levels of metabolite classes in seven wild edible fruits analysed by LC-MS

Table 6.12 Reported bioactive compound present in seven wild edible fruits of Manipur.

S. No	Name of compound	Biological activity	Biological activity** (**Source)
1	Pirbuterol	Beta-2 adrenergic agonist and bronchodilator used for the symptomatic treatment of asthma	https://go.drugbank.com/drugs/DB01291
2	Benzocaine	Benzocaine is a topical local anaesthetic used for the temporary relief of pain and itching associated with minor burns, sunburn, scrapes and insect bites or minor skin irritations.	[22] https://go.drugbank.com/drugs/DB01086
3	Dihydrocapsaicin	Dihydrocapsaicin has been shown to induce hypothermia in rats, a property which may help protect victims of stroke and cardiac arrest.	https://drugs.ncats.io/drug/W9BV32M08A
4	Saxagliptin	An DPP-4 inhibitor used for the management of type 2 diabetes mellitus.	https://go.drugbank.com/drugs/DB06335
5	Stilbamidine	Treating various fungal infections.	https://www.medchemexpress.com/Stilbamidine.html

Table 6.12 (Contd.) Reported bioactive compound present in seven wild edible fruits of Manipur.

S. No	Name of compound	Biological activity	Biological activity** (**Source)
6	Caseadine	Antimicrobial and antioxidant activity and a high antitumor potential	[23]
7	Chlorogenic acid	Hypoglycemic, hypolipidemic, anti- inflammatory, antioxidant, and other pharmacological properties. Specifically, CA relieves the effects of, and prevents, diabetes mellitus (DM)	[24]
8	Apigenin 7-glucoside	Antioxidant, anti-inflammatory, and chemoprevention.	[25]
9	Heteratisine	Potent antiarrhythmic and antifibrillatory	[26]
10	Tubulosine	An antitumor constituent	[27]
11	Cassine	Antimicrobial alkaloid	[28]
12	Alpha-Eucaine	Used as local anesthetic	[29]
13	Gambiriin B1	Antioxidant activity	[30]

Table 6.12 (Contd.) Reported bioactive compound present in seven wild edible fruits of Manipur.

S. No	Name of compound	Biological activity	Biological activity** (**Source)
14	2-Octyl-4-propylthiazole	Use as food additives, flavors, and ingredients.	[31]
15	Scopoletin	Antimicrobial and antifungal activities as well as pharmacological effects Anti-Inflammatory effects, used for rheumatic arthritis therapy, possess hypotensive, xanthine oxidase inhibitory (anticancer), antioxidant activities	[32–37]
16	Procyanidin B7	Procyanidin monomers reduces the risk of coronary heart disease; improved risk factors of the metabolic syndrome such as hypertension, vascular endothelial dysfunction, dyslipidemia, and glucose intolerance	[37]
17	2-(3-Phenylpropyl) tetrahydrofuran)	Sweet, Fruity, and green tasting compound	The Good Scents Company (2009)
18	Catechin	Anti-microbial, anti-viral, anti-inflammatory, anti-allergenic, and anti-cancer effects of catechins. Catechins increase the penetration and absorption of healthy functional foods and bio cosmetics into the body and the skin, thus improving their utility.	[38]
19	Hexyl 2-furoate	A sweet, apple, and floral tasting compound	The Good Scents Company (2009)
20	Kinetin	A plant hormone promotes cell division and plant growth; found in cosmetic products as an anti-aging agent	https://go.drugbank.com/drugs/DB11336
21	beta-Solamarine	Anti-tumour agent and anti-bacterial	[39–41]
22	Oleuropein	Antioxidant, anti-inflammatory, anti-atherogenic, anti-cancer activities, antimicrobial activity, antiviral activity, hypolipidemic and hypoglycaemic effect.	[42]

Table 6.12 (Contd.) Reported bioactive compound present in seven wild edible fruits of Manipur.

