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Article

Metabolic Profiling in Banana Pseudo-Stem Reveals a Diverse Set of Bioactive Compounds with Potential Nutritional and Industrial Applications

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Abstract: Banana (*Musa spp*.) is an ancient and popular fruit plant with highly nutritious fruit. The pseudo-stem of banana represents on average 75% of the total dry mass but its valorization as a nutritional and industrial by-product is limited. Recent advances in metabolomics have paved the way to understand and evaluate the presence of diverse sets of metabolites in different plant parts. This study aimed at exploring the diversity of primary and secondary metabolites in the banana pseudo-stem. Hereby, we identified and quantified 373 metabolites from a diverse range of classes including, alkaloids, flavonoids, lipids, phenolic acids, amino acids and its derivatives, nucleotide and its derivatives, organic acids, lignans and coumarins, tannins, and terpene using the widely-targeted metabolomics approach. Banana pseudo-stem is enriched in metabolites for utilization in the food industry (L-lysine and L-tryptophan, L-glutamic acid, Phenylalanine, Palmitoleic acid, α-Linolenic acid, and Lauric acid, and Adenine) and pharmaceutical industry (Guanosine and Cimidahurinine, Bergapten, Coumarins, Procyanidin A2, Procyanidin B1, Procyanidin B3, Procyanidin B2, and Procyanidin B4, Asiatic acid). The metabolome of banana pseudo-stem with integration across multi-omics data may provide the opportunity to exploit the rich metabolome of banana pseudo-stem for industrial and nutritional applications.

Keywords: Banana pseudo-stem; widely-targeted metabolomics; alkaloids; crop waste valorization

1 Introduction

Bananas (*Musa spp*.) are one of the most important fruits in the world and the fourth most important food crop after rice, wheat, and corn. Banana is an excellent source of starch that is accepted as a staple or supplement diet worldwide including Asia, Africa, and Central and South America. Palatability, cheaper source of instant energy, and richness in macronutrients are some of the characteristics which have paved

the way for banana high acceptance by consumers [1–3]. Besides the use of banana as food or supplemental food, the whole plant has potential commercial use in different industries such as packaging and pharmaceutical [4–7]. Although banana fruit has been the focus of interest for scientists to increase its value with biofortification [8–10] and yield [11], less attention was given to other plant parts, including pseudo-stem and leaves.

Banana plant parts have been used in several food preparations and as traditional medicine. Banana pseudo-stem and flowers are employed in cooking with a decent quantity of macronutrients, i.e., iron and potassium, and also a bunch of antioxidants in the form of flavonoids [12]. Banana pseudo-stem is a by-product of the banana plant, which is trunk shaped consisting of overlapping leaf sheaths. It represents on average 75% of the total dry mass of the plant, therefore represents a potential source of bioactive components. The latest developments in omics have provided more insight into the dynamics and networks of metabolic pathways. Accumulation of current knowledge of metabolites with metabolic flux regulation during plant development can exploit the potential of banana pseudo-stem as a source of primary and secondary metabolites along with its other industrial and nutritional uses. Physiochemical characterization of banana pseudo-stem and its valorization for biofiber and bio-composite [13] have potential prospects to evolve as a source of primary antioxidants [2], bioenergy feedstock [14], and raw material in polymer composites [15].

Recent advances in the fields of mass spectrometry, chromatography, liquid chromatography, capillary electrophoresis have paved the way to a relatively new technique called metabolomics which is termed as the use of high-throughput technology to explore all the metabolites in plant tissues at a specific time or growth period. Multiple studies have been carried out to estimate metabolites in plant tissue, resulting in the identification of thousands of metabolites [16–18]. Reports emphasizing genotypic variation present in carotenoids [19–22], phenolics [23,24], and volatile aroma compounds [25–28] have suggested marked differences in the quantity of metabolites at different stages and different plant-parts/tissues. In banana fruit, comprehensive metabolome characterization revealed it as a rich source of primary and secondary metabolites including organic acids, amino acids, peptides, alkaloids, benzenoides, and phenylpropanoids and derivates [29–32]. This rich metabolome enhances the nutritional quality of banana fruit [2,19,33]. However, no comprehensive study has been conducted to assess the richness of metabolites present in other banana tissues.

In this study, we have identified and quantified a huge number of metabolites present in the banana pseudo-stem by using the widely-targeted metabolomic approach. Our work provides insight into the metabolomics of banana pseudo-stem and the theoretical basis for further improvement of banana plant quality and valorization.

2 Material and Methods

2.1 Plant Material

In this study, the banana variety Guangfen No.1 (*Musa spp*. Pisang Awak sub-group ABB) was used as plant material to characterize the metabolome of the pseudo-stem. The material was provided by the Institute of Fruit Tree Research, Guangdong Academy of Agricultural Sciences, Guangzhou, China. Seedlings were grown on tissue culture and later moved to the nutrient soil medium after four weeks. Plants were kept under the controlled conditions (temperature = 28°C, relative humidity = 60%–80%). The photoperiod was kept at 12 h (1500 ± 200 lx). After six weeks, the banana plantlets had five to six true leaves. Triplicate pseudo-stems were then cut and used for metabolome analyses.

2.2 Metabolic Profiling

As described by Zhang et al. [34], samples were prepared for extract analyses, metabolite identification and quantification following the standard procedure of Wuhan MetWare Biotechnology Co., Ltd., Wuhan, China (www.metware.cn).

2.3 Preparation of Samples and Extraction

Frozen samples from triplicate banana pseudo-stems were crushed to powder using a mixer mill for 1.5 min at 30 Hz frequency. 100 mg powder was used for further extraction using 70% aqueous ethanol at 4°C temperature. Extraction was done overnight followed by centrifugation at 10,000 × g for 10 min. The extracts were absorbed and filtered before further analysis.

2.4 HPLC and ESI-Q TRAP-MS/MS

The extracted samples were analyzed with LC-ESI-MS/MS system using standard analytical conditions as previously described by Cao et al. [35]. Q TRAP system (Triple quadrupole-linear ion trap mass spectrometer) was used for quantification of metabolites. Triple quadrupole scans and linear ion trap were acquired on this system. The standard source parameters were used: ion source, turbo spray; source temperature 500°C; ion spray voltage (IS) 5500 V; ion source gas I (GSI), gas II (GSII), curtain gas (CUR) were set at 55, 60, and 25 psi, respectively; the collision gas (CAD) was high. The qualitative analysis of the material was established on secondary spectrum information using the public database of metabolites. The samples were qualitatively analyzed according to the secondary spectrum information. The isotope signals were removed during the quantitative analysis of samples. Triple Q scans were attained as multiple reaction monitoring (MRM) experiments. Metabolite quantification was accomplished using multiple reaction monitoring (MRM) analysis with triple quadrupole mass spectrometry. In the MRM mode, the quadrupole first filters the precursor ions of the target substance, and excludes ions corresponding to other molecular weight substances to initially eliminate interference. The precursor ions are fragmented by the collision chamber induced ionization to form many fragment ions. Then, through triple quadrupole filtering, the desired fragment ion is selected to eliminate non-target ion interference, so that the quantification is more accurate and the repeatability is better. After obtaining the metabolite mass spectrometry data of different samples, we integrated the peak area of the mass spectrum peaks of all substances, and performed correction on the peaks of the same metabolite in different samples [36].

2.5 Quality Control and Data Analysis

Quality control was performed to check the reliability and reproducibility of the data. Extracted samples were mixed and inserted into every sample and changes were monitored. Datasets with the intensity of the metabolites from the three samples were uploaded to the Analyst 1.6.1 software (AB SCIEX, Ontario, ON, Canada) for descriptive statistical analyses.

3 Results and Discussion

3.1 Overview of the Metabolic Profiling in Banana Pseudo-Stem

Metabolites are organic compounds produced in many plant species as secondary metabolites, including amino acids, alkaloids, fats, and protein. In this study, we explored the metabolome of banana pseudo-stem samples (Fig. 1a) using the widely-targeted metabolomics approach which provides a comprehensive platform for the detection of metabolites in different plant parts [36,37]. We identified a diverse range of metabolites (373) grouped into 10 major known classes based on the structure of metabolites (Fig. 1b). The most abundant metabolites present in the pseudo-stem belong to flavonoids (95), lipids (66), phenolic acids (62), amino acids and its derivatives (44), and alkaloids (30). The other identified metabolites belong to nucleotide and its derivatives (23), organic acids (20), lignans and coumarins (14), tannins (14), and terpene (5). Although multiple studies have been carried out in the past to evaluate different metabolites and diversity in banana germplasm [19–28], this is the first comprehensive metabolic profiling study for evaluating metabolites in pseudo-stem of banana. Metabolite profiling has also been previously reported in *Dendrobium officinale* [35], tomato [38], barley [39,40], and wolfberry [41]. Based on ion abundance, lipids showed the highest concentration, followed by alkaloids and amino acids (Fig. 1c).

