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Analysis of functional groups in selected species of the tribe Paniceae (*Panicoideae*, *Poaceae*) using FTIR spectroscopy

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Abstract

Fourier Transform Infrared (FTIR) spectroscopy was employed to identify and characterize the functional groups in six species from the Paniceae tribe. The FTIR spectra were obtained within the 4000-400 cm^{-1} range, associated with various functional groups' stretching vibrations. This study presents preliminary data on the characteristic peaks corresponding to the functional groups of six plant species, namely *Pennisetum glaucum, Panicum miliaceum, Panicum sumatrense, Paspalum scrobiculatum, Setaria italica*, and *Echinochloa frumentacea*, using caryopsis as the sample. The FTIR analysis confirmed the presence of acids, alcohols, alkanes, alkenes, carboxyl groups, halogenated compounds, and aromatic compounds in the powdered samples. The findings suggest that the caryopsis of the selected species from the Paniceae tribe contains significant bioactive compounds that may contribute to their pharmacological properties.

Keywords: Paniceae, FTIR, *Pennisetum, Panicum, Echinochloa, Setaria, Paspalum*

Introduction

Millet refers to a collective group of small-seeded grains that belong to the tribes Paniceae and Chlorideae within the Poaceae family (commonly known as grasses). Approximately ten thousand years ago, millet served as a staple food before the widespread adoption of wheat and rice (Lu et al., 2009). It is notable for its significant content of certain amino acids, particularly sulphur-containing ones like cysteine and methionine. While millets are relatively high in methionine and provide a good source of essential amino acids, they typically have lower

levels of lysine and threonine (Saleh et al., 2013). Depending on the variety, millets are a valuable source of lipids, vitamin B, minerals, dietary fibre, and polyphenols. According to Mahajan et al. (2021), some of the most significant varieties of millet include Kutki millet (*Panicum sumatrense*), Proso millet (*P. miliaceum*), Pearl millet (*Pennisetum glaucum*), Finger millet (*Eleusine coracana*), Foxtail millet (*Setaria italica*), and Kodo millet (*Paspalum scrobiculatum*). The phytochemicals in millet grains contribute to its substantial health benefits (Coulibaly et al., 2011). Research by Zhang et al. (2014) analyzed the phytochemical properties, antioxidant potential, and anti-proliferative characteristics of three distinct varieties of proso millet. To evaluate these bioactive compounds, it is essential to employ modern analytical techniques such as FTIR, TLC, HPLC, HPTLC, and GC, among others. Fourier Transform Infrared Spectroscopy (FTIR) is particularly valuable for qualitatively analyzing active ingredients in biological and pharmaceutical materials.

According to Lingegowda et al. (2012), this rapid and non-destructive method enables the chemical characterization of samples to determine the presence of functional groups responsible for their biological activity. Typically, this technique is utilized to identify the functional groups present in plant chemical components. It has proven to be essential for recognizing medicinal compounds within the pharmacopoeias of numerous countries and aids in interpreting structures through complementary techniques (Mariswamy et al., 2012). The current study involves Fourier Transform Infrared Spectroscopy (FTIR) analysis of six plant species within the tribe Panaceae, all utilized as millets by tribal communities. The species analyzed are *P. glaucum, P. miliaceum, P. sumatrense, P. scrobiculatum, S. italica*, and *E. frumentacea*. The FTIR analysis provides valuable insights into their chemical properties.

Materials and Methods

Collection and preparation of sample

Caryopses from selected millet species, specifically *Pennisetum glaucum, Panicum miliaceum, Panicum sumatrense, Paspalum scrobiculatum, Setaria italica*, and *Echinochloa frumentacea*, belonging to the Paniceae tribe, were identified and collected from the Thayyannan Kudi tribal area in the Chinnar Wildlife Sanctuary, located in the Idukki district of Kerala, India. Samples were collected in triplicate during the respective fruiting seasons: September to October for *P. glaucum, S. italica*, and *E. frumentacea*, and June to August for *P. miliaceum, P. scrobiculatum*, and *P. sumatrense*. Once collected, the caryopses were ground into a fine powder using a wooden mortar and pestle and subsequently stored in polythene bags. Six samples were labelled and placed into individual polythene bags for proper storage.