S. No	Name of compound	Biological activity	Biological activity** (**Source)
23	2,4,6-Trimethyl-4-phenyl-1,3-dioxane	Flavouring ingredients	The Good Scents Company (2009)
24	Physalin E	Anti-inflammatory effects	[43]
25	Heterophylol	Fever, boils, wounds, skin diseases, convulsions, diuretic, constipation, ophthalmic disorders and snake bite	[44]
26	Venlafaxine	An antidepressant, used in the treatment of generalized anxiety, social anxiety, panic disorder, major depressive disorder (MDD), and consider it a second-line option for management of obsessive-compulsive disorder.	The Good Scents Company (2009)
27	(-)-Epicatechin	Consumption of epicatechin–containing food can help prevent the onset of type II diabetes and many cardiovascular diseases	[45,46]
28	Vulgarin	Vulgarin exhibited a significant antihepatotoxic activity	[47]
29	Koenigicine	Anti-hyperlipidemic and anti-hyperglycemic activities	[48]
30	Beiwutine	Analgesic and inti-inflammatory effects in the treatment of arthritis	[49]
31	Ibutilide	Anti-arrhythmic	[50]

Table 6.12 (Contd.) Reported bioactive compound present in seven wild edible fruits of Manipur.

S. No	Name of compound	Biological activity	Biological activity** (**Source)
32	2-phenethyl propionate	Fragrance material, widely used in cosmetics	[51]
33	Cromolyn	Standard mast cell stabilizer used in many clinical studies to treat various allergic diseases	[52,53]
34	Corchorifatty acid F	Anti-neuroinflammatory effect and antiproliferative activities against cancer cell lines	[54]
35	Gossypetin	Antianxiety and antidepressant activity	[55]
36	Myricitrin	Anti-inflammatory activity	[56]
37	Cynaroside	Antioxidant, antimicrobial, and antimutagenic activity	[57]
38	Entecavir	Antiviral	[58]
39	Nifedipine	Anti-hypertension	[59]
40	Niazicin	Anti-hypertension, anti-tumour, and anti-inflammatory	[60,61]
41	Asperuloside	Anti-viral, anti-malarial, anti-protozoal, anti-tumorigenic, anti-hypertensive, anti-obesity, immunomodulatory, anti-inflammatory and antioxidant agent	[62]

Table 6.12 (Contd.) Reported bioactive compound present in seven wild edible fruits of Manipur.

S. No	Name of compound	Biological activity	Biological activity** (**Source)
42	Trilobolide	Immunostimulatory	[63]
43	(±)-Nicotine	Wide variety of biological functions ranging from gene expression, regulation of hormone secretion and enzyme activities	[64]
44	Pheneturide	Anticonvulsant	[65]
45	Talinolol	Cardioprotective and antihypertensive activity	https://drugcentral.org/drugcard/2557
46	Sulfadimidine	Anti-infective agent	[66] https://drugcentral.org/?q=Sulfadimidine&approval=
47	Valtratum	Antioxidants and anticancer activities	[67]
48	Penciclovir	Antiviral	https://drugcentral.org/?q=Penciclovir&approval=
49	(+)-Chebulic acid	Antispasmodic action, antioxidant, hepatoprotective effect, cytoprotective and immunosuppressive activities	[68,69]
50	Physalin I	Immunosuppressive, anti-malarial and anti-leishmanial agents.	[70]

Table 6.12 (Contd.) Reported bioactive compound present in seven wild edible fruits of Manipur.

S. No	Name of compound	Biological activity	Biological activity** (**Source)
51	Leonurine	Neuroprotective effects in ischemic stroke, Parkinson's disease, and Alzheimer's disease; antioxidation, anti-inflammation, and anti-apoptosis	[71,72]
52	Buspirone	Anxiolytic agent	https://drugcentral.org/?q=Buspirone&approval=
53	Anopterine	Antitumor agent	[73]
54	Dihydromorellofla vone	Anti-inflammatory, anti-HIV, antifungal, antitumor, hypocholesterolemic, and anti-plasmodial	[74]
55	Mumefural	Antioxidant activity	[75]
56	Trichilin A	Anti-infective, anti-inflammatory, antischistosomal, antiplasmodial, anticonvulsant, anti-trypanosomal, antioxidant, antitussive, antimutagenic and hepatoprotective properties.	[76]
57	Chebulagic acid	Antitumor	[77]
58	Amlaic acid	Antiviral (best in the control COVID19), anti-inflammatory	[78,79]

Table 6.12 (Contd.) Reported bioactive compound present in seven wild edible fruits of Manipur.