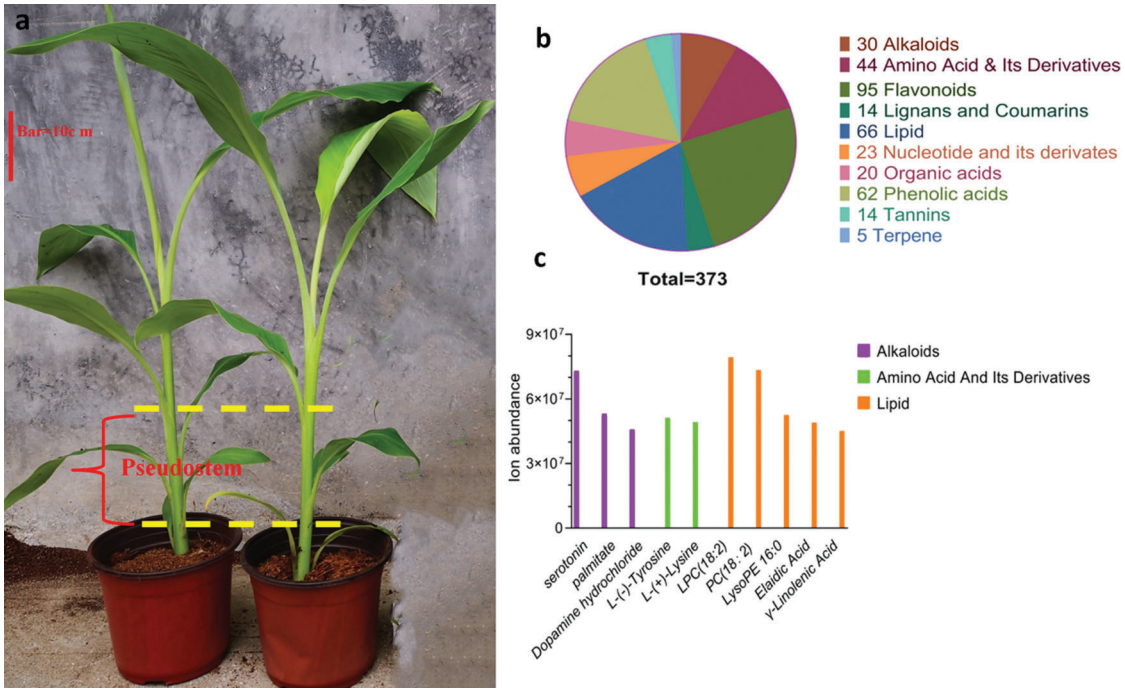

Figure 1: Overview of metabolite profiling of banana pseudo-stem. (a) Picture of the banana plant used for metabolomic analysis. (b) Metabolic profile of all major identified classes of metabolites in banana pseudo-stem. (c) Top 10 most abundant metabolites belonging to three different known classes

3.2 Alkaloids

Alkaloids as secondary metabolites are considered as an important class of naturally occurring organic compounds [42] which are not only an essential part of the human diet but also known for their properties as anti-parasitic [43], anti-plasmodial [44], anti-corrosive [44], anti-oxidative [45], anti-bacterial [46,47], and insecticidal characteristics [48]. In this study, we identified 30 alkaloids (Appendix Tab. A1) from the pseudo-stem of banana. Top 10 most abundant alkaloids found in banana pseudo-stem are (in descending order) Serotonin, 3-{(2-aminoethoxy)(hydroxy) phosphoryl]oxy}-2-hydroxypropyl palmitate, Dopamine hydrochloride, Choline, 3-hydroxypropyl palmitate glc-glucosamine, bis (N,N-diethylethanaminium)-2-acetamido-1,5-anhydro-2-deoxy-1-[-hydroxy(phosphonato)methyl]-D-glucitol, 2-hydroxy 5,8,11,14,17-icosapentaenoyloxy]propyl-2 (trimethylammonio) ethyl phosphate, N-benzylmethylene isomethylamine, Tryptamine, and 3-{[(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl-9,12-octadecenoate (Fig. 2a). Caffeine and Nicotine-hex were also identified, but their abundance was lower among other alkaloids. Previously published reports suggested the presence of alkaloids in banana sap, peel, and leaves as important anti-microbial agents [49–51]. Most of the identified alkaloids have not yet been reported. Characterization of these alkaloids may provide oversight into their biological activities.

3.3 Amino Acid and Its Derivatives

Protein extracts from plants are the important raw material in food, pharmaceutical and cosmetic industries [52,53]. Previous reports have suggested banana flower as an important source of amino acids and flavonoids [54,55]. Here, we identified 44 amino acids and their derivatives from the banana pseudo-stem. Ion abundance of amino acids and their derivatives showed higher frequency than other metabolites present in the banana pseudo-stem (Appendix Tab. A1). L-(-)-Tyrosine (5.12E + 07), L-(+)-Lysine (4.92E + 07), Valine (4.37E + 07), Tryptophan (3.27E + 07), trans-4-Hydroxy-L-proline (2.84E + 07), Proline

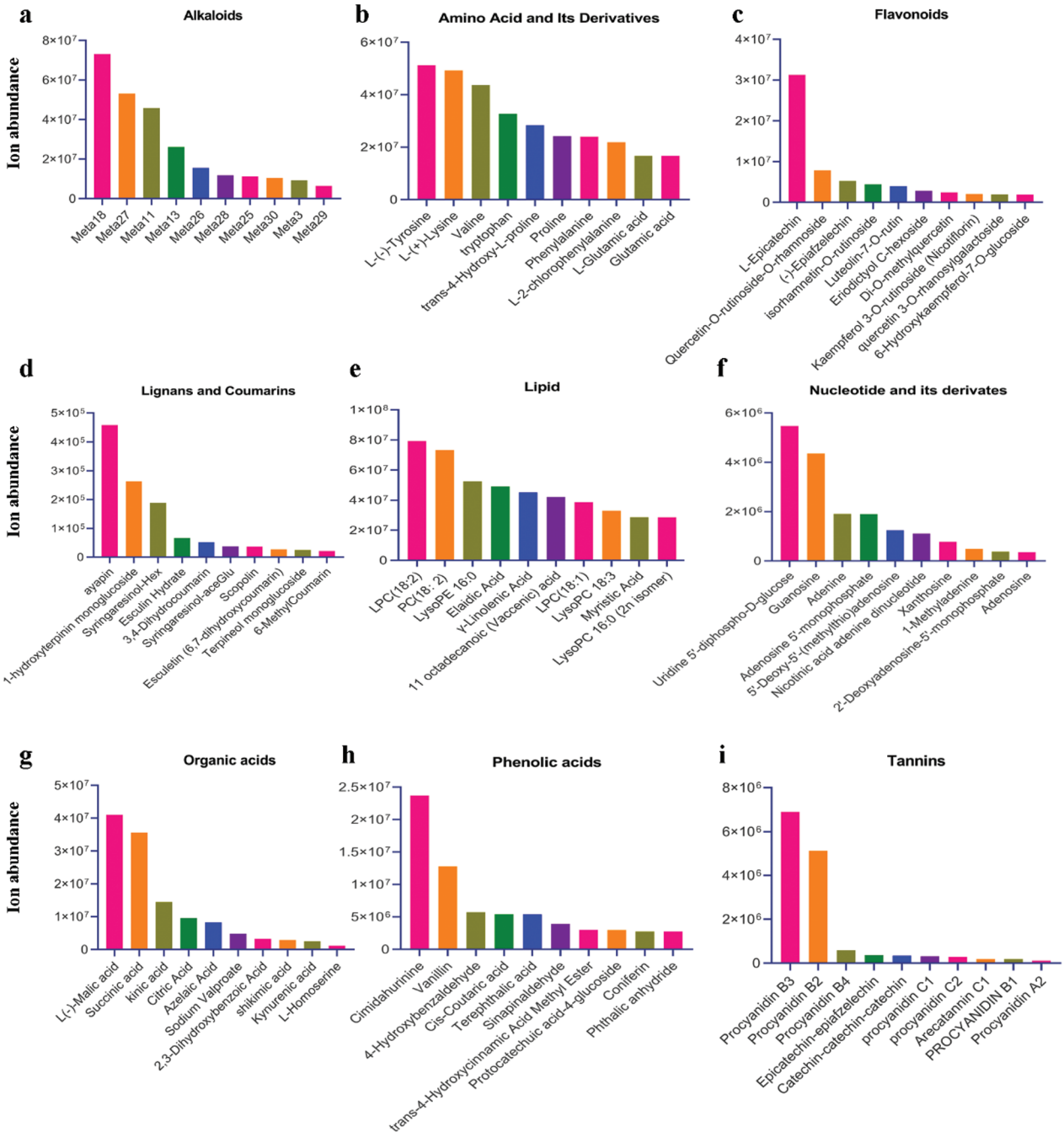

Figure 2: Top 10 metabolites from each structure-based category based on ion abundance. (a) Alkaloids (b) Amino acids and its derivatives (c) Flavonoids (d) Lignans and Coumarins (e) Lipids (f) Nucleotide and its derivatives (g) Organic acids (h) Phenolic acids (i) Tannins

