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EDITED BY
Wricha Tyagi,
International Crops Research Institute for the Semi-Arid Tropics (ICRISAT), India

REVIEWED BY
Wei Cai,
Hunan University of Medicine, China
Rasmieh Hamid,
Education and Extension Organization (AREEO), Iran

*CORRESPONDENCE
Mahima Sharma
mahisharma2403@gmail.com

†These authors have contributed equally to this work

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Metabolomic profiling of finger millet: unlocking the secrets of a nutritious staple food

Vishal Gupta [1†], Mahima Sharma [1*†], Sushil Kumar Gupta [2], Shaily Javeria [1], Zakir Amin [3], Suhail Ashraf [4], Javed Masood Khan [5] and Rajesh N. Udavant [6]

[1]Division of Plant Pathology, Faculty of Agriculture, Sher-e-Kashmir University of Agricultural Sciences and Technology of Jammu, Chatha, India, [2]Directorate of Research, Sher-e-Kashmir University of Agricultural Sciences and Technology of Jammu, Chatha, India, [3]ICAR-Central Institute of Temperate Horticulture, Srinagar, India, [4]Tamil Nadu Agricultural University, Coimbatore, India, [5]Department of Food Science and Nutrition, Faculty of Food and Agricultural Sciences, King Saud University, Riyadh, Saudi Arabia, [6]Department of Entomology, University of Georgia, Tifton, GA, United States

Introduction: Finger millet (*Eleusine coracana*) is gaining increasing recognition as a functional food and a promising source of nutraceuticals for mitigating metabolic disorders, owing to its abundance of bioactive compounds. Despite its nutritional and therapeutic potential, comprehensive metabolomic profiling of its primary and secondary metabolites remains limited. This study aimed to perform an in-depth metabolomic analysis of finger millet landraces cultivated in the temperate region of Padder Valley, District Kishtwar, Union Territory of Jammu and Kashmir, and to assess the therapeutic relevance of these metabolites in preventing metabolic diseases.

Methods: Comprehensive phytochemical profiling was conducted using liquid chromatography coupled with high-resolution tandem mass spectrometry (LC-HRMS/MS) to identify and characterize primary and secondary metabolites in finger millet grains. Inductively coupled plasma mass spectrometry (ICP-MS) was employed to quantify macro- and microelemental contents.

Results: Metabolomic analysis identified a total of 50 primary metabolites, including derivatives of amino acids, fatty acids, and carbohydrates such as dehydroascorbic acid, niacin, xanthine, orotic acid, nicotinuric acid, gluconic acid, propionic acid, decanoic acid, and palmitic acid. Additionally, 135 secondary metabolites were characterized, encompassing heterocyclic compounds, phenolics, flavonoids, alkaloids, and terpenes such as 4-hydroxycyclohexylcarboxylic acid, 2-furoic acid, methyl cinnamate, mesitol, 4-hydroxybenzoic acid, heptalactone, viburtinal, and geranic acid. Elemental analysis revealed the presence of 10 macro- and microelements, with magnesium (Mg), calcium (Ca), potassium (K), and phosphorus (P) being the most abundant.

Discussion: The comprehensive metabolite profiling demonstrates that finger millet is a rich source of bioactive primary and secondary compounds with potential therapeutic benefits. The diversity of metabolites and essential minerals highlights its value as a functional food ingredient for the prevention and management of metabolic disorders. These findings provide a biochemical basis for the development of value-added nutraceutical products derived from finger millet landraces.

KEYWORDS

metabolomic profiling, bioactive compounds, ragi, nutraceutical, phenolics

Highlights

- 53 phenolic compounds have been identified for the first time in finger millet in Jammu and Kashmir.
- Coumarin, and eugenol is the major phenolic compound in finger millet.
- Phenolic compounds significantly contribute to the antioxidant capacity.

Introduction

Food insecurity and malnutrition are serious health problems in developing countries especially India and underdeveloped countries that impact millions of people. Currently, over 1.4 billion people are living in the country which has been increasing progressively, it is critical to address these issues to ensure nutritional equity and self-sufficiency (Baduni et al., 2024). Being the world's primary producer of millet, India has a lot of potential to combat malnutrition and food insecurity. Millets, belong to the Poaceae family of small-seeded edible grasses and are found in arid and marginal areas of both tropical and temperate climates (Yadav et al., 2024). India accounts for 41% of the world's production of millet, according to global data. (Vishal et al., 2024). Millets significantly improve nutritional and food security and increase genetic diversity of the global food basket (Mallick et al., 2024). Millets such as pearl millet (*Pennisetum glaucum*), foxtail millet (*Setaria italica*), porso millet (*Panicum miliaceum*), finger millet (*Eleusine coracana*), barnyard millet (*Echinochlo aesculenta*), kodo millet (*Paspalum scrobiculatum*), sorghum (*Sorghum bicolor*), and little millet (*Panicum sumatrense*) are rich in vital nutrients, gluten-free and low glycaemic index, to make them ideal for people with diabetes, degenerative, and coeliac diseases (Singh et al., 2024). As staple grains for centuries, millets played a significant role in Indian diets, especially in hilly and rural areas due to their low water requirement, drought tolerance, resistance to harsh weather conditions, climate resilience and also reduced input requirement (Vikash et al., 2024). However, with the advent of modern agricultural practices and the widespread cultivation of rice and wheat millet usage has declined sharply, contributing less than 10 per cent to the human diet (Ghosh et al., 2024).

Eleusine coracana, sometimes referred to as ragi, nachni, kodra or finger millet, is widely grown in China, India, and other parts of Africa. The highlands of Eastern Africa, especially Ethiopia and Uganda, are believed to be its birthplace (Tamilselvan et al., 2023). About 5,000 years ago, *E. coracana* was domesticated and then spread to Asia and other parts of Africa. It has the efficacy for addressing food security and malnutrition because of its high content of nutrition. Due to significant amounts of minerals, protein, carbohydrates, and dietary fiber, finger millet has a well-established nutritional value that draws a lot of interest in the present era (Deme et al., 2019). Additionally, micro and macronutrients, is a virtuous source of phytoconstituents, especially phenolic compounds, which help in lowering chronic diseases including cardiovascular diseases, diabetes, and cancer. Proanthocyanidins, hydroxybenzoic (p-hydroxybenzoic and, protocatechuic) acids, flavonoids (apigenin, quercetin, epicatechin, and catechin), and hydroxycinnamic (p-coumaric acid, ferulic acid) are predominant polyphenols present in finger millet (Kalsi et al., 2023). Finger millet has been identified as a prominent source of minerals and protein, although little is known about its phytochemical makeup. Understanding finger millet's phytochemicals and nutritional value may enhance its application as a source of functional food material and help comprehend the associated health benefits (Abioye et al., 2022). In humans, severe chronic diseases include heart disease, cancer, diabetes, and cognitive dysfunction have been linked to the oxidation of cellular molecules by reactive species (Sharma et al., 2023). Dietary antioxidants play a crucial role in protection against oxidative damage and maintaining a healthy metabolic balance. Recent research has increasingly concentrated on plant bioactive compounds due to their several health benefits (Pandey et al., 2023).

Metabolomics as a relatively new field, is capable of analyzing every low molecular weight molecule present in particular organism or tissue. Liquid Chromatography Mass Spectrometer (LC-MS) technology has been employed in several research to detect and assess expression levels of various metabolites. These studies span multiple dimensions, including plant development (Theodoridis et al., 2023), plant-microbe interactions (Spina et al., 2021), human diseases (Zhou and Zhong, 2022), and plant nutrition (Zhong et al., 2022).

Abbreviations: ACN, acetonitrile; FA, formic acid; KEGG, Kyoto Encyclopedia of Genes and Genomes; LC-HRMS, Liquid Chromatography-High Resolution Mass Spectrometry; m/z, mass-to-charge-ratio; MEGA, Molecular Evolutionary Genetics Analysis; mL, Milliliter; RT, retention time.

The phytochemical composition of *Eleusine coracana* remains inadequately explored in existing literature, highlighting the need for a comprehensive analysis of its beneficial compounds. In the current investigation, phytochemical analysis was conducting utilizing LC-MS/MS, while elemental analysis was performed through ICP-MS. The goal of this study was to examine the profiling of phytochemical compounds present in the local landraces of finger millet cultivated in the temperate region of District Kishtwar (Padder Valley) within the Union Territory of Jammu and Kashmir. The development of innovative food products and nutraceutical applications could benefit from an enhanced comprehensive of phytochemical components. This strategy may also contribute to the sustainable advancement of the Indian biome by harnessing the untapped potential of this underutilized crop and promoting biodiversity conservation. These findings of the present study offer a thorough and understandable explanation of the phytochemical and nutritional components of finger millet as well as the metabolic pathways connected to the metabolic compounds that were identified through differential analysis.