Functional group analysis

The primary tool for identifying the presence of functional groups or chemical bonds in a compound is the FTIR spectrometer (Abubakar et al., 2021). To prepare translucent sample discs, 10 mg of each ground caryopsis sample was mixed with 100 mg of KBr to form a pellet. The powdered samples from each plant specimen were then analyzed using an FTIR spectroscope (Perkin Elmer Spectrum IR version 10.61), featuring a resolution of 4 cm^{-1} and a scan range of

400-4000 cm^{-1}. The results were interpreted following the findings of Hemmalakshmi et al. (2017).

Results and discussion

Pennisetum glaucum

Figure 1 and Table 1 display the FTIR spectra of *P. glaucum*. A prominent band at 3281.75 cm^{-1} indicates the presence of an aliphatic primary amine, specifically signifying N-H stretching. Additionally, a peak at 2924.34 cm^{-1} suggests an alkane or saturated aliphatic compound characterized by C=H stretching and asymmetric stretching of the -CH (CH_2) vibrations. The peak observed at 1642.47 cm^{-1} corresponds to C=N stretching (related to imines/oximes), while the peak at 1365.11 cm^{-1} reflects C-H stretching (alkane), and the band at 1149.12 cm^{-1} indicates C-N stretching (amine). The C-N stretching associated with amines appears prominently at 1076.72 cm^{-1}. Notably, the infrared spectra of *P. glaucum* exhibit a significant peak at 995.90 cm^{-1}, indicative of C=C bending (alkene). Many of these bands are in a similar spectral range to those observed in *P. miliaceum* and *P. sumatrense*. Comparable bands were also identified in the water and ethyl extracts of *Dillenia pentagyna* (Singh et al., 2022). Furthermore, several peaks in the fingerprint region, roughly 500-300 cm^{-1}, were excluded due to identification difficulties stemming from their complexity and overlap.

Table 1. FTIR analysis of *Pennisetum glaucum* caryopsis powder

Frequency (cm^{-1})	Frequency range (cm^{-1})	Bond/streching	Functional group
3281.75	3400-3300 3330-3250	N-H stretching	aliphatic primary amine
2924.34	3000-2840/ 2935-2915	C-H stretching/ Asymmetric stretching of -C H(CH_2) vibration	Alkane/Saturated aliphatic compound
1642.47	1690-1640	C=N stretching	Imine / oxime
1365.11	1385-1380 1370-1365	C-H bending	Alkane
1149.12	1250-1020	C-N stretching	Amine
1076.72	1250-1020	C-N stretching	Amine
995.90	1000-675	=C- H bending	Alkene
927.27	1000-675	=C- H bending	Alkene
859.74	1000-675	=C- H bending	Alkene
761.67	1000-675	=C- H bending	Alkene
571.31	620-490, 730-500	C-I, C-Cl	Halogen compound (Chloro compound, Iodo compound) alkyl halides
523.13	620-490, 730-500	C-I, C-Cl	Halogen compound (Chloro compound, Iodo compound) alkyl halides