S. No	Name of compound	Biological activity	Biological activity** (**Source)
59	Granisetron	An antiemetic for cancer chemotherapy patients.	https://drugcentral.org/?q=Granisetron&approval=
60	Quercetin	Antioxidant	[80,81]
61	Tectoridin	Estrogenic, anti-oxidative and hepatoprotective effects	[82–84]
62	Gallic acid	Free radical scavenging effect, induction of cancer cell apoptosis, and protection of cells from UV- or irradiation-induced damage	[85,86]
63	Ellagic acid	Anti-inflammatory and antioxidant activities	[87,88]
64	Putranjivain A	Antidiabetic, antimicrobial, anti-inflammatory, and immune-regulating activities	[89,90]
65	Sanguiin H11	Antimicrobial, antiviral, anticancer, anti-inflammatory, and osteoclastogenesis inhibitory agent; antioxidant	[91,92]

Table 6.12 (Contd.) Reported bioactive compound present in seven wild edible fruits of Manipur.

S. No	Name of compound	Biological activity	Biological activity** (**Source)
66	Isoterchebin	Antioxidant activity	[93]
67	Kaempferol 3-rhamnoside 7-xyloside	Antibacterial and antioxidant	[94]
68	Nordihydrocapsaicin	Anticancer effects, act against high cholesterol levels and obesity, and they are commonly used to treat arthritis pain	[95]
69	Sparfloxacin	Antimicrobial	[96]
70	Diamorphine	Anti-inflammatory and analgesic properties	[97,98] https://drugcentral.org/?q=diamorphine&approval=
71	D-Tartaric acid	Antioxidant agent	[99]

6.4 DISCUSSION

6.4.1 FT-IR

Based on the findings of the FT-IR spectra, all the fruit samples exhibited four prominent peaks within the range of 1500-4000 cm^{-1}. OH-groups or carboxylic acid functional groups were detected in all the fruit samples. Alkenes (C=C stretch) groups were observed in all the fruits except *R. semialata*. The spectra around 574 cm-1 indicated the skeletal model of pyranose ring [100]. The peak at around 1022 cm-1 showed the characteristic amorphous region, C–O of C–O–C and that of the peak around 1371 cm^{-1} indicated C–H symmetric bending of CH_3 [100,101]. The peak at 1648 cm^{-1} indicated the bending behaviour of -OH in adsorbed water. The presence of peak 2931 cm^{-1} suggested the presence of CH2 stretching [102]. Furthermore, the presence of a broad wide peak at 3388 cm^{-1} indicated O-H stretching [100,101].

6.4.2 Antimicrobial activity

The selected microbial strains in the present study are associated with common human diseases, and some of them have been reported as infectious pathogens. *Staphylococcus aureus* is a significant bacterial pathogen responsible for a wide range of clinical conditions, including skin and soft tissue infections, bloodstream infections, pneumonia, urinary tract infections, and more [103]. *Listeria monocytogenes*, a food-borne pathogen, can cause severe and potentially fatal diseases, especially in pregnant women, new-borns, and immunocompromised individuals [104]. *Klebsiella pneumonia* are commonly found in various environments and can cause infections such as pneumonia, urinary tract infections, and bloodstream infections, particularly among vulnerable populations like neonates, the elderly, and immunocompromised individuals. *Klebsiella* is also known to be involved in community-acquired diseases [105]. *Pseudomonas aeruginosa* is a gram-negative bacterium found in the environment, including soil and water. It can cause infections in the blood, lungs (pneumonia), and other parts of the body, especially

following surgery [106]. *Candida albicans* is the most prevalent fungal pathogen in humans and is known to cause mucosal infections like vaginitis and oral-pharyngeal thrush, particularly in immunocompromised individuals. In severe cases, it can lead to bloodstream infections and organ damage [107]. These microorganisms are significant pathogens with the potential to cause various diseases and infections, highlighting the importance of studying their antimicrobial activity and identifying effective strategies for their control.

The antimicrobial activity of the aqueous and ethanolic extracts obtained from wild edible fruits was evaluated against various test organisms. The results indicated that both extracts exhibited antimicrobial activity, with the ethanolic extract demonstrating greater effectiveness compared to the aqueous extract. Among the aqueous extracts, eight fruits showed activity against *S. aureus*, with *P. emblica* displaying the largest inhibition zone (14 mm). However, it was observed that the ethanol extracts of *P. emblica* and *D. indica* did not show any zone of inhibition. This disparity could be attributed to the extraction methods and the solvents used, which may have influenced the extraction efficiency of bioactive compounds.