Materials and methods

Plant material

Seeds of finger millet were collected from local habitat found in Chasoti village (33°34′ N latitude, 75°53′58″ E longitude, at an altitude of 1638 m), of Padder Valley (District Kishtwar), Jammu and Kashmir, India (Figure 1). The collected specimens were transported to Division of Plant Pathology, Faculty of Agriculture, SKUAST Jammu, within 48 hours of collection. Further, the samples were thoroughly rinsed with distilled water to eliminate soil particles and extraneous materials. The seeds were subsequently separated manually for further processing and analysis.

Characterization of finger millet

Molecular characterization of the collected finger millet samples was performed to ensure precise validation. The seeds were germinated under controlled conditions in plant growth chamber on 30°C with 55% humidity and 12 h light, and the resulting seedling tissues were utilized for genomic DNA extraction to facilitate further molecular analyses (Ibrahim et al., 2023). Purified DNA is used as the template for PCR to amplify segments of *matK* and *rbcL* gene sequences. The primers *matK-F* (5′-CTTTGCATTTATTACGGCTC-3′), *matK-R* (5′-GATTGGTTACGGGAGAAAAAG-3′) and *rbcL-F* (5′-GAAGTAGTAGGATTGATTCT-3′), *rbcL-R* (5′-CATCATTATTGTATACTCTTTC-3′) were used to amplification (Molla et al., 2023). The PCR mix (20 µl), which included 10 µl of master mixture, 1 µl of 10 nm each primer, 1 µl of DNA, and 7 µl of milli Q, was supplemented with total DNA (50–500 ng). The following circumstances was performed when the reaction was carried out: 1 min of 94 °C, followed by 32 cycles for 10 sec at 98°C, 56°C and 55°Cfor 15 sec, 68°C for 30 sec, and final elongation of 3 min at 68°C. 1.5% agarose gel electrophoresis was used to isolate and visualise the amplified DNA products under UV light (Supplementary Figure S1). Biologia Research

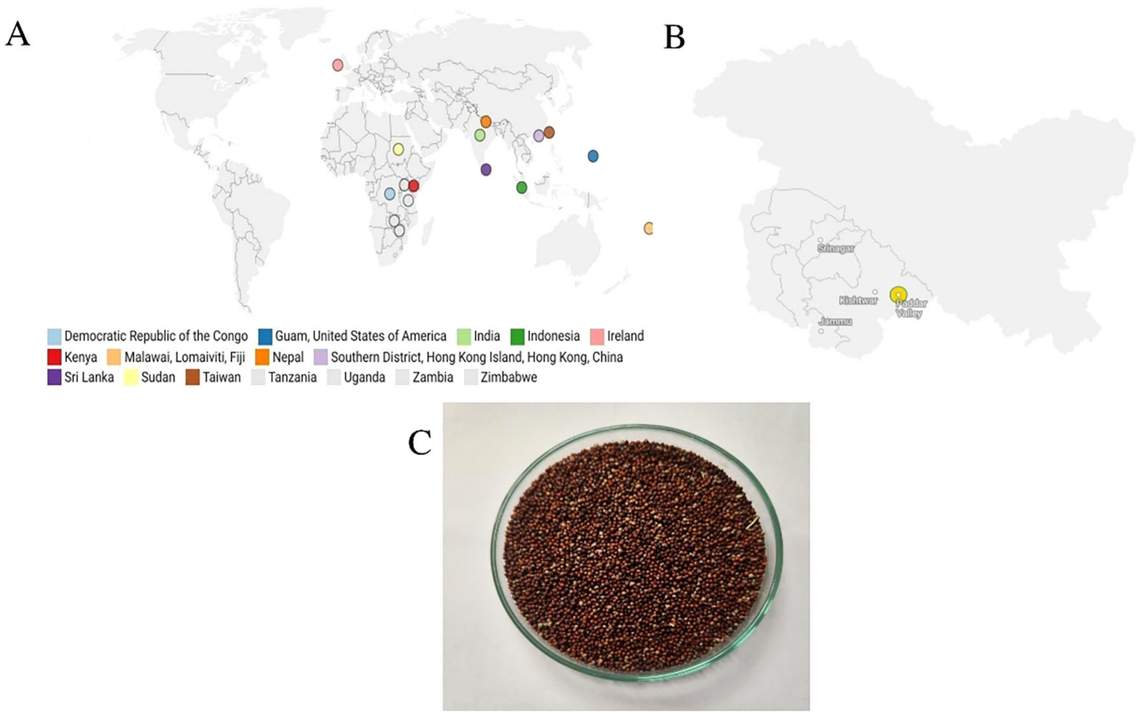

FIGURE 1
(A) Global distribution of finger millet **(B)** Local habitat for collection of finger millet in the UT of Jammu and Kashmir used in current study, **(C)** samples of finger millet seeds from Chasoti village of Padder Valley (District Kishtwar), Jammu and Kashmir, India.

India Pvt Ltd., Karnal, Haryana sequenced the purified partial amplicons. Before being compared to those in the GenBank database using the Basic Local Alignment Search Tool (https://blast.ncbi.nlm.nih.gov/Blast.cgi), the sequences were constructed, altered, and aligned in MEGA11 to determine the sequence homology with closely related taxa. In this research, the plant species exhibiting the highest sequence identity (100%) were selected as closest taxonomic match for molecular identification (Almutairi, 2021).

Preparation of extract

Finger millet dried seeds were coarsely grounded for extraction. 50 g of the powered seed sample from three independent seed batches (n = 3) was placed in a cellulose thimble and extracted using 400 mL of 95% methanol from Merck (Darmstadt, Germany) (65°C) in a Soxhlet apparatus. Exhaustive extraction was applied with solvent for 10–12 hours to ensure a complete extraction procedure (Figure 2). The extract was concentrated at 40°C under reduced pressure by using a rotary evaporator and was stored at 4°C until further use (Malathi et al., 2024).

Elemental composition by ICP-MS

0.5-1.0 gm of homogenized powder of sample was weighed using weighing paper and transferred into polytetrafluoroethylene-Teflon (PTFE-TFM) vessels, performed in triplicate. Add 15 mL dilute nitric acid 70% (v/v), was purchased from Merck (Darmstadt, Germany) into the same vessel. The pre-digestion reactions were allowed to proceed for 20 mins. Then, the vessels were tightly closed and inserted into the 20SVT50 rotor. The rotor was subjected to Multiwave 5000 radiation system at 140°C for 30 mins. After completion of the digestion, the vessels were taken out of the microwave and were allowed to cool down to room temperature (25 °C) for 20 mins. The digests produced were quantitatively transferred into 25 mL volumetric flasks and the flasks were then filled up to mark with ultrapure water. The aqueous solutions were then passed through polyvinylidene difluoride (PVDF) microfilters, prior to metal analysis by ICP-OES. Each sample was digested in triplicates with a blank as the fourth sample (Mafukata et al., 2024).