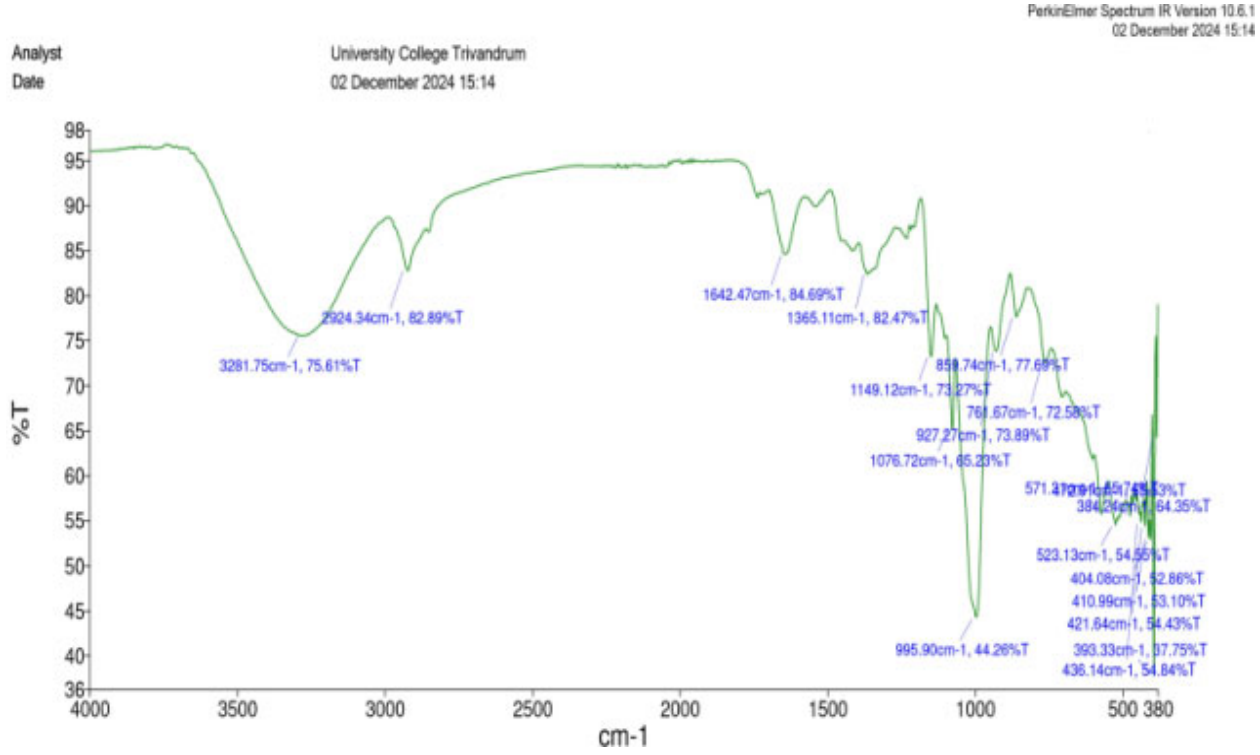

Figure 1. FTIR spectra of *Pennisetum glaucum* caryopsis powder

Figure 2. FTIR spectra of *Panicum miliaceum* caryopsis powder

Panicum miliaceum

The functional groups identified through FTIR analysis of the dried caryopsis of powdered *P. miliaceum* are detailed in Figure 2 and Table 2. The infrared absorption spectra were analyzed to characterize the various bonds present. These bonds ranged from weak to medium strength, with strong bonds noted at 3552, 1654.92, and 2054 cm^{-1}, respectively. The stretching vibration band associated with N-H stretching in aliphatic primary amines was identified at approximately 3280.87 cm^{-1}. Additionally, an alkane, classified as a saturated aliphatic compound, shows C-H stretching and the asymmetric stretching of the -C H(CH_2) vibration at 2924.99 cm^{-1}. The C=C stretching, indicative of alkenes, was observed at 1637.38 cm^{-1}. The O-H group, resulting from the presence of alcohols, produced a peak at 1337.66 cm^{-1}. The C-N stretching associated with amines was identified at 1149.07 cm^{-1}, while in the powdered caryopsis, a peak was noted at 1076.28 cm^{-1}. A prominent peak corresponding to a C–O–C group was also observed at 996.61 cm^{-1}.

Panicum sumatrense

Figure 3 and Table 3 demonstrate that *P. sumatrense* exhibits sixteen peaks. The peaks observed at 2924, 1149, and 1076 cm^{-1} are consistent with those found in *P. glaucum* and *P. miliaceum*, along with additional peaks at 859 and 571 cm^{-1} for *P. glaucum*, and at 996 and 419 cm^{-1} for *P. miliaceum*. Notably, a peak characteristic of N-H stretching in aliphatic primary amines was recorded at 3279.85 cm^{-1}. As saturated aliphatic compounds, the presence of alkanes is indicated by C-H stretching and asymmetric -C H(CH_2) vibrations observed at 2924.36 cm^{-1}. The

Table 2. FTIR analysis of *Panicum miliaceum* caryopsis powder

Frequency (cm^{-1})	Frequency range (cm^{-1})	Bond/streching	Functional group
3280.87	3400-3300 3330-3250	N-H stretching	Aliphatic primary amine
2924.99	3000-2840/ 2935-2915	C-H stretching/ Asymmetric stretching of -C H(CH_2) vibration	Alkane/Saturated aliphatic compound
1637.38	1662-1626	C=C stretching	alkene
1337.66	1420-1330	O-H bending	alcohol
1149.07	1250-1020	C-N stretching	amine
1076.28	1250-1020	C-N stretching	amine
996.61	1000-675	=C- H bending	Alkene
930.21	1000-675	=C- H bending	Alkene
860.44	1000-675	=C- H bending	Alkene
572.08	550–690	(C–Br)	Halogen compound [Bromocompounds]
518.01	500–730	C-Cl	Halogen compound [Chlorocompound]
462.19	490–620	C–I)	Halogen compound