*In a, Meta 18 is serotonin, Meta 27 is 3-{(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl palmitate, Meta 11 is Dopamine hydrochloride, Meta 13 is Choline, Meta 26 is 3-hydroxypropyl palmitate glc-glucosamine, Meta 28 is bis(N,N-diethylethanaminium)-2-acetamido-1,5-anhydro-2-deoxy-1-[-hydroxy(phosphonato) methyl]-D-glucitol, Meta 25 is 2-hydroxy-5,8,11,14,17-icosapentaenoyloxy]propyl-2-(trimethylammonio)ethyl phosphate, Meta 30 is N-benzylmethylene isomethylamine, Meta 3 is Tryptamine, and Meta 29 is 3-{[(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl-9,12-octadecenoate.

(2.42E + 07), Phenylalanine (2.40E + 07), L-2-chlorophenylalanine (2.19E + 07), L-Glutamic acid (1.67E + 07), and Glutamic acid (1.67E + 07) showed rich ion abundance in descending order (Fig. 2b). In contrast, N-Acetyl-L-tyrosine, Proline betaine, L-Homocitrulline, 2,6-Diaminooimelic acid, N-Phenylacetylglycine, Nα-Acetyl-L-arginine, Serine were less abundant. L-lysine and L-tryptophan have marked share (more than 50%) in the amino acid market [56]. Utilization of L-glutamic acid as a flavor enhancer and Phenylalanine as peptide sweetener is also well established [56,57]. Therefore, banana pseudo-stem has high potential for the amino acid market.

3.4 Flavonoids

Flavonoids are major secondary metabolites present in plants playing an important role in pigmentation, anti-microbial, and antioxidants activities [58]. Our results led to the identification of 95 metabolites belonging to flavonoids (Appendix Tab. A1) which were the most abundant (95) metabolites identified in the banana pseudo-stem. L-Epicatechin, Quercetin-O-rutinoside-O-rhamnoside, (-)-Epiafzelechin, isorhamnetin-O-rutinoside, Luteolin-7-O-rutin, Eriodictyol C-hexoside, Di-O-methylquercetin, Kaempferol 3-O-rutinoside (Nicotiflorin), Quercetin 3-O-rhanosylgalactoside, and 6-Hydroxykaempferol-7-O-glucoside were the most abundant phenolic compounds present in the banana pseudo-stem (Fig. 2c). Earlier reports have emphasized the presence and importance of phenolic compounds as antioxidants and antimicrobial agents in different plant species, i.e., *Linum capitatum* [59], *Cephalaria pastricensis* [60], *Zea mays* [61], and *S. anisochila* [62]. Anthocyanins are responsible for different fruit colors, i.e., red, orange, purple, and blue in plants [63]. Previous reports also suggest the presence of phenolic compounds in different parts of the banana plant (viz. leaves, flower, fruit) and the diversity of these compounds in different genotypes [23,24]. A step forward towards quantification and characterization of these naturally occurring flavonoids in banana pseudo-stem can provide a better insight into their utilization.

3.5 Lignans and Coumarins

Both lignans and coumarins are known for their antitumor and antibacterial activities in the pharmaceutical industry [46] and are extracted from many source plants including *Haplophyllum* species [64], *Melicope hayesii* [65], Chinese herbs [66], banana [67], and other plants [67]. Here, we identified and quantified 14 metabolites from this class including Pinoresinol-Hex, Pinoresinol-aceGlu Syringaresinol-Hex, Syringaresinol-aceGlu, 6-MethylCoumarin, Coumarin, Esculetin (6,7-dihydroxycoumarin), Bergapten, Scopolin, Esculin hydrate, 3,4-Dihydrocoumarin, 1-hydroxyterpinin monoglucoside, Terpineol monoglucoside, and Ayapin (Fig. 2d). Various lignans have been reported for their role in antimicrobial activities against gram positive bacteria and some viruses [67]. Bergapten is used as an effective treatment of psoriasis [68], but the other identified lignans in this study haven't been characterized yet. Coumarin compounds extracted from different plants (tonka beans, clover, woodruff, cassia, and lavender) have well-known role in the treatment of cancer, brucellosis, and burns [69].

3.6 Lipid

Fatty acids are well known to present in banana fruit pulp and peel [70]. In total, 66 metabolites were identified in this category. Most abundant lipids found in banana pseudo-stem are presented in Fig. 2e, including LPC(18:2), PC(18:2), LysoPE 16:0, Elaidic acid, γ-Linolenic acid, 11 octadecanoic (Vaccenic) acid, LPC(18:1), LysoPC 18:3, Myristic acid, and LysoPC 16:0 (2n isomer). Palmitoleic acid, Punicic acid, α-Linolenic ccid, and Lauric acid, considered as important lipids found in different plants [71], were also present in banana pseudo-stem.

3.7 Nucleotide and Its Derivates

A total of 23 nucleotides and its derivatives were identified in the banana pseudo-stem. Uridine 5'-diphospho-D-glucose, Guanosine, Adenine, Adenosine 5'-monophosphate, 5'-Deoxy-5'-(methylthio)

adenosine, Nicotinic acid adenine dinucleotide, Xanthosine, 1-Methyladenine, 2'-Deoxyadenosine-5'-monophosphate, and Adenosine were the most abundant metabolites in this class (Fig. 2f). Adenine is referred to as the energy currency of the cell and is an important metabolite playing a major role in the plant physiology and metabolism [72]. Guanosine acts as a mediator in the catabolism of guanine nucleotides which is involved in the biosynthesis of caffeine in some plants [73].

3.8 Organic Acids

Organic acids, mainly nonvolatile organic acids, are known for their active role in fruit flavor [74] and fruit ripening in banana [75]. The presence of citric acid, malic acid, oxalic acid and tartaric acid in fruit is well documented [75] but less is known about their prevalence in other plant parts. Organic acids play a crucial role in carbon metabolism as a mediator and act as a key component in nutrient stress tolerance [76]. Here, we identified 20 organic acid metabolites in the banana pseudo-stem (Appendix Tab. A1). L (-)-Malic acid, Succinic acid, Kinic acid, Citric acid, Azelaic acid, Sodium valproate, 2,3-Dihydroxybenzoic acid, Shikimic acid, Kynurenic acid, and L-Homoserine were major organic acids present in banana pseudo-stem (Fig. 2g).

3.9 Phenolic Acids

Phenolic acids are the most abundant polyphenols present in plants known for their broad-spectrum role in plant-microbe interaction and anti-microbial activities [77,78]. Cimidahurinine, Vanillin, 4-Hydroxybenzaldehyde, *Cis*-Coutaric acid, Terephthalic acid, Sinapinaldehyde, *trans*-4-Hydroxycinnamic acid methyl ester, Protocatechuic acid-4, glucoside, Coniferin, and Phthalic anhydride (Fig. 2g). Cimidahurinine is an important phenolic compound with its vital role in inhibiting melanin production and as an antioxidant [79]. The ethnopharmacological approach for extraction and utilization of phenolic compounds can help to increase the value addition of banana pseudo-stem.