The aqueous extracts of *G. xanthochymus* and *E. floribundus* were active against *L. monocytogens*, whereas three out of fifteen ethanol extracts were inactive against this organism. Six fruits exhibited activity in their aqueous extracts against *K. pneumonia*, while 12 fruits showed activity in their ethanol extracts. Regarding *P. aeruginosa*, five fruits displayed activity in their aqueous extracts, whereas only one fruit out of the 15 tested did not show any activity in its ethanol extract. None of the aqueous extracts from the 15 fruits showed antifungal activity against the fungal strain *C. albicans*. However, the ethanol extracts of eight fruits exhibited antifungal activity against *C. albicans*. Notably, ethanol extracts from fruits such as *Averrhoa carambola*, *Elaeocarpus floribundus*, *Garcinia pedunculata*, *Garcinia xanthochymus*, and *Spondias pinnata* displayed antimicrobial activity against all the tested organisms.

Although ethanol is known for its broad-spectrum antimicrobial activity, it is worth mentioning that the aqueous extracts of the eight fruits in this study demonstrated

antibacterial potential. This finding further supports the effectiveness of certain plant extracts as natural antimicrobials. This observation is consistent with earlier research conducted on crude extracts of plant leaves, as documented by Obeidat et al. in 2012 [108]. Additionally, several studies have reported the antimicrobial activity of various wild edible fruits. For instance, wild jujube (*Ziziphus lotus*) from Morocco [109], *S. pinnata* from Bangladesh [110], *Antidesma bunius* from Al-Orman Botanical Garden, Giza, Egypt [111], *Garcinia xanthochymus* from Similipal Biosphere Reserve, Odisha [112], *Rubus ellipticus* from Uttarakhand [113], and 12 wild edible fruits of South Africa [113] have all demonstrated antimicrobial properties.

Considering these findings, the ethanolic extracts were deemed more suitable for compound analysis. However, for the purpose of this study, the aqueous extracts were analysed due to their demonstrated antimicrobial activity and the traditional utilization of these wild edible fruits as decoctions. Hence, it is crucial to identify and analyse the active compounds present in the aqueous extracts, as they may differ from those present in the ethanolic and other solvent extracts. Further investigations are warranted to determine the specific bioactive compounds responsible for the observed antimicrobial activity and their potential applications in pharmaceutical and healthcare sectors.

6.4.3 Analysis of aqueous extract by LC-MS

Plants are known to harbour a diverse array of compounds, many of which possess pharmacological activities with the potential for therapeutic applications. However, a substantial number of these compounds remain unidentified in terms of their specific bioactivities. Ongoing research efforts continually unveil new plant-derived compounds, which may serve as valuable sources for the development of novel drugs. In line with this pursuit, the current study aimed to investigate the metabolic profiles of the crude aqueous extracts obtained from seven wild edible fruits using Liquid Chromatography-Mass Spectrometer (LC-MS) analysis.

The application of LC-MS analysis enabled the comprehensive identification and characterization of a considerable number of metabolites present in the fruit extracts. In total, 71 reported metabolites were successfully identified and assigned in this study. These identified metabolites have been previously acknowledged for their documented bioactive properties and are associated with potential health benefits. Through the utilization of LC-MS, valuable insights into the chemical composition of the fruit extracts were obtained, thereby facilitating the exploration and assessment of their bioactive potential.

The dominant group of identified metabolites in this study were alkaloids and derivatives, comprising 3.91% to 40.47% of the total. Alkaloids, which represent a highly diverse class of chemical compounds, are among the largest groups of natural products, with approximately 27,000 alkaloids described to date [114]. These alkaloids exhibit significant clinical potential for the treatment of various diseases. Numerous studies have demonstrated their novel bioactivity and clinical applications, as well as the positive impact of structure modifications on enhancing their activity, improving pharmacokinetics, and ensuring higher safety levels [115]. For instance, previous research has reported anti-fungal, cardioprotective, immunoregulatory, anti-malarial, anti-inflammatory, antioxidant, cerebro-protective, anti-mutagenic, vaso-relaxing, anxiolytic, and analgesic activities associated with alkaloids [116]. Notable examples of plant alkaloids include morphine and codeine, which are widely used as narcotic analgesics, apomorphine (a derivative of morphine) employed in Parkinson's disease treatment, the muscle relaxant papaverine, and the antimicrobial agents sanguinarine and berberine. Furthermore, several potent anti-cancer drugs have been developed from plant compounds [117]. In the present study, several reported alkaloids, including caseadine, chebulagic acid, cassine, heteratisine, beiwutine, and diamorphine, were identified, exhibiting diverse biological activities such as antibacterial, antiviral, antioxidant, antiarrhythmic, and anti-fibrillatory effects. Detailed information on these alkaloids is given in Table 6.12.