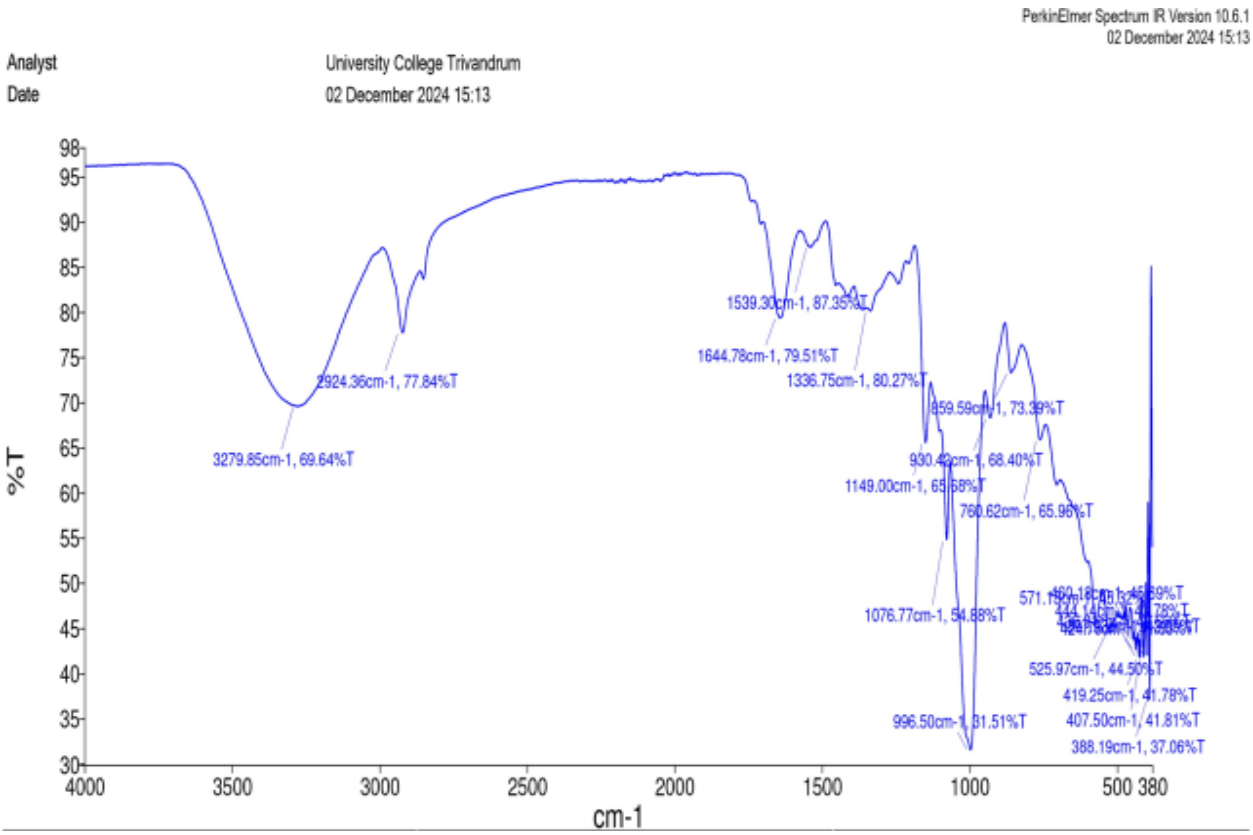

Figure 3. FTIR spectra of *Panicum sumatrense* caryopsis powder

Table 3. FTIR analysis of *Panicum sumatrense* caryopsis powder

Frequency (cm^{-1})	**Frequency range (cm^{-1})**	**Bond/streching**	**Functional group**
3279.85	3400-3300 3330-3250	N-H stretching	Aliphatic primary amine
2924.36	3000-2840/ 2935-2915	C-H stretching/ Asymmetric stretching of -C H(CH_2) vibration	Alkane/Saturated aliphatic compound
1644.78	1662-1626	C=C stretching	alkene
1539.30	1420-1330	O-H bending	alcohol
1336.75	1420-1330	O-H bending	alcohol
1149.00	1250-1020	C-N stretching	amine
1076.77	1250-1020	C-N stretching	amine
996.50	1150–911	C–O–C group	
930.42	1150–911	C–O–C group	
571.13	500–730	C-Cl	Halogen compound [Chloro compound]
525.97	500–730	C-Cl	Halogen compound [Chloro compound]

powdered extract also reveals C=C stretching at 1644.78 cm^{-1}, O-H bending at 1539.30 cm^{-1}, and O-H stretching at 1336.75, 1149.00, and 1076.72 cm^{-1}, respectively.