3.10 Tannins and Terpene

Tannins can be found in many plants, i.e., pomegranate [80], sorghum [81], and tea [82]. These phenolic compounds are known for their beneficial effects on protein metabolism, rumen degradation of dietary protein and increasing absorption of amino acids in the small intestine [83]. Procyanidin B3, Procyanidin B2, Procyanidin B4, Epicatechin-epiafzelechin, Catechin-catechin-catechin, Procyanidin C1, Procyanidin C2, Arecatannin C1, Procyanidin B1, and Procyanidin A2 were identified as the top 10 most abundant tannins (Fig. 2h) among the 14 tannins (Appendix Tab. A1) found in banana pseudo-stem. Proanthocyanidins also are known as condensed tannins, i.e., Procyanidin A2, Procyanidin B1, Procyanidin B3, Procyanidin B2, and Procyanidin B4 are used as an anti-tumor-promoting effect. Although these phenolic compounds are extracted as a complex mixture from different plants, recent advances can promote their extraction and further utilization as an important bioproduct in the pharmaceutical industry.

Terpenoids, a class of secondary metabolites, are well-known for their use in pharmaceuticals, industrial compounds, insecticides, and the food industry [84,85]. In this study, we identified seven terpenoids including 24,30-dihydroxy-12(13)-enolupinol, 2-Hydroxyoleanolic acid, Oleanolic acid-3-O-beta-D, pyran xylose (1→3)-beta-D-pyran glucuronide, Asiatic acid, and Maslinic acid (Fig. 2i). Asiatic acid and its derivates are used as antidiabetic agents in glycogen phosphorylase inhibition pathways [86].

4 Conclusions

The banana pseudo-stem is an excellent source of secondary metabolites. In total, 373 metabolites were identified belonging to alkaloids, amino acid and its derivatives, nucleotide and its derivates, lignans and

coumarins, flavonoids, lipids, organic acids, phenolic acids, tannins and terpene. Most of the identified metabolites have not been previously reported in banana.

Metabolic profile of banana pseudo-stem suggests the presence and availability of large number of metabolites. Alkaloids, amino acids and its derivatives (L-lysine and L-tryptophan, L-glutamic acid, Phenylalanine), flavonoids, lipids (Palmitoleic acid, α-Linolenic acid, and Lauric acid), nucleotides (Adenine, Guanosine), and organic acids have wide roles as important nutritional components of the human diet. While phenolics acids (Cimidahurinine), lignans (Bergapten), coumarins, tannins (Procyanidin A2, Procyanidin B1, Procyanidin B3, Procyanidin B2, and Procyanidin B4), terpene (Asiatic acid) have been extensively used in the pharmaceutical industry. Presence of the above-mentioned metabolites with the integration of modern fields of omics, banana pseudo-stem can evolve as a valuable source in the food and medicine industry besides its use as biofiber, bio-composite and as a raw material in the polymer industry.

In this study, we profiled the metabolome of pseudo-stem in developing plants. Since, the exploitation of banana pseudo-stem as a by-product could be feasible mainly in developed plants (after harvesting banana fruit), it is probable that the metabolic profiles of the pseudo-stem in developing and developed plants are different. Therefore, we suggest a future study to evaluate the metabolic profile of banana pseudo-stem in developed plants. With the provided knowledge of banana pseudo-stem metabolites, a targeted approach for understanding the genetic background and diversity in germplasm can be useful to exploit and valorize the wasted banana pseudo-stem in human nutrition and other important fields.

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Conflicts of Interest: The authors declare that they have no conflicts of interest to report regarding the present study.

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Appendix

Table A1: Metabolite profile of banana pseudo-stem

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta18	serotonin	Alkaloids	71934000	78459000	68812000	73068333
Meta27	3-{(2-aminoethoxy)(hydroxy) phosphoryl]oxy}-2-hydroxypropyl palmitate	Alkaloids	47489000	48883000	62942000	53104667
Meta11	Dopamine hydrochloride	Alkaloids	47730000	43345000	46389000	45821333
Meta13	Choline	Alkaloids	24203000	25568000	28486000	26085667
Meta26	3-hydroxypropyl palmitate glc-glucosamine	Alkaloids	12808000	15296000	18770000	15624667
Meta28	bis(N,N-diethylethanaminium) -2-acetamido-1,5-anhydro-2-deoxy-1-[-hydroxy (phosphonato) methyl]-D-glucitol	Alkaloids	10779000	10826000	13812000	11805667
Meta25	2-hydroxy-5,8,11,14,17-icosapentaenoyloxy]propyl-2-(trimethylammonio)ethyl phosphate	Alkaloids	11172000	10024000	12424000	11206667
Meta30	N-benzylmethylene isomethylamine	Alkaloids	10324000	11377000	9650800	10450600
Meta3	Tryptamine	Alkaloids	9579400	8719400	9414000	9237600
Meta29	3-{[(2-aminoethoxy)(hydroxy) phosphoryl]oxy}-2-hydroxypropyl-9,12-octadecenoate	Alkaloids	5059100	6635600	7640200	6444966.7
Meta12	Hordenine	Alkaloids	7486600	5448500	3875900	5603666.7
Meta4	Spermine	Alkaloids	2786900	3347300	2143500	2759233.3
Meta7	N-Acetyl-5-hydroxytryptamine	Alkaloids	921930	979170	1210900	1037333.3
Meta6	Indole-3-carboxaldehyde	Alkaloids	645630	411780	743490	600300
Meta24	3-{(2-aminoethoxy)(hydroxy) phosphoryl]oxy}-2-12-octadecadienoate	Alkaloids	404190	424710	510140	446346.67
Meta16	10-Formyl-THF	Alkaloids	291150	297410	274580	287713.33
Meta14	“N’,N”“,N”“’-p-coumaroyl-cinnamoyl-caffeoyl spermidine”	Alkaloids	207800	229360	356780	264646.67
Meta15	Indole	Alkaloids	181480	202930	205850	196753.33
Meta20	N-Acetylputrescine	Alkaloids	193310	195850	198560	195906.67
Meta19	L-Carnitine	Alkaloids	157000	228350	150730	178693.33
Meta8	2-Aminoadipic acid	Alkaloids	93456	105540	198780	132592
Meta9	L-Hyoscyamine	Alkaloids	129880	65351	154040	116423.67
Meta23	9a-Hydroxysophoramine	Alkaloids	118700	96862	107780	107780.67

(Continued)

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta22	sessilifoliamide C	Alkaloids	70393	82472	144010	98958.333
Meta5	Indole-5-carboxylic acid (98%)	Alkaloids	113500	59428	107690	93539.333
Meta21	Shikonin	Alkaloids	84593	109490	85129	93070.667
Meta17	6-hydroxynicotinic acid	Alkaloids	94510	84466	92447	90474.333
Meta1	Fer-agmatine	Alkaloids	5782.8	1593.6	62700	23358.8
Meta10	Caffeine	Alkaloids	24194	16224	21637	20685
Meta2	Nicotine-Hex	Alkaloids	3997.8	3142.6	2450.8	3197.0667
Meta40	L-(-)-Tyrosine	Amino Acid and Its Derivatives	54030000	50757000	48677000	51154667
Meta57	L-(+)-Lysine	Amino Acid and Its Derivatives	45511000	50160000	52043000	49238000
Meta51	Valine	Amino Acid and Its Derivatives	43510000	47497000	40168000	43725000
Meta74	tryptophan	Amino Acid and Its Derivatives	29773000	33973000	34299000	32681667
Meta36	trans-4-Hydroxy-L-proline	Amino Acid and Its Derivatives	16153000	36692000	32349000	28398000
Meta73	Proline	Amino Acid and Its Derivatives	22880000	22865000	26732000	24159000
Meta52	Phenylalanine	Amino Acid and Its Derivatives	23424000	25946000	22740000	24036667
Meta48	L-2-chlorophenylalanine	Amino Acid and Its Derivatives	21495000	21813000	22415000	21907667
Meta56	L-Glutamic acid	Amino Acid and Its Derivatives	16532000	15609000	17960000	16700333

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta50	Glutamic acid	Amino Acid and Its Derivatives	16113000	14730000	19116000	16653000
Meta32	Pipecolic acid (Pip)	Amino Acid and Its Derivatives	18058000	10484000	17007000	15183000
Meta49	alpha-Aminocaproic acid	Amino Acid and Its Derivatives	12527000	14590000	12663000	13260000
Meta43	L-Isoleucine	Amino Acid and Its Derivatives	12767000	14108000	12743000	13206000
Meta38	L-Leucine	Amino Acid and Its Derivatives	11526000	14356000	11955000	12612333
Meta42	L-Valine	Amino Acid and Its Derivatives	10819000	11568000	9758000	10715000
Meta64	L-Methionine	Amino Acid and Its Derivatives	3691000	4237400	3016300	3648233.3
Meta37	L-AsparticAcid	Amino Acid and Its Derivatives	3346000	3743200	2463000	3184066.7
Meta69	2-Aminoisobutyric acid	Amino Acid and Its Derivatives	2531400	2628000	2970500	2709966.7
Meta67	Methionine sulfoxide	Amino Acid and Its Derivatives	2179600	2688500	1741900	2203333.3
Meta41	L-Histidine	Amino Acid and Its Derivatives	1366000	1618100	1767900	1584000