Liquid chromatography-high resolution mass spectrometry identification

LC-HRMS was used to identify secondary metabolites in the methanol extract of finger millet, using a previously described method with some modifications (Anggraeni et al., 2025). This study represents a preliminary profiling of finger millet. The analysis was performed in three independent replicates to ensure consistency. Biologia Research India Pvt Ltd., Karnal, Haryana performed the LC-HRMS/MS analysis. Extracted metabolite samples were analyzed for identifying and relatively quantifying using LC-HESI-MS/MS method on Vanquish Flex UHPLC coupled with Orbitrap Fusion™ Lumos™ Tribrid™ MS from Thermo Scientific. The polar metabolites were eluted by running the samples on Hypersil GOLD VANQUISH column (150mm x

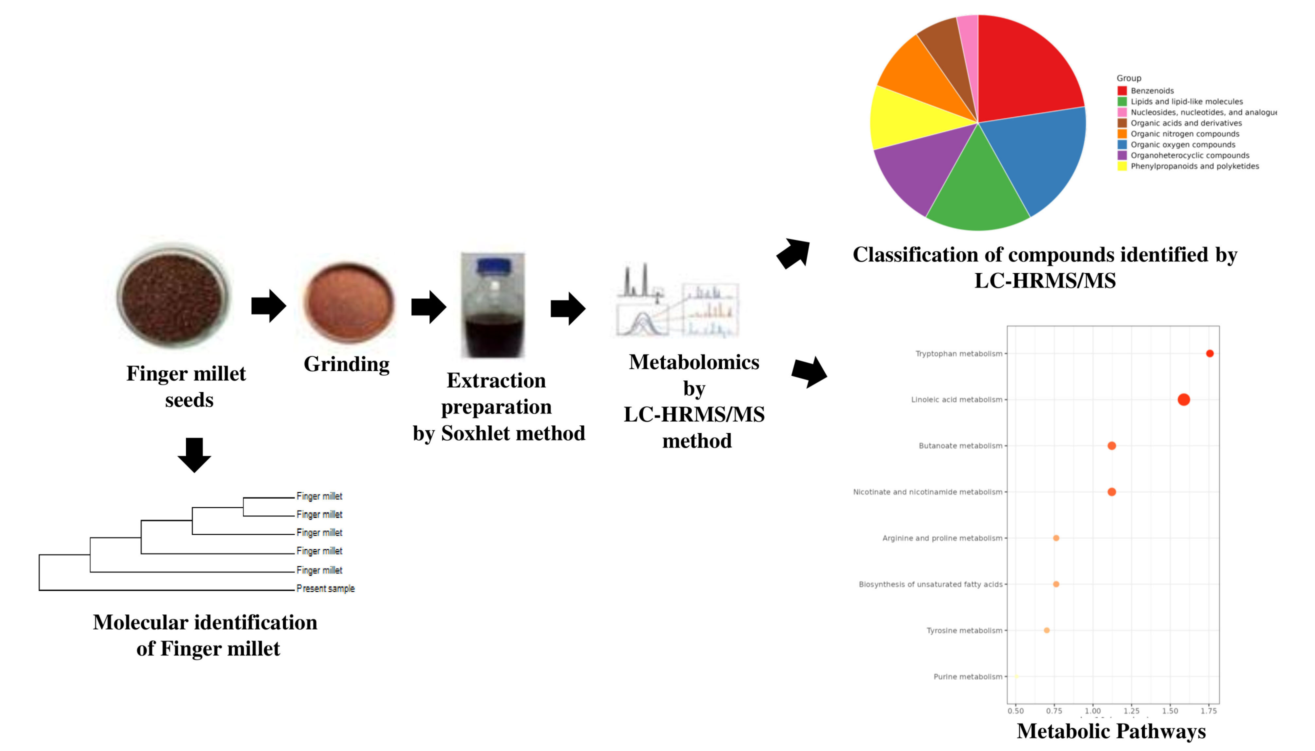

FIGURE 2
Workflow of LC−HRMS based untargeted metabolomic analysis of finger millet.

2.1mm; 1.9 µ) column at column temperature of 40 °C. For UHPLC run, 0.1% formic acid in water and 0.1% formic acid in acetonitrile were used as mobile phase A and mobile phase B, respectively. The gradient run includes %B from 1 to 25 in 3.5 minutes, 25 to 35 in 4 minutes, 35 to 95 in 2.8 minute, a stable 95% for 3.7 minutes and re-equilibration at 1% for 6 minutes. The H-ESI was used for ionization at static spray voltage of 3400 (v) for positive ions. The full scans and MS2 scans were acquired at 120000 at scan range 50–1500 m/z. The ddMS2 spectra were acquired using Orbitrap detector at 60000 resolutions with HCD fragmentation using stepped collision energy at 20, 40, 75%. The raw spectral data were processed using Compound discoverer 3.3.2.3.1 Software and mzCloud server and ChemSpider database search.

Kyoto encyclopedia of genes and genomes annotation and metabolic pathway analyses of differential identified compounds

Identified metabolites were annotated using the Kyoto Encyclopedia of Genes and Genomes (KEGG) compound database (http://www.kegg.jp/kegg/compound/) and annotated metabolites were mapped to the KEGG Pathway database (http://www.kegg.jp/kegg/pathway.html) using software MetaboAnalyst. Pathways with significantly regulated metabolites were then fed into metabolite set enrichment analysis, and their significance was determined by hypergeometric test p-values (Supplementary Tables S1, S2). The KEGG pathways with corrected *p*-values of less than 0.05 were considered significantly enriched by differentially expressed genes (Cao et al., 2022; Han et al., 2024).

Statistical analysis

Every experiment was conducted three times, and the means of the results are provided. To compute the mean and standard deviation, SPSS-22 statistical software (SPSS, Inc., Chicago, IL, USA) was used.

Results

Molecular identification

The *matK* and *rbcL* gene sequencing was utilized to identify finger millet sample, and a phylogenetic tree was made using MEGA 11 software. The Tamura 3-parameter model with lowest BIC and highest AIC values served as the basis for the maximum likelihood tree of the present millet sample, which was built using MEGA 11 and based on the study of *matK* and *rbcL* gene sequences. Every area with lacking information and gaps was eliminated. With gaps filled by pairwise deletion, the estimated transition/transversion bias (R) was 2.2. The bootstrap consensus tree was inferred from 1,000 to 3,000 iterations, and the maximum likelihood approach was used to reconstruct the evolutionary history. *Eleusine coracana*, the current millet sample, is well depicted in the dendrogram (Figure 3) that illustrates the

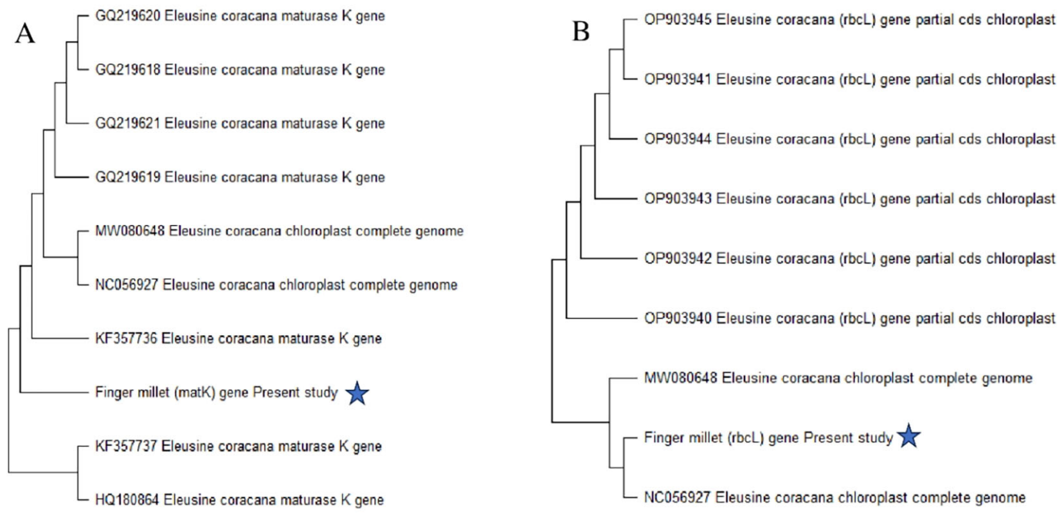

FIGURE 3
Maximum likelihood phylogenetic tree on basis of matK and rbcL sequence of *Eleusine coracana:* **(A)** depicts phylogenetic tree on basis of matK and **(B)** depicts according to rbcL sequence of *Eleusine coracana*.

TABLE 1 ICP-MS analysis of finger millet.

S. No.	Minerals	Sample concentration (mg/100gram)
1	Ca	326.17 ± 0.8
2	Mg	138.24 ± 0.2
3	Zn	2.62 ± 1.4
4	Mn	2.13 ± 0.4
5	Fe	3.73 ± 0.4
6	Cu	0.67 ± 0.8
7	Se	0.04 ± 0.6
8	P	249.47 ± 0.8
9	K	416.93 ± 0.2
10	Na	1.27 ± 0.2

evolutionary relationship. The sequences utilized in this investigation have been added to GenBank with accession numbers PQ753526 (*rbcL*) and PQ728252 (*matK*).

ICP-MS analysis

Elemental analysis was carried out for the finger millet. A total of 10 macroelements and microelements were present at different concentrations (Table 1). The major elements found were calcium (Ca), potassium (K), phosphorus(P), and magnesium (Mg). Among all the analyzed elements, potassium was found to have the highest concentration. It is an essential mineral for the efficient functioning of tissues, the body's cells, and organs. Increased potassium intake in diets can help maintain healthy blood pressure levels. The elements that are present in low concentrations are manganese

TABLE 2 Secondary metabolite phytochemical profiling of the *Eleusine coracana* seed extract analyzed by LC-HRMS/MS.