In the present study, organic acids were found to contribute to a significant proportion (3.24%-39.35%) of the identified metabolites. Organic acids are commonly present in

ripe fruits and are responsible for imparting sourness to them [118]. The concentrations of organic acids and sugars play a crucial role in determining fruit flavour and quality [119]. Organic acids, particularly citric acid, have been associated with antimicrobial activity and skin health [120,121]. The content of organic acids in fruit flesh can be influenced by various environmental factors and cultivation practices, such as temperature, light intensity, cultivar, rootstock, mineral nutrition, water availability, and fruit load/pruning [122]. Organic acids, including citric and ascorbic acids, possess pH-lowering properties and inhibit or kill spoilage-causing organisms in food products. Hence, they are commonly used as preservatives in the food processing industry [123]. Fruit acids play a crucial role in promoting food digestion and enhancing blood circulation. Furthermore, the acid content in fruits can influence the stability of phenolic compounds. Phenolic compounds are a diverse group of plant-derived compounds known for their antioxidant properties and potential health benefits [124]. Wild edible fruits contain various bioactive compounds, particularly organic acids, vitamin C, and E, which have been reported to exhibit biological activity against lipid peroxidation [125]. In the analysed fruit samples, specific organic acids such as benzocaine, isocitrate, medicanine, L-ascorbic acid-2-glycoside, and tartaric acid were identified. Among them, benzocaine is a known drug and topical local anaesthetic used for temporary pain and itch relief associated with minor burns, sunburn, scrapes, insect bites, or skin irritations [22]. Previous research by Gao, 2012 demonstrated the antibacterial activity of different types of organic acids extracted from Japanese apricot fruits against *Escherichia coli*, *Bacillus subtilis*, and *Streptococcus suis* [126].

The analysed fruits in this study exhibited a sugar content ranging 3.8% to 31%. As previously discussed, the concentrations of organic acids and sugars play a crucial role in determining fruit flavour and quality [119]. Sugars, particularly glucose and sucrose, are the main contributors to the sweetness, texture, and juiciness of fruits [127]. For instance, Gao et al. (2012) reported that jujube fruits from the Loess Plateau of China were predominantly composed of glucose and sucrose [128]. Furthermore, *Ficus carica*, commonly known as fig, is renowned for its sweetness in the market, attributed to its high sugar content [124]. The presence of sugars in fruits enhances

their palatability and contributes to their overall sensory appeal. It is noteworthy that the identified sugars in this study were predominantly glycosides, such as Asperuloside, a secondary metabolite belonging to iridoid glycosides known for their pharmacological properties, including antiviral, antimalarial, antiprotozoal, antitumorigenic, antihypertensive, anti-obesity, immunomodulatory, anti-inflammatory, and antioxidant effects [62].

The fatty acid/lipid content of the analysed fruits ranged from 3.59% to 19.94%. Among the fruits, *G. pedunculata* exhibited the highest fatty acid content, while *P. emblica* had the lowest. One of the identified fatty acids, corchorifatty acid, belongs to the group of linoleic acids and derivatives. This fatty acid has been associated with various bioactive properties, including anti-neuroinflammatory effects and antiproliferative activities against cancer cell lines [54]. Additionally, valtratum and anopterin, which possess antitumor, anticancer, and antioxidant activities, were also identified [67,73]. Linoleic acids is considered an essential fatty acid that can reduce the risk of coronary heart diseases [129,130], coronary artery diseases [131], lowers risk of type 2 diabetes mellitus [132], renal disease [133], and regulates plasma cholesterol [134]. The composition of fatty acids in fruits is influenced by factors such as variety, geographical location, climate conditions, and the stage of fruit development [135].