(Continued)

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta61	L-Glutamine	Amino Acid and Its Derivatives	1433700	1868300	1303100	1535033.3
Meta63	L-Tyramine	Amino Acid and Its Derivatives	1367600	1124000	1376700	1289433.3
Meta39	L-(-)-Threonine	Amino Acid and Its Derivatives	1159900	1101000	1198100	1153000
Meta34	L-Asparagine Anhydrous	Amino Acid and Its Derivatives	796820	1041500	805330	881216.67
Meta70	N,N-Dimethylglycine	Amino Acid and Its Derivatives	753880	565890	753860	691210
Meta58	N6-Acetyl-L-lysine	Amino Acid and Its Derivatives	372240	412490	286880	357203.33
Meta72	3,4-Dihydroxy-DL-phenylalanine	Amino Acid and Its Derivatives	140000	399210	300810	280006.67
Meta53	leucylphenylalanine	Amino Acid and Its Derivatives	228310	231640	157010	205653.33
Meta46	Asp-phe	Amino Acid and Its Derivatives	175260	152640	176420	168106.67
Meta55	L-Citrulline	Amino Acid and Its Derivatives	179020	133360	188590	166990
Meta66	S-(5'-Adenosy)-L-homocysteine	Amino Acid and Its Derivatives	148450	143940	176730	156373.33

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta44	L-(+)-Arginine	Amino Acid and Its Derivatives	108710	123320	124180	118736.67
Meta33	1,2-N-methylpipecolic acid (NmePip)	Amino Acid and Its Derivatives	102380	104780	101370	102843.33
Meta65	5-Hydroxy-L-tryptophan	Amino Acid and Its Derivatives	134620	86441	52896	91319
Meta71	H-HomoArg-OH	Amino Acid and Its Derivatives	78618	72733	75924	75758.333
Meta54	Acetyl tryptophan	Amino Acid and Its Derivatives	56259	69399	82460	69372.667
Meta60	1-Methylhistidine	Amino Acid and Its Derivatives	54771	57716	87565	66684
Meta45	N-Acetyl-L-tyrosine	Amino Acid and Its Derivatives	59769	71569	58968	63435.333
Meta31	Proline betaine (ProBet)	Amino Acid and Its Derivatives	42348	45995	49287	45876.667
Meta35	L-Homocitrulline	Amino Acid and Its Derivatives	38908	37735	53550	43397.667
Meta62	2,6-Diaminooimelic acid	Amino Acid and Its Derivatives	35010	32597	40355	35987.333
Meta68	N-Phenylacetylglycine	Amino Acid and Its Derivatives	15533	42799	21193	26508.333

(Continued)

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta59	Nα-Acetyl-L-arginine	Amino Acid and Its Derivatives	29001	18240	12073	19771.333
Meta47	Serine	Amino Acid and Its Derivatives	17663	22115	15763	18513.667
Meta135	L-Epicatechin	Flavonoids	31172000	23351000	39517000	31346667
Meta85	Quercetin-O-rutinoside-O-rhamnoside	Flavonoids	7124900	6940800	9624200	7896633.3
Meta113	(-)-Epiafzelechin	Flavonoids	5649900	3102100	7087500	5279833.3
Meta76	isorhamnetin-O-rutinoside	Flavonoids	3974000	3583900	5759500	4439133.3
Meta161	Luteolin-7-O-rutin	Flavonoids	4788900	2872000	4225900	3962266.7
Meta128	Eriodictyol C-hexoside	Flavonoids	2949500	2058200	3418300	2808666.7
Meta132	Di-O-methylquercetin	Flavonoids	2752600	2460000	2019700	2410766.7
Meta134	Kaempferol 3-O-rutinoside (Nicotiflorin)	Flavonoids	2602600	1335800	2090700	2009700
Meta79	quercetin 3-O-rhanosylgalactoside	Flavonoids	1987100	1664000	2138200	1929766.7
Meta166	6-Hydroxykaempferol-7-O-glucoside	Flavonoids	1831500	2414300	1378500	1874766.7
Meta78	Quercetin-3-O-glucoside-7-O-rhamnoside	Flavonoids	1910600	1646600	2053800	1870333.3
Meta123	Luteolin 8-C-hexosyl-O-hexoside	Flavonoids	1889100	1617700	1978600	1828466.7
Meta125	Tricin 7-O-hexoside	Flavonoids	2048400	1285900	2055100	1796466.7
Meta91	Catechin	Flavonoids	1558600	1135200	2072000	1588600
Meta149	Bioquercetin	Flavonoids	1551700	1294100	1553400	1466400
Meta159	Diosmetin-7-O-galactoside	Flavonoids	1475100	879220	1720900	1358406.7
Meta86	isorhamnetin-O-rutinoside-O-rhamnoside	Flavonoids	1113500	1158000	1600500	1290666.7
Meta98	Cyanidin 3–rutinoside (Keracyanin chloride)	Flavonoids	1659900	990860	722330	1124363.3
Meta115	phloretin 2'-O-glucoside	Flavonoids	792480	594520	863700	750233.33
Meta157	Anthocyanin 3-O-beta-D-glucoside	Flavonoids	913520	516680	648120	692773.33
Meta141	Luteolin 7-O-glucoside (Cynaroside)	Flavonoids	798700	405780	423590	542690
Meta111	gossypitrin	Flavonoids	518100	372410	528150	472886.67

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta142	Kaempferol 3,7-dirhamnoside (Kaempferitrin)	Flavonoids	364930	258020	668820	430590
Meta143	Quercetin 3-O-glucoside (Isotrifoliin)	Flavonoids	453110	333020	439450	408526.67
Meta160	Quercetin 3-O-beta-D-glucoside	Flavonoids	433640	276570	496460	402223.33
Meta94	Hyperin	Flavonoids	365790	237750	388180	330573.33
Meta139	Hesperetin 5-O-glucoside	Flavonoids	317190	261660	360310	313053.33
Meta124	Tricin 7-O-hexosyl-O-hexoside	Flavonoids	310350	246980	334490	297273.33
Meta163	lonicerin	Flavonoids	363340	199780	328470	297196.67
Meta77	Kaempferol-3-O-glucoside-7-O-rhamnoside	Flavonoids	365700	200260	320810	295590
Meta138	Isorhamnetin 3-O-neohesperidoside	Flavonoids	217490	251990	379800	283093.33
Meta83	isorhamnetin-O-rutinoside-O-glucoside	Flavonoids	229780	357680	212390	266616.67
Meta87	(-)-Epigallocatechin	Flavonoids	30877	18451	747540	265622.67
Meta109	Naringenin-7-O-glucoside	Flavonoids	276600	193420	290230	253416.67
Meta93	Rutin	Flavonoids	246120	212130	231910	230053.33
Meta102	Spiraeoside	Flavonoids	246760	192400	239000	226053.33
Meta97	Isoquercitrin	Flavonoids	219500	143640	266320	209820
Meta155	Phellodendroside	Flavonoids	117470	375710	28918	174032.67
Meta105	Fustin	Flavonoids	158290	131430	222040	170586.67
Meta146	Luteolin – 7 – 0 – glucoside	Flavonoids	147080	160090	121260	142810
Meta133	Methyl gallate	Flavonoids	222630	84027	80502	129053
Meta131	Tricin 5-O-hexoside	Flavonoids	134450	125370	107130	122316.67
Meta116	avicularin	Flavonoids	124620	71708	151710	116012.67
Meta121	Chrysoeriol O-malonylhexoside	Flavonoids	93791	130250	103900	109313.67
Meta81	Kaempferol-O-rutinoside-O-glucoside	Flavonoids	129900	126820	63141	106620.33
Meta127	Chrysoeriol 7-O-hexoside	Flavonoids	81668	59428	121210	87435.333
Meta112	Astilbin	Flavonoids	84818	64392	94689	81299.667
Meta119	Quercetin-3-O-α-L-arabinopyranoside (guaijaverin)	Flavonoids	77047	52450	112000	80499
Meta129	Luteolin C-hexoside	Flavonoids	79460	71919	85993	79124
Meta153	Apigenin-6-C-2 -glucuronylxyloside	Flavonoids	61061	41852	109400	70771