Name	RT [min]	m/z	Molecular weight	Molecular formula	Delta mass [PPM]	Activity
Sugar alcohols						
Volemitol	5.18	211.082	212.089	$C_7 H_{16} O_7$	1.5	Antioxidant
D-(-)-Mannitol	5.07	181.072	182.079	$C_6 H_{14} O_6$	1.88	Antioxidant
D-(+)-Arabitol	4.77	151.061	152.068	$C_5 H_{12} O_5$	2.43	Antibiotic
1-Deoxy-L-mannitol	3.30	165.077	166.084	$C_6 H_{14} O_5$	2.64	Antioxidant
6-Methyltetrahydro-2H-pyran-2,5-diol	8.41	287.148	132.079	$C_6 H_{12} O_3$	4.33	–
Quinoline						
Xanthurenic acid	1.28	206.045	205.038	$C_{10} H_7 N O_4$	2.77	Neuroactive
Hydroxy-1,4-benzoquinone	1.80	123.009	124.016	$C_6 H_4 O_3$	4.58	Cytotoxic
Hydroxynaphthoic acid	7.74	377.104	188.048	$C_{11} H_8 O_3$	3.84	Allelopathic
Benzoquinone	0.68	167.035	108.021	$C_6 H_4 O_2$	3.83	Antimicrobial
Phenolic aldehyde						
β-Resorcylaldehyde	0.54	137.024	138.032	$C_7 H_6 O_3$	2.98	Anti-inflammatory
Benzaldehyde	2.28	276.100	106.042	$C_7 H_6 O$	4.38	Antimicrobial
3-(4-Hydroxyphenyl)-2-oxiranecarbaldehyde	0.54	163.040	164.047	$C_9 H_8 O_3$	1	–
Phenolic compounds						
Vanilpyruvic acid	3.50	209.045	210.053	$C_{10} H_{10} O_5$	1.86	–
Vanillin	0.53	151.040	152.047	$C_8 H_8 O_3$	2.62	Antioxidant
Urolithin B	8.91	447.085	212.047	$C_{13} H_8 O_3$	1.95	Anti-inflammatory
Umbelliferone	0.74	161.024	162.032	$C_9 H_6 O_3$	2.33	Antioxidant
Scopoletin	0.78	191.035	192.042	$C_{10} H_8 O_4$	2.18	Antioxidant

(Continued)

TABLE 2 Continued

Name	RT [min]	m/z	Molecular weight	Molecular formula	Delta mass [PPM]	Activity
Phenolic compounds						
Schisandrin C	12.17	385.166	384.158	$C_{22}H_{24}O_6$	4.03	Antioxidant
Salicylic acid	0.74	137.024	138.032	$C_7H_6O_3$	2.99	Antimicrobial
Protocatechuic acid	0.72	153.019	154.027	$C_7H_6O_4$	2.93	Antioxidant
Phloroglucinol	4.08	125.024	126.032	$C_6H_6O_3$	4.42	Phloroglucinol
Phenylpropiolic acid	1.80	145.030	146.037	$C_9H_6O_2$	4.08	Anticancer
Phenylglyoxylic acid	0.49	149.024	150.032	$C_8H_6O_3$	2.93	–
Phenylethyl alcohol	0.66	181.087	122.073	$C_8H_{10}O$	3.65	Antimicrobial
Phenol	0.73	93.034	94.042	C_6H_6O	3.32	Antioxidant
p-Cresol	0.38	107.050	108.057	C_7H_8O	3.2	Antimicrobial
Naphthalene-2,3-diol	0.94	159.045	160.05	$C_{10}H_8O_2$	2.49	–
N-[2-Hydroxy-4(sulfooxy)phenyl]acetamide	6.15	145.028	247.015	$C_8H_9NO_6S$	0.85	–
Methyl cinnamate	1.79	161.061	162.068	$C_{10}H_{10}O_2$	4.15	Antimicrobial
Mesitol	0.66	135.081	136.089	$C_9H_{12}O$	3.17	Antioxidant
Meconic acid	0.35	198.988	199.996	$C_7H_4O_7$	2.22	–
Lithospermoside	6.99	330.119	329.111	$C_{14}H_{19}NO_8$	1.57	Antioxidant
Isovanillic acid	0.41	167.035	168.042	$C_8H_8O_4$	3.18	–
Hydroquinone	0.73	109.029	110.037	$C_6H_6O_2$	3.86	–
Homovanillic acid	0.81	181.051	182.058	$C_9H_{10}O_4$	2.24	–
Guaietolin	0.65	211.098	212.105	$C_{11}H_{16}O_4$	2.79	Antimicrobial
Guaiacol	0.94	123.045	124.052	$C_7H_8O_2$	3.55	Antimicrobial
Eugenol	1.75	163.077	164.084	$C_{10}H_{12}O_2$	3.82	Antimicrobial
Dihydrophloroglucinol	0.92	187.061	128.047	$C_6H_8O_3$	3.56	–
Coumarin	0.71	145.030	146.037	$C_9H_6O_2$	3.65	Antimicrobial
Benzoic acid	10.11	121.029	122.037	$C_7H_6O_2$	1.8	Antimicrobial
Benzeneacetamide-4-O-sulphate	7.65	273.054	231.020	$C_8H_9NO_5S$	1.46	–
Aceturic acid	1.18	98.025	117.043	$C_4H_7NO_3$	3.45	–
5-carboxyvanillic acid	0.35	211.025	212.032	$C_9H_8O_6$	2.22	Antioxidant
4-Hydroxyphthalic acid	0.41	181.014	182.022	$C_8H_6O_5$	3.38	–
4-Hydroxycyclohexylcarboxylic acid	1.12	189.077	144.079	$C_7H_{12}O_3$	4.39	–
4-Hydroxybenzoic acid	1.12	137.024	138.032	$C_7H_6O_3$	4.13	Antimicrobial
4-Hydroxy-3-nitrophenylacetic acid	0.54	196.025	197.032	$C_8H_7NO_5$	2.64	–
4-Ethylguaiacol	0.49	151.076	152.084	$C_9H_{12}O_2$	2.93	Antimicrobial
4,5-Dihydroxyphthalic acid	0.36	197.009	198.016	$C_8H_6O_6$	2.18	–
3-Hydroxybenzoic acid	3.37	137.024	138.031	$C_7H_6O_3$	1.24	Antimicrobial
3-(4-Hydroxy-3-methoxyphenyl)-2-methylpropanoic acid	0.48	209.082	210.089	$C_{11}H_{14}O_4$	2.72	–
3,4-Dihydroxyphthalic acid	0.43	197.009	198.016	$C_8H_6O_6$	2.44	–

(Continued)