Paspalum scrobiculatum

Figure 4 displays the FTIR spectra, while Table 4 summarizes the peak values of *P. scrobiculatum* caryopsis powder. Notably, the peak observed at 3280 cm^{-1} shows similarities to the spectra of *P. miliaceum* and *S. italica*. Furthermore, the FTIR fingerprint spectra at 1076 and 1149 cm^{-1} for *P. scrobiculatum* exhibit a comparable spectral pattern to those of *P. glaucum*, *P. sumatrense, P. miliaceum, S. italica*, and *E. frumentacea*. The peak at 1365 cm^{-1} also shows similarities with *P. glaucum* and E. frumentacea. *S. italica* features a characteristic peak at 1742 cm^{-1}, while *P. glaucum* presents a comparable measurement at 1642 cm^{-1}, aligning with its apex value. Additionally, *P. miliaceum* and *E. frumentacea* display similarities at a peak of 860 cm^{-1}, whereas *P. glaucum, P. sumatrense*, and *E. frumentacea* show similarities at a peak of 571 cm^{-1}.

The prominent peak observed at 3280.23 cm^{-1} indicates N-H stretching associated with aliphatic primary amines. In contrast, the stretching vibrations of O-H, characteristic of alcohols, correspond to a band located at 2925.03 cm^{-1}. The peak at 1742.14 cm^{-1} is associated with C-H bending in aromatic compounds, while C-H bending in alkanes is represented by the peak at 1642.98 cm^{-1}, along with additional

Table 4. FTIR analysis of *Paspalum scrobiculatum* caryopsis powder

Frequency (cm^{-1})	**Frequency range (cm^{-1})**	**Bond/streching**	**Functional group**
3280.23	3400-3300 3330-3250	N-H stretching	Aliphatic primary amine
2925.03	3000-2840/ 2935-2915	C-H stretching/ Asymmetric stretching of -C H(CH2) vibration	Alkane/Saturated aliphatic compound
1742.14	2000-1650	C-H bending	aromatic compound
1642.98	2000-1650	C-H bending	aromatic compound
1365.22	1385-1380 1370-1365	C-H bending	alkane
1149.40	1250-1020	C-N stretching	amine
1076.42	1250-1020	C-N stretching	amine
997.04	1000-675	=C- H bending	Alkene
929.89	1000-675	=C- H bending	Alkene
860.45	1000-675	=C- H bending	Alkene
571.6	620-490, 730-500	C-I, C-Cl	Halogen compound (Chloro compound, Iodo compound) alkyl halides
524.3	620-490, 730-500	C-I, C-Cl	Halogen compound (Chloro compound, Iodo compound) alkyl halides