(Continued)

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta144	Afzelechin (3,5,7,4'-Tetrahydroxyflavan)	Flavonoids	48077	69107	86564	67916
Meta147	catechin-(7,8-bc)-4β-(3,4-dihydroxyphenyl)-dihydro-2-(3H)-pyranone	Flavonoids	49803	81204	62864	64623.667
Meta75	quercetin-O-rutinoside.t-hexose	Flavonoids	62105	68926	52112	61047.667
Meta165	sudachiin C	Flavonoids	52221	49076	79753	60350
Meta164	sudachiin B	Flavonoids	41533	42158	76681	53457.333
Meta168	6-Hydroxykaempferol-7,6-O-Diglucoside	Flavonoids	50382	48183	44485	47683.333
Meta99	Cyanidin chloride	Flavonoids	45439	45023	42718	44393.333
Meta130	Tricin O-saccharic acid	Flavonoids	30732	20026	79001	43253
Meta92	Tangeretin	Flavonoids	32858	34307	61864	43009.667
Meta162	Quercetin 3,7-bis-O-beta-D-glucoside	Flavonoids	43332	41284	38374	40996.667
Meta88	Nobiletin	Flavonoids	20589	28016	59340	35981.667
Meta108	4,2',4',6'-Tetrahydroxychalcone	Flavonoids	38359	23276	41365	34333.333
Meta126	Chrysoeriol 7-O-rutinoside	Flavonoids	38070	24338	30395	30934.333
Meta167	6-Hydroxykaempferol-3,6-O-Diglucoside	Flavonoids	40120	14512	21790	25474
Meta96	Kaempferol 7-O-glucosdie	Flavonoids	24241	11658	21763	19220.667
Meta117	Catechin gallate, CG	Flavonoids	16515	11111	19334	15653.333
Meta101	(-)-catechin gallate	Flavonoids	15584	14645	14784	15004.333
Meta100	gallate catechin gallate, GCG	Flavonoids	13786	14108	16829	14907.667
Meta103	Trifolin	Flavonoids	17562	9919.4	16661	14714.133
Meta122	8-C-hexosyl-hesperetin O-hexoside	Flavonoids	16973	12321	13126	14140
Meta148	Herbacetin	Flavonoids	14064	13065	14173	13767.333
Meta110	isoschaftoside	Flavonoids	11443	8584.5	16574	12200.5
Meta145	2,6-Dimethyl-7-octene-2,3,6-triol	Flavonoids	10021	9826.5	13213	11020.167
Meta114	eriocitrin	Flavonoids	9447.4	10677	5641	8588.4667
Meta136	Phloretin	Flavonoids	8364.1	5801.9	10610	8258.6667
Meta82	isorhamnetin-O-glucoside-O-glucoside	Flavonoids	8260.1	7799.2	8589.4	8216.2333
Meta152	Natsudaidain 3-O-(5-glucosyl-3-hydroxy-3-methylglutarate)-glucoside)	Flavonoids	7934.7	5816.4	9505.8	7752.3

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta84	syringetin-O-rutinoside-O-glucoside	Flavonoids	8450.9	7905	6611.1	7655.6667
Meta80	isorhamnetin-O-rutinoside-O-rutinoside	Flavonoids	6319.4	11225	4929.1	7491.1667
Meta95	Eriodictyol	Flavonoids	6325.6	2646.3	12313	7094.9667
Meta107	Narirutin	Flavonoids	5066.6	4230.3	4904.8	4733.9
Meta154	3',4',7-Trihydroxyflavone	Flavonoids	6031.8	4554.8	3070.1	4552.2333
Meta169	6-Hydroxykaempferol-3-O-rutin-6-O-glucoside	Flavonoids	9	3915.9	6701.2	3542.0333
Meta104	Kaempferin	Flavonoids	4467.1	3874	1856.3	3399.1333
Meta158	Luteolin-7-O-glucuronide	Flavonoids	9855.2	9	9	3291.0667
Meta137	Delphinidin 3-O-glucoside (Mirtillin)	Flavonoids	9	9	6855.9	2291.3
Meta150	Hispidulin	Flavonoids	2770.9	983.64	2357.6	2037.38
Meta120	Peonidin	Flavonoids	1845.3	1667.1	2571.2	2027.8667
Meta156	Pratensein	Flavonoids	1751.1	592.12	1927.4	1423.54
Meta90	Baicalin	Flavonoids	2317.3	9	9	778.43333
Meta140	Isovitexin 7-O-glucoside (Saponarin)	Flavonoids	9	9	1906.5	641.5
Meta89	Naringin	Flavonoids	9	9	9	9
Meta106	Cyanidin 3-O-galactoside	Flavonoids	9	9	9	9
Meta118	luteolin 7-O-glucuronide	Flavonoids	9	9	9	9
Meta151	Scutellarin	Flavonoids	9	9	9	9
Meta170	Pinoresinol-Hex	Lignans and Coumarins	12765	7129.6	40394	20096.2
Meta171	Pinoresinol-aceGlu	Lignans and Coumarins	4482.4	5113.6	9	3201.6667
Meta172	Syringaresinol-Hex	Lignans and Coumarins	179550	184960	201790	188766.67
Meta173	Syringaresinol-aceGlu	Lignans and Coumarins	21332	77221	12687	37080
Meta174	6-MethylCoumarin	Lignans and Coumarins	24399	21864	18290	21517.667
Meta175	Coumarin	Lignans and Coumarins	2861.6	1920.9	2521.9	2434.8

(Continued)

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta176	Esculetin (6,7-dihydroxycoumarin)	Lignans and Coumarins	27288	32019	20769	26692
Meta177	Bergapten	Lignans and Coumarins	18057	13156	18212	16475
Meta178	Scopolin	Lignans and Coumarins	34708	46430	26657	35931.667
Meta179	Esculin Hydrate	Lignans and Coumarins	48963	112530	38121	66538
Meta180	3,4-Dihydrocoumarin	Lignans and Coumarins	50663	45378	58454	51498.333
Meta181	1-hydroxyterpinin monoglucoside	Lignans and Coumarins	289200	237920	261470	262863.33
Meta182	Terpineol monoglucoside	Lignans and Coumarins	11653	8501.6	52822	24325.533
Meta183	ayapin	Lignans and Coumarins	576140	390660	408670	458490
Meta243	LPC (18:2)	Lipid	88597000	73255000	76469000	79440333
Meta239	PC (18: 2)	Lipid	76066000	70135000	73978000	73393000
Meta210	LysoPE 16:0	Lipid	46213000	48913000	62369000	52498333
Meta196	Elaidic Acid	Lipid	51435000	53218000	42392000	49015000
Meta192	γ-Linolenic Acid	Lipid	46829000	43853000	44623000	45101667
Meta199	11 octadecanoic (Vaccenic) acid	Lipid	44440000	41268000	40494000	42067333
Meta246	LPC (18:1)	Lipid	30256000	39022000	46615000	38631000
Meta203	LysoPC 18:3	Lipid	28902000	34497000	35653000	33017333
Meta188	Myristic Acid	Lipid	28801000	30357000	26973000	28710333
Meta228	LysoPC 16:0 (2n isomer)	Lipid	27426000	27905000	30528000	28619667
Meta241	Hexadecyl sphingosine	Lipid	19603000	20690000	18808000	19700333
Meta245	LPC (16:1)	Lipid	16637000	17031000	22453000	18707000
Meta204	LysoPC 16:0	Lipid	15765000	16850000	21474000	18029667
Meta240	isoPC (18:2)	Lipid	17480000	18192000	11073000	15581667
Meta215	4-Hydroxysphinganine	Lipid	13066000	11472000	11622000	12053333