TABLE 2 Continued

Name	RT [min]	m/z	Molecular weight	Molecular formula	Delta mass [PPM]	Activity
Phenolic compounds						
3,4-Dihydroxyphenylglycol	7.21	171.064	170.057	$C_8 H_{10}O_4$	0.44	Antioxidant
2-Furoic acid	0.98	111.009	112.016	$C_5 H_4 O_3$	3.6	Antimicrobial
2,4-Dihydroxybenzoic acid	0.40	153.019	154.027	$C_7 H_6 O_4$	3.23	Antimicrobial
1,2-Benzoquinone	0.53	153.019	108.021	$C_6 H_4 O_2$	3.57	Cytotoxic
(E)-p-coumaric acid	2.63	163.040	164.047	$C_9 H_8 O_3$	2.25	Antioxidant
(E)-Isoferulic acid	3.46	193.051	194.058	$C_{10} H_{10} O_4$	2.26	Anti-inflammatory
(E)-Ferulic acid	0.70	193.051	194.058	$C_{10} H_{10} O_4$	2.34	Antimicrobial
(2Z)-3-(3-Hydroxyphenyl)-2-methylacrylaldehyde	1.12	161.061	162.068	$C_{10} H_{10} O_2$	3.89	–
(2E)-3-(3,4-Dimethoxyphenyl)acrylic acid	0.77	207.066	208.074	$C_{11} H_{12} O_4$	2.38	–
Alkaloids						
Roquefortine L	12.01	202.590	403.166	$C_{22} H_{21} N_5 O_3$	4.98	Antimicrobial
Putaminoxin	0.59	211.134	212.141	$C_{12} H_{20} O_3$	2.75	Antimicrobial
Naphthalen-2-amine	4.81	142.066	143.073	$C_{10} H_9 N$	2.22	–
D-(-)-Quinic acid	5.60	191.056	192.068	$C_7 H_{12} O_6$	2.08	Antioxidant
Chaksine	13.61	473.286	450.297	$C_{22} H_{38} N_6 O_4$	3.92	–
6-hydroxypseudooxynicotine	8.87	452.227	194.105	$C_{10} H_{14} N_2 O_2$	0.47	–
4-O-α-D-Glucopyranosylmoranoline	6.45	326.144	325.137	$C_{12} H_{23} N O_9$	1.14	–
3-Methyloxindole	0.67	146.061	147.068	$C_9 H_9 N O$	2.8	–
3-hydroxy-3-methyloxindole	0.96	162.056	163.063	$C_9 H_9 N O_2$	2.57	–
2-pyridone	0.72	140.035	95.037	$C_5 H_5 N O$	4.45	–
Terpenoids						
γ-Heptalactone	1.14	127.076	128.084	$C_7 H_{12} O_2$	3.98	–
Viburtinal	0.71	159.045	160.052	$C_{10} H_8 O_2$	3.26	Antimicrobial
Tulipalin A	0.53	195.066	98.037	$C_5 H_6 O_2$	2.96	Cytotoxic
Trans-geranic acid	0.47	167.108	168.115	$C_{10} H_{16} O_2$	3.02	Antimicrobial
Maraniol	0.95	203.071	204.079	$C_{12} H_{12} O_3$	2.67	–
Glycyrin	12.00	383.149	382.142	$C_{22} H_{22} O_6$	2.37	Anti-inflammatory
Geranyl formate	12.81	183.137	182.130	$C_{11} H_{18} O_2$	0.23	–
Geranyl acetate	0.47	195.139	196.146	$C_{12} H_{20} O_2$	2.1	Antimicrobial
Gallic acid	0.53	169.014	170.021	$C_7 H_6 O_5$	2.32	Antioxidant
DL-Mevalonic acid	0.43	129.056	148.073	$C_6 H_{12} O_4$	2.93	–
Abietatriene	13.80	271.241	270.234	$C_{20} H_{30}$	0.3	–
6-Methylhept-5-en-2-one	0.48	185.118	126.104	$C_8 H_{14} O$	3.93	–
4-Methyl-2-propyltetrahydro-2H-pyran-4-yl acetate	0.50	199.134	200.141	$C_{11} H_{20} O_3$	2.52	–

(Continued)

TABLE 2 Continued

Name	RT [min]	m/z	Molecular weight	Molecular formula	Delta mass [PPM]	Activity
Heterocyclic compounds						
Thiophene	0.46	82.996	84.003	$C_4 H_4 S$	3.04	Anti-inflammatory
Thiazole	0.40	83.991	84.998	$C_3 H_3 N S$	1.95	–
Quinolone	4.17	144.046	145.053	$C_9 H_7 N O$	3.87	Antibacterial
Pyrrole	2.97	66.035	67.042	$C_4 H_5 N$	2.09	–
Lumazine	1.12	163.026	164.034	$C_6 H_4 N_4 O_2$	3.94	Antimicrobial
Isoxazolin-5-one	10.10	84.009	85.016	$C_3 H_3 N O_2$	1.44	Antimicrobial
Isoplumbagin	0.71	187.040	188.047	$C_{11} H_8 O_3$	3.3	Anticancer
Indole	1.83	116.051	117.058	$C_8 H_7 N$	4.55	–
Furoic acid	1.85	202.038	169.004	$C_3 H_7 N O_5 S$	1.89	Antimicrobial
Furan	1.12	135.045	68.026	$C_4 H_4 O$	3.73	Anticancer
4,5-Dihydroxy-3-oxo-1-cyclohexene-1-carboxylic acid	0.66	171.030	172.037	$C_7 H_8 O_5$	2.63	–
2-(Methylthio)benzothiazole	2.58	404.039	181.002	$C_8 H_7 N S_2$	2.53	–
2-(3-Hydroxy-3,4,5,6-tetrahydro-1H-cyclopenta-furan-4-yl)-3-methoxy-3-oxopropanoic acid	9.65	243.087	242.079	$C_{11} H_{14} O_6$	3.62	–
Organic compounds						
1-Acetylcyclohexyl acetate	10.18	183.102	184.110	$C_{10} H_{16} O_3$	1.37	–
2,5-Dimethyl-4-ethoxy-3(2H)-furanone	1.15	215.093	156.079	$C_8 H_{12} O_3$	4.05	–
Propenal	0.84	55.019	56.026	$C_3 H_4 O$	2.88	–
Phenylacetaldehyde	1.66	119.050	120.057	$C_8 H_8 O$	3.32	–
Methyl Phenyl Disulfide	1.06	157.014	156.007	$C_7 H_8 S_2$	3.84	–
Isatin	10.22	146.061	147.032	$C_8 H_5 N O_2$	1.34	Antibacterial
Indole-3-carbidol	2.96	146.025	147.068	$C_9 H_9 N O$	2.63	–
Heptenal	0.59	171.103	112.089	$C_7 H_{12} O$	3.63	Antimicrobial
Glyoxylic acid	5.08	133.014	74.0	$C_2 H_2 O_3$	4.17	–
Furfuryl acetone	3.51	137.061	138.068	$C_8 H_{10} O_2$	2.06	Antimicrobial
Furfuranol	2.10	97.029	98.037	$C_5 H_6 O_2$	3.94	Antimicrobial
Formylpyruvate	5.50	115.004	116.011	$C_4 H_4 O_4$	2.67	–
Ethylpropyldisulfide	1.63	137.045	136.038	$C_5 H_{12} S_2$	1.8	Antifungal
Cumene	0.66	119.087	120.094	$C_9 H_{12}$	3.37	–
Butyronitrile	1.83	70.065	69.057	$C_4 H_7 N$	0.2	–
Acetophenone	0.46	119.050	120.057	$C_8 H_8 O$	3.06	–
4-Oxo-2-propylpentanoic acid	0.52	157.087	158.094	$C_8 H_{14} O_3$	2.16	–
4-Methylthio-4-methyl-2-pentanone	1.41	147.084	146.077	$C_7 H_{14} O S$	3.16	–
4-Hydroxy-5-methyl-3-furanone	4.86	113.024	114.032	$C_5 H_6 O_3$	3.14	–
4,7-Dihydroxycoumarin	0.50	179.033	178.026	$C_9 H_6 O_4$	1.81	Anti-inflammatory

(Continued)

TABLE 2 Continued

Name	RT [min]	m/z	Molecular weight	Molecular formula	Delta mass [PPM]	Activity
Organic compounds						
4,5,7-Trihydroxycoumarin	2.97	193.014	194.021	$C_9 H_6 O_5$	2.39	Antimicrobial
3,4-Dimethylthiophene	2.04	113.042	112.035	$C_6 H_8 S$	4.88	–
2-methylcitric acid	4.96	205.035	206.043	$C_7 H_{10} O_7$	2.27	–
Dhurrin	7.01	334.09	311.100	$C_{14} H_{17} N O_7$	0.31	–
Flavonoids						
Catechol	0.41	109.043	110.058	$C_6 H_6 O_2$	4.47	Antioxidant
Flaviolin	0.46	205.012	206.083	$C_{10} H_6 O_5$	2.17	Antioxidant
Pyrogallol	1.18	125.058	126.063	$C_6 H_6 O_3$	3.61	Antioxidant
Kumarone	0.76	161.073	162.023	$C_{11} H_{14} O$	2.13	Anti-inflammatory
Purpurogallin	0.47	219.048	220.093	$C_{11} H_8 O_5$	2.89	Antioxidant
Esters						
Tetrahydrofurfuryl acetate	0.67	143.071	144.079	$C_7 H_{12} O_3$	2.72	–
Methyl sorbate	1.14	125.061	126.068	$C_7 H_{10} O_2$	3.51	Antimicrobial
Ethyl levulinate	3.69	189.077	144.079	$C_7 H_{12} O_3$	3.51	Antioxidant
Ethyl benzoylacetate	0.60	191.071	192.079	$C_{11} H_{12} O_3$	2.77	–
Benzyl formate	3.99	135.045	136.053	$C_8 H_8 O_2$	4.2	–
Acevaltrate	11.25	241.107	480.200	$C_{24} H_{32} O_{10}$	1.42	–
Acid derivatives						
Suberic acid	1.00	174.089	173.082	$C_8 H_{14} O_4$	2.93	–
Crotonic acid	0.50	86.037	84.024	$C_4 H_6 O_2$	2.62	–
Hormones						
Indoleacetylaspartate	6.467	290.057	288.036	$C_{14} H_{14} N_2 O_5$	1.59	–

PPM is a widely accepted unit used in high-resolution mass spectrometry to express the mass deviation. This value reflects the instrumental mass accuracy, which is critical for high-confidence metabolite identification. A low Delta Mass (typically within ±5 PPM) is considered indicative of a high-confidence match.