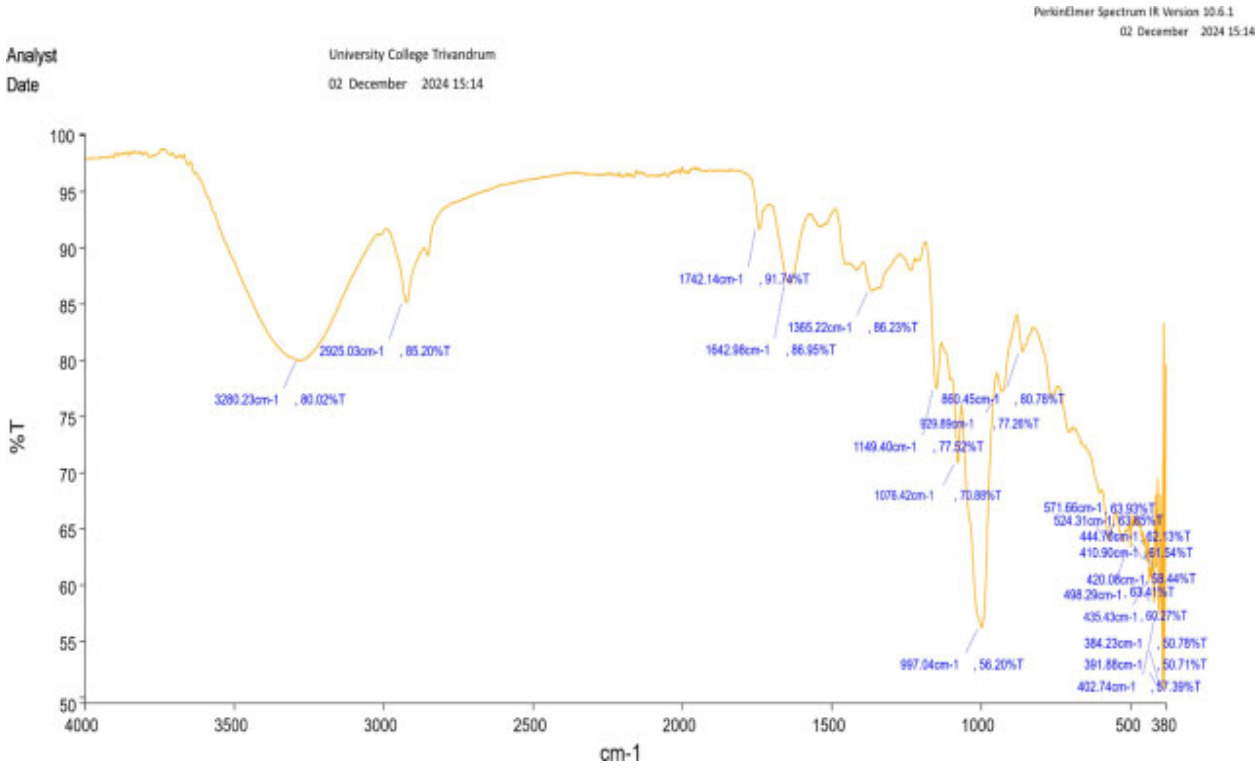

Figure 4. FTIR spectra of *Paspalum scrobiculatum* caryopsis powder

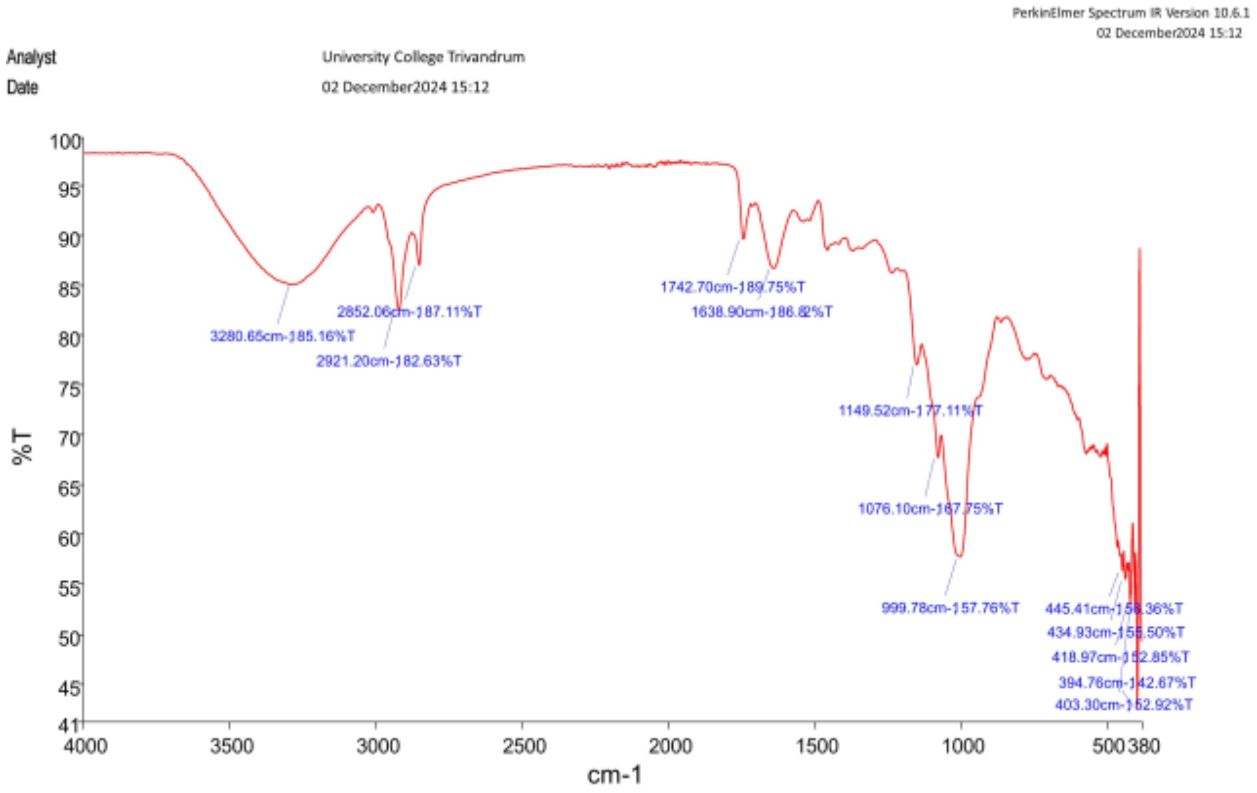

Figure 5. FTIR spectra of *Setaria italica* caryopsis powder

frequencies at 1149.40 and 1076.42 cm-1. The absorption peaks observed at 997.04, 929.89, and 860.45 cm-1 are attributed to C-H bending vibrations in alkenes.