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta234	Palmitoleic acid	Lipid	10445000	11225000	10308000	10659333
Meta249	LPC (18:0)	Lipid	8275900	8763500	11852000	9630466.7
Meta190	1-Stearoyl-sn-glycero-3-phosphocholine	Lipid	8074200	8687600	11119000	9293600
Meta205	LysoPE 18:1 (2n isomer)	Lipid	6097000	9113800	11285000	8831933.3
Meta191	LysoPE 18:1	Lipid	5038500	6640700	7915300	6531500
Meta217	LysoPC 15:0	Lipid	7590200	5300700	6547600	6479500
Meta244	2,3-dihydroxypropyl-9,12,15-octadecatrienoate-hexose-hexose	Lipid	4688500	6314300	8288100	6430300
Meta223	9,10-EODE	Lipid	4434200	4806200	8955900	6065433.3
Meta213	MAG (18:3) isomer3	Lipid	5036700	7706200	3701200	5481366.7
Meta209	LysoPE 18:2 (2n isomer)	Lipid	4492900	5148500	5641900	5094433.3
Meta221	MAG (18:3) isomer1	Lipid	5691700	5698600	3242900	4877733.3
Meta211	Punicic acid	Lipid	2997900	2934200	5043700	3658600
Meta230	LysoPE 16:0 (2n isomer)	Lipid	3198200	3230400	3266000	3231533.3
Meta238	9,10,13-trihyroxy-11-octadecadienoic acid	Lipid	3186500	2799400	2272700	2752866.7
Meta195	cis-10-Heptadecenoic acid	Lipid	2869300	2620500	2683800	2724533.3
Meta231	hexadecanoic acid 2,3-dihydroxypropyl ester	Lipid	2957300	2773300	2352100	2694233.3
Meta200	MAG (18:3) isomer5	Lipid	1920000	4150800	1142500	2404433.3
Meta212	MAG (18:2)	Lipid	2311300	3084400	1759000	2384900
Meta235	9S-hyroxy-10E,12E-octadecadienoic acid	Lipid	1928800	1781300	2699300	2136466.7
Meta186	13-Hydroxy-9,11-octadecadienoic acid	Lipid	1958700	1811400	2616600	2128900
Meta187	9-Hydroxy-10,12-octadecadienoic acid	Lipid	1888600	1622500	2583900	2031666.7
Meta229	LysoPC 18:0	Lipid	1775300	1779100	1896800	1817066.7
Meta197	Hendecanoic acid	Lipid	1530600	1652200	1516700	1566500
Meta185	9,10-Dihydroxy-12-octadecenoic acid	Lipid	1678000	876550	1802500	1452350
Meta224	9-HOTrE	Lipid	969050	1129500	1975000	1357850
Meta202	D-erythro-Dihydrosphingosine	Lipid	1362900	1145700	1171700	1226766.7
Meta184	13-Oxo-9-hydroxy-10-octadecenoic acid	Lipid	1145900	997450	1468100	1203816.7
Meta220	LysoPC 17:0	Lipid	1043400	1024000	1200800	1089400
Meta207	LysoPE 14:0	Lipid	786730	702020	1213600	900783.33

(Continued)

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta198	Stearic Acid	Lipid	1065100	666290	697280	809556.67
Meta201	MAG (18:1) isomer2	Lipid	498800	1090100	279770	622890
Meta233	Eicosadienoic acid	Lipid	576390	725190	484740	595440
Meta219	MAG (18:1) isomer1	Lipid	396630	921490	208570	508896.67
Meta227	LysoPC 14:0 (2n isomer)	Lipid	482470	469720	570420	507536.67
Meta237	9,12,13-trihyroxy-10,15-octadecadienoic acid	Lipid	386600	398510	401190	395433.33
Meta208	LysoPC 18:3 (2n isomer)	Lipid	236480	366140	450480	351033.33
Meta242	2,3-dihydroxypropyl-9,12-octadecadienoate-hexose-hexose	Lipid	295370	555080	147140	332530
Meta247	glyceryl linoleate	Lipid	273460	405140	245370	307990
Meta226	12,13-EODE	Lipid	304100	249280	361180	304853.33
Meta206	LysoPC 16:2 (2n isomer)	Lipid	170220	210550	240920	207230
Meta225	13-HOTrE(r)	Lipid	208130	149930	257640	205233.33
Meta216	LysoPC 15:1	Lipid	163410	170010	228750	187390
Meta218	MAG (18:3) isomer2	Lipid	73110	152590	80933	102211
Meta214	MAG (18:3) isomer4	Lipid	96233	130320	78859	101804
Meta193	α-Linolenic Acid	Lipid	47341	57666	53532	52846.333
Meta189	Choline alfoscerate	Lipid	44809	31936	56739	44494.667
Meta232	Eicosenoic acid	Lipid	70615	9	53475	41366.333
Meta222	Lauric acid	Lipid	30983	42939	33621	35847.667
Meta248	Glycerin Monopalmitate	Lipid	15086	34735	52131	33984
Meta236	9-hydroxy-12-oxo-10-octadecenoic acid	Lipid	33141	28424	36952	32839
Meta194	cis-4,7,10,13,16,19-Docosahexaenoic Acid (C22:6n3)	Lipid	3637.3	5593.6	3677.1	4302.6667
Meta259	Uridine 5'-diphospho-D-glucose	Nucleotide and its derivates	4780600	5342700	6278800	5467366.7
Meta266	Guanosine	Nucleotide and its derivates	4480200	4544300	4049200	4357900
Meta260	Adenine	Nucleotide and its derivates	1974400	1726800	2024200	1908466.7
Meta257	Adenosine 5'-monophosphate	Nucleotide and its derivates	2039900	1647700	2007900	1898500

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta267	5'-Deoxy-5'-(methylthio) adenosine	Nucleotide and its derivates	1240000	1206200	1261400	1235866.7
Meta256	Nicotinic acid adenine dinucleotide	Nucleotide and its derivates	1237500	1173600	916800	1109300
Meta252	Xanthosine	Nucleotide and its derivates	683360	1023100	628350	778270
Meta254	1-Methyladenine	Nucleotide and its derivates	582400	515660	368890	488983.33
Meta269	2'-Deoxyadenosine-5'-monophosphate	Nucleotide and its derivates	405450	372000	349760	375736.67
Meta262	Adenosine	Nucleotide and its derivates	418510	352150	307390	359350
Meta264	Guanine	Nucleotide and its derivates	276430	233520	263670	257873.33
Meta271	N6-Succinyl Adenosine	Nucleotide and its derivates	177410	262080	208670	216053.33
Meta261	2-Hydroxy-6-aminopurine	Nucleotide and its derivates	168760	305540	95043	189781
Meta250	Cytosine	Nucleotide and its derivates	169240	156070	200860	175390
Meta268	Uridine 5'-diphosphate	Nucleotide and its derivates	153740	141700	213760	169733.33
Meta265	Allopurinol	Nucleotide and its derivates	174720	130290	167660	157556.67
Meta272	7-methylguanine	Nucleotide and its derivates	177520	129350	85450	130773.33
Meta270	Uridine 5'-monophosphate	Nucleotide and its derivates	75648	93188	136400	101745.33

(Continued)

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta258	Guanosine 5'-monophosphate	Nucleotide and its derivates	46663	72466	31300	50143
Meta251	5-Methylcytosine	Nucleotide and its derivates	37633	63198	47164	49331.667
Meta263	Uracil	Nucleotide and its derivates	17996	19101	21703	19600
Meta255	Lumazine	Nucleotide and its derivates	10387	7296.1	8965.7	8882.9333
Meta253	β-Nicotinamide mononucleotide	Nucleotide and its derivates	5459.2	3012.8	2704.6	3725.5333
Meta277	L(-)-Malic acid	Organic acids	36301000	41831000	44842000	40991333
Meta274	Succinic acid	Organic acids	26413000	52845000	27641000	35633000
Meta278	kinic acid	Organic acids	12787000	16460000	14164000	14470333
Meta279	Citric Acid	Organic acids	6369000	9044600	13320000	9577866.7
Meta275	Azelaic Acid	Organic acids	10430000	6899500	7335900	8221800
Meta285	Sodium Valproate	Organic acids	4779000	5246400	4404400	4809933.3
Meta283	2,3-Dihydroxybenzoic Acid	Organic acids	3528200	2582400	3738400	3283000
Meta273	shikimic acid	Organic acids	3119100	2685300	2868700	2891033.3
Meta289	Kynurenic acid	Organic acids	2486700	2351100	2546300	2461366.7
Meta284	L-Homoserine	Organic acids	1317300	981570	1193100	1163990
Meta292	γ-aminobutyric acid	Organic acids	791090	512850	637870	647270
Meta288	phosphoenolpyruvic acid	Organic acids	247530	329110	406130	327590
Meta281	Fumaric acid	Organic acids	262510	108200	253320	208010