(Mn), copper (Cu), iron (Fe), zinc (Zn), sodium (Na), and selenium (Se).

Phytochemical profile of *Eleusine coracana* by LC-HRMS/MS

A developed and broad untargeted metabolomics method was conducted to the comprehensive phytochemical profile investigation of *Eleusine coracana* seed metabolites utilizing LC-HRMS/MS. Peaks were examined manually for signal/noise (s/n) > 10 in resulting data matrix, which included around 4000 signals with an MS2 spectrum overall. Duplicate signals were then eliminated as previously mentioned. Ultimately, the product ion spectra (MS2) yielded 521 very reproducible metabolite signatures. 185 were allegedly detected with the commercial standards based on fragmentation pattern, retention time (RT), and mass-to-charge-ratio (m/z) values of each metabolite. Aside from a few primary metabolites, the results included 13 fatty acid derivatives, 19 amino acids and their derivatives, 6 nucleotide derivatives, 7 carbohydrate derivatives, and 5 vitamin-related substances. An overview of all annotated compounds is given in Tables 2, 3. Our study also putatively identified several secondary metabolites, including 53 phenolic compounds, 5 flavonoids, 13 terpenoids, 10 alkaloids, 13 heterocyclic compounds, 24 organic compounds, 6 ester compounds, 5 sugar alcohols, 4 quinoline compounds, and 2 acid derivatives. Significantly, in case of primary metabolites, four vitamin biosynthesis-related metabolites, including dehydroascorbic acid, niacin, vitamin C, D-pantothenic acid, 5′-O-β-D-glucosyl pyridoxine; various nucleotide derivatives including xanthine, orotic acid, nicotinuricacid, epiguanine, 7-carboxy-7-deazaguanine, allantoin; carbohydrate derivatives such as gluconic acid δ-lactone, methyl α-D-mannoside, xylitol, 2-deoxyhexopyranose; various fatty acid derivatives such as

TABLE 3 Primary metabolite phytochemical profiling of the *Eleusine coracana* seed extract analyzed by LC-HRMS/MS.

Name	RT [min]	m/z	Molecular weight	Molecular formula	Delta mass [PPM]
Carbohydrate derivatives					
δ-Gluconic acid δ-lactone	1.892	177.041	178.048	$C_6 H_{10} O_6$	3.46
Xylitol	4.297	151.061	152.069	$C_5 H_{12} O_5$	3.87
Methyl α-D-mannoside	3.563	193.072	194.079	$C_7 H_{14} O_6$	2.85
L-(-)-Malic acid	4.212	133.014	134.022	$C_4 H_6 O_5$	4.02
Hydroxyacetone phosphate	5.239	152.996	154.003	$C_3 H_7 O_5 P$	2.13
6-Deoxy-3-O-methyl-β-D-galactopyranose	4.163	177.077	178.084	$C_7 H_{14} O_5$	3.66
2-Deoxyhexopyranose	4.993	163.061	164.068	$C_6 H_{12} O_5$	2.45
Nucleotide derivatives					
Xanthine	3.782	151.026	152.033	$C_5 H_4 N_4 O_2$	2.79
Orotic acid	0.49	155.010	156.017	$C_5 H_4 N_2 O_4$	2.23
Nicotinuric acid	1.133	179.046	180.054	$C_8 H_8 N_2 O_3$	3.12
Epiguanine	4.002	164.058	165.065	$C_6 H_7 N_5 O$	3.4
7-Carboxy-7-deazaguanine	2.081	193.037	194.044	$C_7 H_6 N_4 O_3$	3.23
(S)-(+)-allantoin	3.831	157.037	158.044	$C_4 H_6 N_4 O_3$	2.15
Vitamins					
Vitamin C	5.13	175.025	176.032	$C_6 H_8 O_6$	2.42
Niacin	2.903	122.058	123.024	$C_6 H_5 N O_2$	3.08
Dehydroascorbic acid	1.762	173.067	174.017	$C_6 H_6 O_6$	3.6
D-pantothenic acid	12.238	439.230	219.111	$C_9 H_{17} N O_5$	2.22
5′-O-β-D-Glucosylpyridoxine	6.998	332.134	331.127	$C_{14} H_{21} N O_8$	2.22
Amino acid derivatives					
N-Acetyl-L-phenylalanine	0.713	206.082	207.090	$C_{11} H_{13} N O_3$	3.28
N-Acetyl-L-leucine	1.351	172.098	173.105	$C_8 H_{15} N O_3$	2.55
N-Acetyl-L-glutamic acid	7.051	379.135	189.064	$C_7 H_{11} N O_5$	4.63
N-Acetyl-D-quinovosamine	4.919	204.088	205.095	$C_8 H_{15} N O_5$	1.33
N-(3-Carboxypropanoyl)-5-hydroxynorvaline	7.223	467.188	233.090	$C_9 H_{15} N O_6$	1.19
Maleamic acid	0.509	114.020	115.063	$C_4 H_5 N O_3$	3.14
L-Pyroglutamic acid	3.458	188.056	129.042	$C_5 H_7 N O_3$	2.91
L-Proline	1.17	114.056	115.063	$C_5 H_9 N O_2$	4.26
L-Histidinol phosphate	8.502	222.064	221.057	$C_6 H_{12} N_3 O_4 P$	2.74
L-(−)-threo-3-Hydroxyaspartic acid	1.981	150.039	149.032	$C_4 H_7 N O_5$	0.64
L-(+)-Aspartic acid	1.134	132.030	133.038	$C_4 H_7 N O_4$	3.67
Isovalerylglycine	1.783	218.104	159.090	$C_7 H_{13} N O_3$	4.95
DL-Glutamine	4.999	145.062	146.032	$C_5 H_{10} N_2 O_3$	2.87
D-(+)-Tryptophan	4.818	203.082	204.090	$C_{11} H_{12} N_2 O_2$	1.83
Aminolevulinic acid	1.125	130.051	131.058	$C_5 H_9 N O_3$	4.04

(Continued)

TABLE 3 Continued

Name	RT [min]	m/z	Molecular weight	Molecular formula	Delta mass [PPM]
Amino acid derivatives					
γ-Thiomethyl glutamate	3	194.248	193.163	$C_6 H_{11} N O_4 S$	3.71
6-Acetamido-2-oxohexanoic acid	4.035	168.324	187.012	$C_8 H_{13} N O_4$	3.33
4-Methyleneglutamic acid	4.972	158.027	159.086	$C_6 H_9 N O_4$	2.12
3-Sulfamoylalanine	8.028	186.034	168.063	$C_3 H_8 N_2 O_4 S$	2.37
Fatty acid derivatives					
Triacetic acid	4.947	143.035	144.042	$C_6 H_8 O_4$	2.49
Sorbic acid	3.913	93.034	112.052	$C_6 H_8 O_2$	3.39
Propionic acid	0.792	73.029	74.036	$C_3 H_6 O_2$	2.41
Palmitic Acid	15.237	535.471	256.240	$C_{16} H_{32} O_2$	0.11
Decanoic acid	10.209	171.139	172.146	$C_{10} H_{20} O_2$	0.89
8-Hydroxy-5,6-octadienoic acid	0.624	215.093	156.079	$C_8 H_{12} O_3$	3.59
6-Oxohexanoic acid	0.883	189.077	130.063	$C_6 H_{10} O_3$	3.07
3E-octenoic acid	0.46	141.092	142.099	$C_8 H_{14} O_2$	2.46
3-Hydroxysebacic acid	0.811	217.108	218.115	$C_{10} H_{18} O_5$	2.27
2-Hydroxyundecanoate	13.933	425.288	201.149	$C_{11} H_{21} O_3$	3.5
1-Nonanoic acid	0.662	157.123	158.131	$C_9 H_{18} O_2$	2.35
1-Hexanal	0.531	99.081	100.089	$C_6 H_{12} O$	3.5
9-Oxononanoic acid	0.719	171.103	172.110	$C_9 H_{16} O_3$	3.18

PPM is a widely accepted unit used in high-resolution mass spectrometry to express the mass deviation. This value reflects the instrumental mass accuracy, which is critical for high-confidence metabolite identification. A low Delta Mass (typically within ±5 PPM) is considered indicative of a high-confidence match.

propionic acid, decanoic acid, palmitic acid, 6-oxohexanoic acid, triacetic acid, 6-oxohexanoic acid were detected in the seeds of *Eleusine coracana*.

