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Phytochemical Profiling and Metabolic Pathway Analysis of Wild Edible Plants: *Alternanthera sessilis* and *Alternanthera tenella* from Rampachodavaram, Andhra Pradesh, India.

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Abstract:

The present study investigates the phytometabolite composition of *Alternanthera sessilis* and *Alternanthera tenella*, two wild edible plants recognized for their medicinal and nutritional value. LC–MS/MS analysis coupled with mzCloud spectral library matching identified 117 compounds, spanning major phytochemical classes including flavonoids, phenolics, triterpenoids, sterols, amino acids, and fatty acids. Pathway analysis linked these metabolites to amino acid, lipid, flavonoid, phenylpropanoid, and purine metabolism. The results highlight these species as valuable sources of bioactive metabolites with potential applications in nutraceutical and pharmaceutical formulations.

Key words: Phytochemicals, Metabolic pathway, wild edible plants

1. Introduction

Wild edible plants (WEPs) play an important role in traditional medicine and food systems, providing essential micronutrients and secondary metabolites with therapeutic properties. *Alternanthera sessilis* (sessile joyweed) and *A. tenella* (joyweed) are common leafy greens used in South and Southeast Asia. Traditional use reports their benefits in treating inflammation, liver disorders, and diabetes. However, detailed metabolomic profiling of these species remains underexplored.

This study aims to elucidate their phytochemical diversity and map identified metabolites to biological pathways using LC–MS and bioinformatic annotation.

2. Materials and Methods

2.1 Sample Preparation

Fresh aerial parts of *A. sessilis* and *A. tenella* were extracted using methanol (70% v/v). The extracts were filtered, concentrated, and analysed using LC–MS/MS.

2.2 Instrumentation and Data Processing

Metabolite profiling was conducted using Thermo Fisher Scientific's Compound Discoverer 3.2 software linked to the mzCloud database. Identifications were based on MS^2 spectral similarity (>95%) and compound library confidence scores.

2.3 Pathway Annotation

Identified compounds were cross-referenced with KEGG and PlantCyc databases to associate them with major metabolic pathways. Visualization was performed using Python's NetworkX and Matplotlib libraries.

3. Results

3.1 Compound Classification

The identified metabolites belong to several phytochemical classes (Fig. 1). Flavonoids and phenolic acids dominated the profile, reflecting potent antioxidant capacity. Amino acid derivatives and fatty acids indicated metabolic diversity consistent with biological origin.

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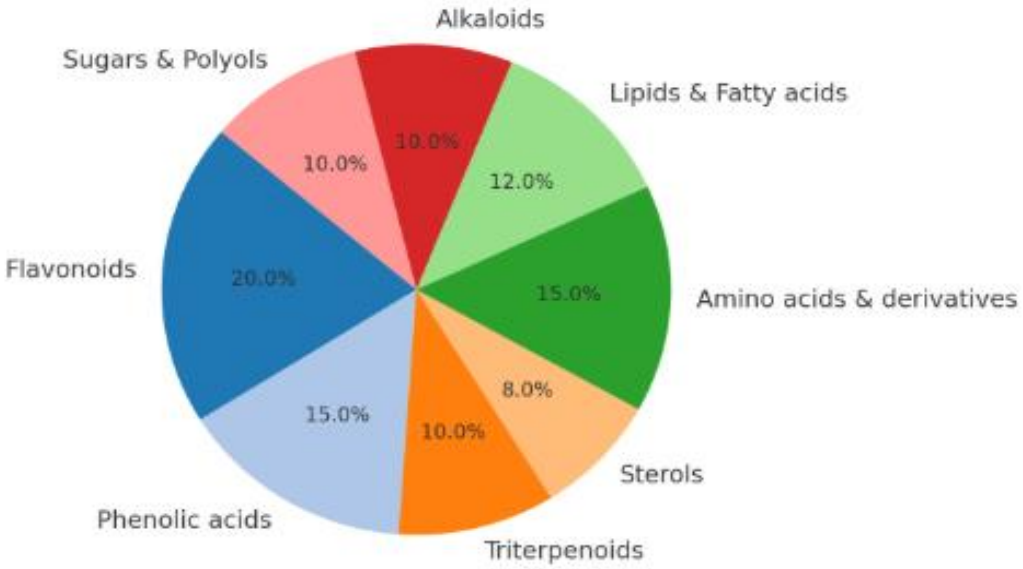
Figure 1. Compound classification in *Alternanthera sessilis* and *A. tenella*