The analysis of the seven wild fruits of Manipur revealed the presence of various phenolic compounds, which are known for their diverse bioactive properties. These compounds accounted for a range of 1.55% to 17.62% of the total composition of the fruits. Among the identified phenolic acids, gallic acid, ellagic acid, and chebulic acids were prominent. Gallic acid is well-known for its antioxidant properties, which help in scavenging harmful free radicals and protecting cells from oxidative damage [136]. Additionally, gallic acid has shown the ability to induce apoptosis in cancer cells and provide cellular protection against UV or irradiation-induced damage [85,86]. Ellagic acid, on the other hand, exhibits antioxidant, anti-inflammatory activities, and potentially preventing chronic diseases [87,88]. Furthermore, chlorogenic acid, another identified phenolic compound, contributes to various bioactivities including

hypoglycaemic, hypolipidemic, anti-inflammatory, antioxidant, and other pharmacological properties. Notably, chlorogenic acid has been reported to alleviate the effects of, and prevent, diabetes mellitus (DM) [24].

The analysis revealed that benzenoids and derivatives accounted for 4.67% to 17.46% of the total composition of the fruits. Of particular interest is the identification of amlaic acid in *P. emblica*, which has recently been reported for its potential in controlling COVID-19 and its anti-inflammatory properties [78,79]. Amlaic acid is also noteworthy as it is associated with the perception of bad tastes, making it a potential marker for flavour quality [137]. In addition to its taste-related properties, amlaic acid exhibits strong antioxidant and antibacterial activities, and it is believed to possess other important biological activities as well. Another benzenoid compound identified is heterophyllol, which has a long history of traditional use in treating various ailments such as fever, boils, wounds, skin diseases, convulsions, and more. It is also employed as a diuretic, for constipation relief, and in the management of ophthalmic disorders and snake bites [44]. Furthermore, an anticonvulsant compound called pheneturide was also identified, which suggests potential neurological effects of these fruits [65].

Tannin metabolites were found to contribute between 0% to 15.04% of the total composition of the fruits analysed. Tannin-rich extracts of fruits have demonstrated various bioactive properties, including antidiabetic, anti-inflammatory, and immune-regulating activities, anti-oxidant, anti-cancerous, anti-allergic, anti-inflammatory, anti-helminthic and anti-microbial activities [89,138]. Notably, the identification of putranjivain and sanguiin H11 in this study highlights their potential biological activities [89,90]. Additionally, tannins are known for their astringent properties and their ability to bind and precipitate proteins [139,140]. They have been traditionally used for their antimicrobial and wound healing properties. The presence of tannin metabolites in the analysed fruits suggests their potential contribution to the overall health benefits and therapeutic properties of these fruits.

The analysis of the fruits revealed the presence of various flavonoids, which accounted for a range of 0.53% to 14.68% of the total composition. Among the identified flavonoids, catechin stood out as a well-known compound with a wide array of bioactive properties. Catechins have been found to possess antimicrobial, antiviral, anti-inflammatory, anti-allergenic, and anti-cancer effects. Additionally, catechins can enhance the absorption and penetration of healthy functional foods and biocosmetics into the body and skin, thereby improving their effectiveness. This makes catechin a valuable component in the development of functional foods and skincare products [38]. Another notable flavonoid identified was quercetin, which is renowned for its antioxidant properties. Quercetin has been extensively studied for its role in neutralizing harmful free radicals and protecting cells from oxidative damage. In addition to its antioxidant activity, flavonoids, including quercetin, have been shown to possess antiviral and anticancer properties, making them promising compounds for potential therapeutic applications [141].

The LC-MS analysis revealed the presence of additional steroid compounds, including physalin I, in the wild edible fruits of Manipur. Physalin I is known for its various bioactive properties, such as being an immunosuppressive, anti-malarial, and anti-leishmanial agent [70].

6.5 CONCLUSION

This chapter focuses on the identification of functional groups present in fifteen wild edible fruits that were studied. Additionally, the presence of potent bioactive compounds in selected fruit samples was examined in relation to their antimicrobial activity. The obtained results revealed the presence of various functional groups in the fruits and confirmed their antimicrobial properties. The LC-MS analysis further revealed that a substantial number of phytochemicals detected in the fruit samples exhibit bioactive characteristics, including antioxidative, anti-inflammatory, anti-carcinogenic, and antimicrobial properties. However, it is important to note that further research utilizing different extraction techniques and methodologies is

required. This will enable a deeper understanding of their chemical composition and the possible discovery of additional beneficial compounds with diverse bioactivities. Such detailed investigations will contribute to the expansion of our knowledge of the medicinal and nutritional value of these fruits and support their utilization in the development of functional foods, nutraceuticals, and pharmaceutical products.

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