The phenolic compounds in the seed were coumarin, guaiacol, eugenol, phloroglucinol, 4-hydroxycyclohexylcarboxylic acid, 2-furoic acid, 1,2-benzoquinone, 4-hydroxybenzoic acid, phenylpropiolic acid, methyl cinnamate, schisandrin C, mesitol, dihydrophloroglucinol. Similarly, terpenoids compounds detected in seeds of *Eleusine coracana* were γ-heptalactone, viburtinal, geranic acid, 6-methylhept-5-en-2-one, maraniol, gallic acid, glycyrinetc; alkaloids compounds including roquefortine L, 2-pyridone, chaksine, putaminoxin, 3-methyloxindole; phytohormone include indoleacetylaspartate; acid derivatives such as suberic acid and crotonic acid.

Classification of metabolites detected using LC-MS/MS

Untargeted metabolomics of *Eleusine coracana* collected from the temperate region of District Kishtwar (Padder Valley), revealed putative compounds belonging to 9 different superclasses of compounds such as hydrocarbon derivatives, nitrogen, lipid, and oxygen compounds, heterocyclic compounds, phenylpropanoids, benzenoids, organosulfur compounds, organic acids and its derivatives (Figure 4). Further, detected metabolites were classified into 25 different main classes such as coumarin, cinnamic acid, indole and keto acid derivatives, fatty acyls, pyridine derivatives, furans, lactones, heteroaromatic compounds, carboxylic acid derivatives among others.

KEGG annotation analysis of identified metabolites

KEGG analyses were carried out to classify the functions of differentially identified metabolites and clarify biological pathways and functions in finger millet seeds. KEGG analysis results demonstrated that the metabolic pathways were mapped to identified metabolites in finger millet seed. Based on the findings presented in Figure 5, 185 differential metabolites were identified as participating in the biosynthesis of amino acids, carbohydrate metabolism, citric acid pathway, metabolism of nitrogen, glutathione and porphyrin, biosynthesis of fatty acid, terpenoid biosynthesis, metabolism of propanoate. Notably, pathways involved in carbohydrate metabolism highlighting the grain's role as a rich source of complex carbohydrates. Additionally, enrichment in amino acid biosynthesis pathways

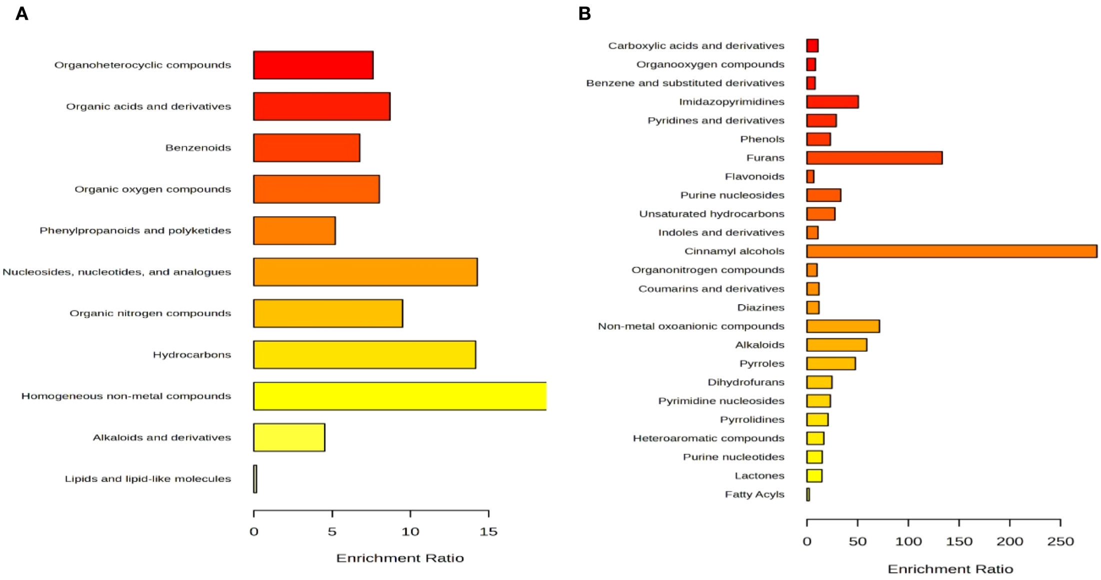

FIGURE 4
Detection and analysis of compounds according to LC–HRMS/MS. **(A)** indicate bar graph of the superclass of 185 differential identified metabolites; **(B)** indicate bar graph of the main class of 185 differential identified metabolites detected in the *Eleusine coracana* seed extract analyzed by LC-HRMS/MS.

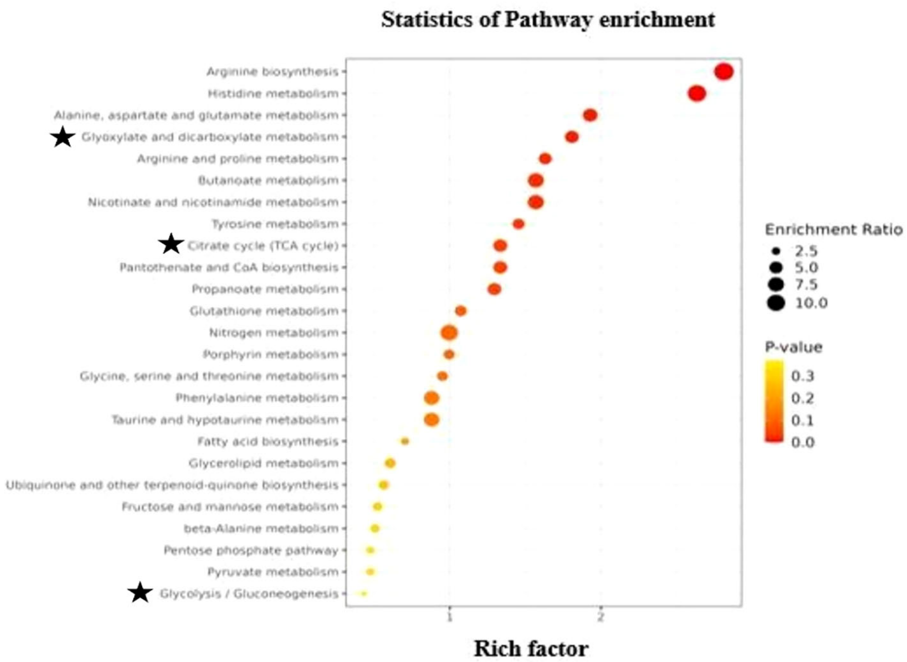

FIGURE 5
Scatter plot of top 25 KEGG pathways for differential identified metabolites in the seeds of *Eleusine coracana*. Abscissa, or rich factor, indicates the percentage of metabolites in a certain route that have been differentially identified. Circle color denoted ranges of corrected P value, while circle area showed number of metabolites that were differentially identified. The ratio of the number of metabolites in the associated pathway that were differentially identified to total number of metabolites that the pathway detected and annotated is known as the rich factor. The degree of enrichment increases with the value.

underscores its protein content, while phenylpropanoid biosynthesis points to the presence of antioxidant compounds contributing to finger millet's health-promoting properties. Phenylpropanoids help plants withstand pests and diseases, and research on Arabidopsis shows that the phenylpropanoid metabolic pathway is activated by salt and drought stress. Amino acid production is essential to an organism's growth and development. Plants under LT stress typically had higher levels of free amino acids than control plants, suggesting that amino acid production responds favorably to stress (Pandohee et al., 2023). Research has demonstrated that in transgenic alfalfa lines containing myoinositol phosphate synthase (MIPS), abiotic stressors including cold, drought, and salt stressors cause IP1 to be generated, while H_2O_2 and NO stressors cause high expression of MIPS. In plant tissues, glutathione metabolism is essential for preserving antioxidant qualities and controlling redox-sensitive signal transduction (Yang et al., 2024). Plant tolerance to range of biotic and abiotic environmental stressors is directly correlated with glutathione levels (Ye et al., 2024).