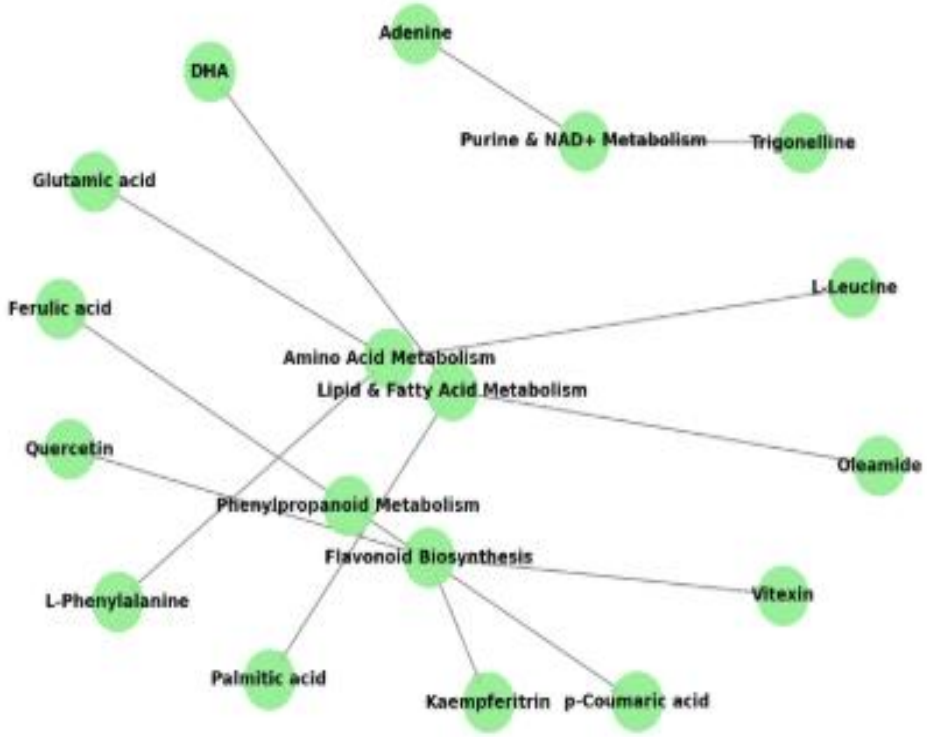


3.2 Metabolic Pathway Analysis

Key metabolites were mapped across five core pathways (Fig. 2):

- **Amino acid metabolism:** L-Leucine, Phenylalanine, Glutamic acid
- **Lipid metabolism:** DHA, Oleamide, Palmitic acid
- **Flavonoid biosynthesis:** Kaempferitrin, Vitexin, Quercetin
- **Phenylpropanoid metabolism:** Ferulic acid, p-Coumaric acid
- **Purine & NAD⁺ metabolism:** Adenine, Trigonelline

Figure 2. Metabolic pathway network of major identified metabolites in *A. sessilis* and *A. tenella*



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4. Discussion

The abundance of flavonoids (vitexin, kaempferol, quercetin) and phenolic acids (ferulic acid, ellagic acid) supports the antioxidant and anti-inflammatory efficacy of these plants. Lipid derivatives like DHA and oleamide highlight their potential neuroprotective and cardioprotective properties. Amino acid and purine derivatives indicate a role in stress adaptation and redox balance.These findings corroborate traditional claims regarding the medicinal use of these species and underscore their nutraceutical potential. The metabolic diversity observed reinforces the adaptability and bioactivity of wild edible plants. The metabolic diversity revealed through LC–MS/MS underscores the bioactive potential of these plants. The dominance of flavonoids (vitexin, kaempferol) and phenolics (ferulic acid, ellagic acid) supports their antioxidant and anti-inflammatory properties. Lipid derivatives such as DHA and oleamide highlight cardioprotective and neuroprotective potential, while triterpenoids (oleanolic, ursolic acids) suggest anti-inflammatory and hepatoprotective activity. Amino acid and purine metabolites indicate roles in redox regulation and stress response.Together, these compounds validate traditional uses of *A. sessilis* and *A. tenella* and promote their potential as functional food ingredients and nutraceutical resources.