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta291	2-Hydroxybutanoic acid	Organic acids	133780	67054	116330	105721.33
Meta286	D-Galacturonic acid (GalA)	Organic acids	121460	87931	90280	99890.333
Meta287	aldehydo-D-galacturonate	Organic acids	117880	98010	80932	98940.667
Meta276	SubericAcid	Organic acids	65145	56076	78083	66434.667
Meta282	Citraconic acid	Organic acids	50889	9	9	16969
Meta290	Sebacate	Organic acids	848.44	9	684.53	513.99
Meta280	D-Xylonic acid lithium salt	Organic acids	9	9	9	9
Meta382	Cimidahurinine	Phenolic acids	16483000	49595000	4882400	23653467
Meta341	Vanillin	Phenolic acids	12717000	11569000	14184000	12823333
Meta343	4-Hydroxybenzaldehyde	Phenolic acids	4932100	4246300	8031800	5736733.3
Meta386	Cis-Coutaric acid	Phenolic acids	8080800	3721600	4499200	5433866.7
Meta366	Terephthalic acid	Phenolic acids	4794000	5366200	6047700	5402633.3
Meta370	Sinapinaldehyde	Phenolic acids	3671800	3104100	4986400	3920766.7
Meta349	trans-4-Hydroxycinnamic Acid Methyl Ester	Phenolic acids	3351100	2957400	2758900	3022466.7
Meta373	Protocatechuic acid-4-glucoside	Phenolic acids	2484500	4392600	2081500	2986200
Meta346	Coniferin	Phenolic acids	2088200	2805200	3400500	2764633.3
Meta393	Phthalic anhydride	Phenolic acids	2728600	2760400	2757800	2748933.3
Meta362	1-O-beta-D-Glucopyranosyl sinapate	Phenolic acids	2152300	2842300	2148100	2380900
Meta361	2,5-dihydroxy benzoic acid O-hexside	Phenolic acids	2446900	2659800	1964600	2357100
Meta379	1-O-[(E)-caffeoyl]-β-D-glucopyranose	Phenolic acids	1661400	2358300	2783700	2267800

(Continued)

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta355	caffeic acid	Phenolic acids	1984000	1831000	2638500	2151166.7
Meta385	sorbic acid	Phenolic acids	1927300	1817300	2549100	2097900
Meta365	Syringic acid O-glucoside	Phenolic acids	2047300	1176400	2108800	1777500
Meta344	4-hydroxybenzoic acid	Phenolic acids	1818000	1211500	1843200	1624233.3
Meta335	Syringic acid	Phenolic acids	1554100	1264600	1089400	1302700
Meta338	chlorogenic acid	Phenolic acids	1828600	756890	1261800	1282430
Meta354	Cryptochlorogenic acid	Phenolic acids	1127700	716390	1309700	1051263.3
Meta367	p-Coumaric acid	Phenolic acids	889860	724670	1504300	1039610
Meta336	Vanillic acid	Phenolic acids	1149600	761600	1019400	976866.67
Meta353	trans-ferulic acid	Phenolic acids	998390	762620	1051300	937436.67
Meta333	Hydrocinnamic acid	Phenolic acids	868360	693930	1193300	918530
Meta334	Ferulic acid	Phenolic acids	959970	734490	1018800	904420
Meta357	Salidroside	Phenolic acids	638060	1292600	422470	784376.67
Meta352	Syringic aldehyde	Phenolic acids	676730	537160	669420	627770
Meta351	4-aminobenzoic acid	Phenolic acids	405060	475190	335460	405236.67
Meta391	Cryptochlorogenic acid	Phenolic acids	410410	170010	279500	286640
Meta342	3-(4-Hydroxyphenyl)-propionic acid	Phenolic acids	266680	238720	342280	282560
Meta389	Trans-3-O-p-coumaric quinic acid	Phenolic acids	426560	144510	229300	266790
Meta350	Methyl ferulate	Phenolic acids	224980	298880	145330	223063.33
Meta378	1-O-[(E)-p-cumaroyl]-β-D-glucopyranose	Phenolic acids	341920	244040	82823	222927.67

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta388	Trihydroxycinnamoylquinic acid	Phenolic acids	200470	279660	141930	207353.33
Meta374	Eugenol monoglucose	Phenolic acids	193670	201120	193080	195956.67
Meta360	3-O-Feruloyl quinic acid	Phenolic acids	206720	186620	146800	180046.67
Meta380	3-O-(E)-p-coumaroyl quinic acid	Phenolic acids	283490	96748	130110	170116
Meta377	Plantainoside A	Phenolic acids	19952	296620	21670	112747.33
Meta345	Sinapyl alcohol	Phenolic acids	99471	41803	171550	104274.67
Meta372	oxalic acid	Phenolic acids	107870	87922	58677	84823
Meta337	coniferyl alcohol	Phenolic acids	77354	21903	140530	79929
Meta358	Sinapic acid	Phenolic acids	83581	42831	98745	75052.333
Meta390	Cis-3-p-coumaric quinic acid	Phenolic acids	63684	31638	32549	42623.667
Meta340	3-Aminosalicylic acid	Phenolic acids	44078	32320	50472	42290
Meta356	Cinnamic acid	Phenolic acids	40553	38313	45084	41316.667
Meta387	3-Hydroxy-4-isopropylbenzylalcohol 3-glucoside	Phenolic acids	45868	67417	9	37764.667
Meta368	Neochlorogenic acid (5-O-Caffeoylquinic acid)	Phenolic acids	22283	38180	29134	29865.667
Meta369	Methyleugenol	Phenolic acids	34100	25439	27978	29172.333
Meta359	Hydroxy-methoxycinnamate	Phenolic acids	19795	45280	15022	26699
Meta348	echinacoside	Phenolic acids	20782	32798	22636	25405.333
Meta383	Beta-D-furanofructosyl-alpha-D-(6-mustard acyl) glucoside	Phenolic acids	6891.5	39479	13904	20091.5
Meta332	3,4-dicaffeoylquinic acid	Phenolic acids	9097.3	20624	29688	19803.1
Meta339	p–Hydroxyphenyl acetic acid	Phenolic acids	20926	20394	8502.1	16607.367

(Continued)

Table A1 (continued).

Compound ID	Compound name	Class	Pseudostem1	Pseudostem2	Pseudostem3	Average
Meta371	Isochlorogenicacid B	Phenolic acids	18428	18820	8551.2	15266.4
Meta392	dihydro-p-coumarat	Phenolic acids	10593	12054	16097	12914.667
Meta364	3-O-p-coumaroyl shikimic acid O-hexoside	Phenolic acids	9	30401	9	10139.667
Meta347	p-Coumaraldehyde	Phenolic acids	6763.7	11648	6467.7	8293.1333
Meta376	Isochlorogenic acid C	Phenolic acids	11235	10118	9	7120.6667
Meta375	Isochlorogenic acid A	Phenolic acids	8421.7	8653.5	9	5694.7333
Meta363	1-O-p-Coumaroyl quinic acid	Phenolic acids	6409.5	7544.9	9	4654.4667
Meta381	Esculetin	Phenolic acids	9	9	9	9
Meta384	Beta-D-furanofructosyl-alpha-D-(3-mustard acyl) glucoside	Phenolic acids	9	9	9	9
Meta399	Procyanidin B3	Tannins	5893100	4294600	10523000	6903566.7
Meta398	Procyanidin B2	Tannins	4602500	3239400	7536200	5126033.3
Meta403	Procyanidin B4	Tannins	539270	350600	848760	579543.33
Meta397	Epicatechin-epiafzelechin	Tannins	291610	222680	569300	361196.67
Meta396	Catechin-catechin-catechin	Tannins	242600	135380	661380	346453.33
Meta400	procyanidin C1	Tannins	243880	121550	560370	308600
Meta401	procyanidin C2	Tannins	227390	124380	507130	286300
Meta405	Arecatannin C1	Tannins	153280	79422	334600	189100.67
Meta395	PROCYANIDIN B1	Tannins	137360	123210	305980	188850
Meta394	Procyanidin A2	Tannins	153050	142100	49288	114812.67
Meta407	gambiriin A-1	Tannins	57278	34184	102790	64750.667
Meta404	Arecatannin B1	Tannins	45673	17697	69741	44370.333
Meta406	gambiriin B-3	Tannins	14029	4757.9	15597	11461.3
Meta402	Cinnamtannin B2	Tannins	9	9	8730.4	2916.1333
Meta410	24,30-dihydroxy-12(13)-enolupinol	Terpene	134270	175540	160420	156743.33
Meta411	2-Hydroxyoleanolic acid	Terpene	156730	161470	116780	144993.33
Meta409	Oleanolic acid-3-O-beta-D-pyran xylose (1→3) -beta-D-pyran glucuronide	Terpene	47416	127820	30834	68690
Meta412	Asiatic acid	Terpene	2377.6	1615.9	1201.2	1731.5667
Meta408	Maslinic acid	Terpene	9	9	9	9