Discussion

The assessment of food and crop products as well as functional genomic research have made extensive use of metabolite profiling and chemometrics, which further guides breeding methods for enhancing and optimizing balance of food components (Li et al., 2021). Several metabolites can be identified and quantified in a single extract by applying the broad target metabolomics technique with LC-HRMS/MS (Dan et al., 2021). Metabolomics has been widely used to examine various compounds found in food products. Numerous significant metabolites with a range of physiological and bioactive roles have been identified by metabolomics investigation of several cereal crops, including millets (Wu et al., 2022). During the barnyard millet's developmental stages, a total of 35 metabolites were found (Meniya et al., 2023). Sugar and sugar alcohols were most abundant of these compounds, followed by amino acids, organic acids, and sterols, in that order. Putative metabolites from 15 different groups of chemicals, including flavonoids, amino acids, organic acid and its derivatives, were identified by untargeted metabolomics of two distinct foxnut kinds that were gathered from various geographical locations (Bao et al., 2022). Numerous physiological effects on the human body, including antioxidative, antimicrobial, neuro-protective, anti-diabetic, antipyretic, anti-inflammatory, anti-depressive, anti-septic, antibiotic, anti-angiogenic, immunomodulatory activities, and anti-carcinogenic, have been demonstrated by number of these compounds that were identified in the current study (Saxena et al., 2024). Plant products include coumarin, which has been shown to have anti-inflammatory, antibacterial, antioxidant, and neuroprotective properties (Vishal et al., 2024). Pervious study observed that catechin and epicatechin were found to be the main polyphenols in all the finger millet samples (Xiang et al., 2019). Quinic acid is an alkaloid molecule with anti-inflammatory, antibacterial, and antioxidant properties that is found in plant metabolites (Deme et al., 2019). The current study also identified abietatriene, a diterpene with range of biological characteristics, such as anti-inflammatory, antibacterial, antiparasitic, antifungal, antioxidant, and antiviral actions (Kuźma and Gomulski, 2022). Results from several studies using animal models and cell cultures indicate that abietatriene has significant advantages by halting cellular DNA damage over time (Sena et al., 2024). Because of its flavour, glycyrin, also referred to as sugar alcohol, is frequently employed as a sweetener in the food sector. Furthermore, studies have shown that glycerin is useful as a skin protectant and to treat glaucoma (Pan et al., 2024).The antioxidant and anti-inflammatory potential of several phenolic compounds found in nutritional bar's metabolome, including ferulic acid, guaiacol, eugenol, and guaietolin, have been thoroughly investigated (Pan et al., 2020).

Phenolic chemicals can withstand gastrointestinal digestion and stay intact as they pass through the colon because they are found in bound form in cereals, such as millet. These substances may have protective effects on the colon after being released by microbial fermentation (Sun et al., 2022). This phenomenon may help explain how whole grains can prevent colon cancer. Ferulic acid was found to significantly decrease production and expression of inflammatory markers include tumour necrosis factor-α (TNF-α), nitric oxide (NO), and interleukin-1β (IL-1β) while increasing levels of anti-inflammatory factor β-endorphin (β-EP) in a human HMC-3 microglial cell model (Vishal et al., 2024). Previous study showed that phenolic compounds such as syringic acid, hydroxyl caffeic acid, caffeic acid, coumaric acid ethyl ester, ellagic acid glucoside, 3-hydroxycoumarin, and feruloyl tartaric acid were identified in seed coat of finger millet (Soujanya et al., 2024). Antibacterial, anti-inflammatory, and antioxidant capabilities are mainly possessed by the hydroxybenzoic acid. Most fruits have a low hydroxybenzoic acid concentration, however, berries including blackberries, blackcurrants, strawberries, raspberries, and pomegranates can have very high levels of this compound (Carrillo et al., 2023; Kumar et al., 2024a). Coumarin, a naturally occurring phenolic compound identified in finger millet, exhibits multiple therapeutic activities. It acts as an anticoagulant by inhibiting vitamin K epoxide reductase, thereby reducing blood clot formation. Additionally, coumarin and its derivatives have been shown to possess anti-inflammatory and antioxidant properties by modulating inflammatory cytokines and scavenging reactive oxygen species (ROS), which are critical in the prevention of chronic diseases such as cardiovascular disorders and cancer (Sharma and Mallubhotla, 2022; Hussain et al., 2019; Kumar et al., 2024b). Eugenol, another key metabolite, is well known for its potent antimicrobial, analgesic, and anti-inflammatory effects. It exerts these effects primarily through the inhibition of COX-2 and NF-κB signaling pathways, which are involved in inflammation and pain signaling. Eugenol also disrupts microbial membranes, making it effective against a broad range of pathogens. Its antioxidant capacity further contributes to its role in protecting cells from oxidative damage, supporting its application in managing oxidative stress-related conditions (Ulanowska et al., 2021; Sharma et al., 2024).

Furthermore, flavonoids were identified as the primary phenolic compound class present in *Eleusine coracana* seeds by the LC-MS approach for phenolic compound quantification (Buelvas et al., 2021), the most abundant phenolic components in the crude extract of *Eugenia pollicina* leaves were flavonoids. Seeds of *Eugenia uniflora* primarily contain phenolics from the flavonoid class, including quercitrin and kaempferol pentoside (Fidelis et al., 2022). Both internal and external factors, including physical, chemical, and biological ones, affect the quantity of phenolic compounds. Moreover, the amount of total phenolic chemicals in plant tissues is similarly influenced by photosynthesis and carbon production (Araujo et al., 2021).

By analyzing the millet's primary and secondary metabolites, we have been able to examine their detailed profiles and try to better understand their roles (Girardelo et al., 2020). The current study employed UHPLC-ESI-QTOF-MS, a potent, dependable, and combinative analytical approach, to quickly characterize a number of phytochemicals in extracts from two Lamiaceae plants (Cocan et al., 2018). It is evident from comparing our results with those of relevant literature that the phenolic compounds (gallic acid, ferulic acid) of porso and foxtail millets was comparable to that of the study suggested by (Pujari and Hoskeri, 2022). Thus, *Eleusine coracana* proved to be a prominent source of phenolic, flavonoid, and terpene chemicals, and its exploitation can find intriguing uses in pharmaceutical, cosmetic, functional food, food supplement, and novel product creation (Dey et al., 2022).

Conclusion

This study provides a comprehensive nutritional and bioactive profiling of underutilized finger millet (*Eleusine coracana*) landraces from Padder Valley, District Kishtwar, Jammu and Kashmir, India. LC-HRMS/MS analysis identified key metabolites, including catechol, flaviolin, pyrogallol, ferulic acid, protocatechuic acid, coumarin, eugenol, cumene, and guaietolin, alongside significant fatty acids, alkaloids, terpenes, and hydrocarbons. These compounds exhibit diverse bioactivities, such as antioxidant, anti-diabetic, antibacterial, and anti-obesity effects, underscoring the potential of finger millet as a functional food ingredient and source of nutraceuticals. The findings highlight the crop's capacity to contribute to dietary diversification, address chronic illnesses, and combat malnutrition. While the results demonstrate substantial therapeutic potential, they are based on metabolomic and in silico analyses. Therefore, future studies should focus on *in vivo* validation, mechanistic investigations, and targeted quantification to confirm the physiological relevance of these bioactive compounds and explore their applications in nutrition, health, and functional food development.

Data availability statement

The datasets presented in this study can be found in online repositories. The names of the repository/repositories and accession number(s) can be found in the article/Supplementary Material.

Author contributions

VG: Conceptualization, Data curation, Formal Analysis, Investigation, Supervision, Visualization, Writing – original draft, Writing – review & editing. MS: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing. SK: Investigation, Supervision, Visualization, Writing – original draft, Writing – review & editing. SJ: Formal Analysis, Investigation, Writing – original draft, Writing – review & editing. ZA: Investigation, Visualization, Writing – original draft, Writing – review & editing. SA: Validation, Visualization, Writing – original draft, Writing – review & editing. JK: Data curation, Funding acquisition, Visualization, Writing – review & editing. RU: Formal analysis, Funding acquisition, Visualization, Writing – review & editing.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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Supplementary material

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fpls.2025.1570787/full#supplementary-material

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