Table 1. Key Phytometabolites Identified from *Alternanthera sessilis* and *A. tenella*

Compound Name	Formula	Molecular Weight (Da)	Match %	Classification
Glycolic acid	$C_2H_4O_3$	76.02	100.0	Endogenous; Cosmetic
L-(+)-Lactic acid	$C_3H_6O_3$	90.03	99.7	Endogenous; Therapeutic
NP-014839	$C_{19}H_{22}O_3$	298.16	99.1	Endogenous; Natural product
NP-006255	$C_{17}H_{26}O_4$	294.18	98.6	Endogenous; Natural product
Azelaic acid	$C_9H_{16}O_4$	188.10	98.4	Endogenous; Industrial
NP-002999	$C_{27}H_{32}O_{15}$	596.17	97.1	Polyphenolic natural product
NP-012534	$C_{15}H_{24}O_5$	284.16	96.6	Endogenous; Natural product
Palmitic acid	$C_{16}H_{32}O_2$	256.24	86.2	Endogenous; Lipid
Docosahexaenoic acid (DHA)	$C_{22}H_{32}O_2$	328.25	99.5	Polyunsaturated fatty acid
Quercetin	$C_{15}H_{10}O_7$	302.23	97.8	Flavonoid
Kaempferol	$C_{15}H_{10}O_6$	286.23	97.2	Flavonoid
Vitexin	$C_{21}H_{20}O_{10}$	432.38	96.9	Flavone glycoside
Ferulic acid	$C_{10}H_{10}O_4$	194.18	95.6	Phenolic acid
p-Coumaric acid	$C_9H_8O_3$	164.16	95.3	Phenolic acid
Oleanolic acid	$C_{30}H_{48}O_3$	456.70	93.4	Triterpenoid
β-Sitosterol	$C_{29}H_{50}O$	414.71	92.9	Sterol
Ursolic acid	$C_{30}H_{48}O_3$	456.70	92.7	Triterpenoid
Trigonelline	$C_7H_7NO_2$	137.14	98.3	Alkaloid
Adenine	$C_5H_5N_5$	135.13	99.3	Nucleobase
Choline	$C_5H_{13}NO$	103.17	98.5	Quaternary amine

Table 2. Summary of Major Pathways and Associated Metabolites

Pathway	Representative Metabolites	Functional Role
Amino Acid Metabolism	L-Leucine, Phenylalanine, Glutamic acid	Protein synthesis, stress adaptation
Fatty Acid Metabolism	DHA, Palmitic acid, Oleamide	Energy storage, anti-inflammatory
Flavonoid Biosynthesis	Kaempferitrin, Vitexin, Quercetin	Antioxidant, anti-inflammatory
Phenylpropanoid Metabolism	Ferulic acid, p-Coumaric acid	Cell wall structure, antioxidant
Purine & NAD^+ Metabolism	Adenine, Trigonelline	Redox balance, DNA/RNA repair

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5. Conclusion

Metabolomic profiling of *Alternanthera sessilis* and *A. tenella* revealed a rich diversity of bioactive compounds contributing to their therapeutic and nutritional value. Their chemical composition supports use in functional food development, while pathway mapping provides molecular insight for future pharmacological studies. LC–MS/MS metabolomic profiling of *Alternanthera sessilis* and *A. tenella* revealed 117 compounds, with strong representation of flavonoids, amino acids, and lipids. Pathway mapping confirms multifunctional biological relevance, supporting their use in traditional medicine and as nutrient-rich greens. Future research should include quantitative analyses and in vivo validation of their pharmacological actions.

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