Setaria italica

The prominent peak observed at 3280.23 cm-1 indicates N-H stretching associated with aliphatic primary amines (Figure 5 and Table 5). In contrast, the stretching vibrations of O-H, characteristic of alcohols, correspond to a band located at 2925.03 cm-1. The peak at 1742.14 cm-1 is associated with C-H bending in aromatic compounds, while C-H bending in alkanes is represented by the peak at 1642.98 cm-1, along with additional frequencies at 1149.40 and 1076.42 cm-1. The absorption peaks observed at 997.04, 929.89, and 860.45 cm-1 are attributed to C-H bending vibrations in alkenes.

Echinochloa frumentacea

The FTIR spectra of *E. frumentacea* reveal a prominent band at 3281.89 cm^{-1} (Figure 6 and Table 6), indicating the presence of N-H stretching, characteristic of secondary amines. The fingerprint spectra of *E. frumentacea*, particularly at 996 cm^{-1}, demonstrate a spectral pattern closely matching those of P. miliaceum and *P. sumatrense*. The peak observed at 2924.19 cm^{-1} is related to C-H stretching, while the asymmetric stretching of the -C H(CH_2) vibration suggests the presence of certain saturated aliphatic or alkene compounds. The identification of alkanes is further supported by the C=C stretching peak at. Additionally, the bands at 1365.11 and 1639.33 cm^{-1} indicate C-H and O-H bending, respectively, characteristic of alkanes and alcohols. The peaks at 1149.23 and 1076.32 1639.33 cm^{-1} confirm C-N stretching, affirming the presence of amines. Furthermore, the peak at 1238.16 1639.33 cm^{-1} reflects C-N stretching/C-O stretching, suggesting the potential presence of either amines or acids. The observed frequency bands at 996.66, 931.86, and 860.21 1639.33 cm^{-1} correspond to the bending of the =C-H bond in alkenes, while C-N stretching

Table 5. FTIR analysis of *Setaria italica* caryopsis powder

Frequency (cm^{-1})	Frequency range (cm^{-1})	Bond/streching	Functional group
3280.65	3400-3300 3330-3250	N-H stretching	Aliphatic primary amine
2921.20	3000-2840/ 2935-2915	C-H stretching/ Asymmetric stretching of -C H(CH_2) vibration	Alkane/Saturated aliphatic compound
2852.06	3200-2700	O-H stretching	alcohol
1742.70	1820-1670	C=O stretching	Carboxyl
1638.90	1650-1566	C=C stretching	cyclic alkene
1149.59	1250-1020	C-N stretching	amine
1076.10	1250-1020	C-N stretching	amine
999.78	1000-675	=C- H bending	Alkene

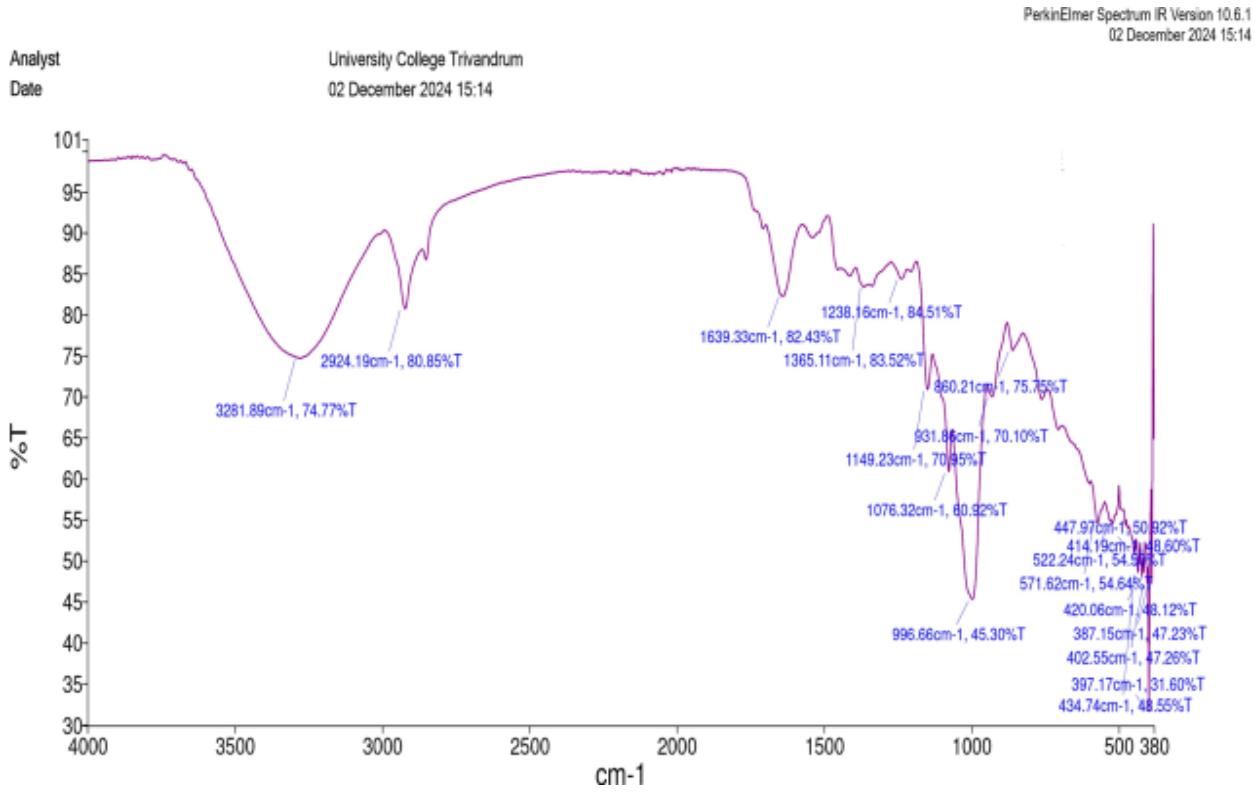

Figure 6. FTIR spectra of *Echinochloa frumentacea* caryopsis powder

(amine) occurs at frequencies of 571.62 and 522.24 1639.33 cm^{-1}. When comparing the infrared spectra of *P. scrobiculatum, S. italica, E. frumentacea, P. glaucum, P. miliaceum,* and *P. sumatrense*, it is clear that certain functional groups - such as amines, alkanes, C-O bonds, aromatic alkenes, and primary alcohol stretches - are present in all examined plant species. A more comprehensive investigation is warranted to characterize the various phytochemical compounds present in these plants thoroughly.

Conclusions

The FTIR analysis of six Paniceae species collected from the Thayyannan Kudi tribal area within the Chinnar Wildlife Sanctuary revealed the presence of several functional groups. Specifically, the analysis identified amines, alkanes, C-O bonds, aromatic alkenes, and stretches of primary alcohols. A comparison of the infrared spectra of *Paspalum scrobiculatum, Setaria italica, Echinochloa frumentacea,* and various species (including *Pennisetum glaucum, Panicum miliaceum*, and *Panicum sumatrense*) shows that they share several prominent peaks associated with specific functional groups. Further detailed investigation is required to characterize the diverse phytochemical compounds in these selected plant species, which may facilitate future formulation efforts.

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Table 6. FTIR analysis of *Echinochloa frumentacea* caryopsis powder

Frequency (cm^{-1})	Frequency range (cm^{-1})	Bond/streching	Functional group
3281.89	3350-3310	N-H stretching	Secondary amine
2924.19	3000-2840/ 2935-2915	C-H stretching/ Asymmetric stretching of -C H(CH_2) vibration	Alkane/Saturated aliphatic compound
1639.33	1662-1626	C=C stretching	Alkene
1365.11	1370-1365/ 1420-1330	C-H bending/ O-H bending	Alkane/ alcohol
1238.16	1250-1020 1320-1210	C-N stretching C-O stretch	Amine/ acid
1149.23	1250-1020	C-N stretching	Amine
1076.32	1250-1020	C-N stretching	Amine
996.66	1000-675	=C- H bending	Alkene
931.86	1000-675	=C- H bending	Alkene
860.21	1000-675	=C- H bending	Alkene
571.62	620-490, 730-500	C-I, C-Cl	Halogen compound (Chloro compound, Iodo compound) alkyl halides
522.24	620-490, 730-500	C-I, C-Cl	Halogen compound (Chloro compound, Iodo compound) alkyl halides

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Authors' contributions: All authors participated in the planning, execution, analysis and writing of this study.

Conflict of interest: Authors declare no conflict of interest.

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