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Qualitative phytochemical screening and FTIR spectroscopic analysis of *Sesamum indicum* L.

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Abstract
Sesamum indicum L. (Pedaliaceae) is one of the oldest condiments and economically important oilseed crop and medicinally important plant due to presence of wide range of secondary metabolites. The biologically active compounds present in plants are called phytochemicals. These phytochemicals are derived from various parts of plants such as leaves, stem and roots. These phytochemicals are used as sources of direct medicinal agents. The present study aim is to analyses the phytochemicals present in *Sesamum indicum* L. by using Qualitative phytochemical analysis and Fourier-transform infrared spectroscopy (FTIR). Preliminary phytochemical screening of the different five extract of the plant showed the presence of alkaloids, proteins, flavonoids, carbohydrate, Phytosterol, Phenols and tannins. FTIR findings indicated the presence of characteristic functional groups like alkanes, alcohols, amines, carboxylic acid, azide, aldehyde and isothiocyanate etc. The findings of this paper will be useful for identification of crude drugs obtained from this plant and pharmacological studies in future.

Keywords: FTIR, *Sesamum indicum* L., phytochemicals

Introduction
Plants are a beneficial source of various bioactive compounds that directly or indirectly treat various human ailments [1]. Phytochemicals are responsible for the medicinal activities of the plants [2]. The phytochemical constituents that play a significant role in medicines can be identified using crude extracts/drugs from plants [3].
Fourier-transform infrared spectroscopy (FTIR) is a high-resolution analytical technique to identify the bioactive compounds based on their functional group and reveal the structure of the compounds [4, 5]. In Fourier-transform infrared spectroscopy (FTIR), molecules show absorption in a characteristic range of frequencies. The organic compounds are mainly absorbed in the 4000-400 cm^{-1} range, which is key in identifying and characterising the compounds in the respective extracts [6].
Sesame (*Sesamum indicum* L.) from the family Pedaliaceae is a flowering plant in the genus Sesamum. It is an annual crop grown between 1.6 and 3.3 ft high. It has opposite leaves, 4 to 14 cm long. The flowers may vary in colour, with some being blue, white or purple [7]. The seeds are small in size, ranging between 3 and 4 mm long by 2 mm wide and 1 mm thick. The seeds are oval and slightly flattened [8]. It is one of the most important oilseeds crop worldwide, and it has been cultivated for its edible seeds since ancient times for use as a traditional health food and its medicinal benefits [9, 10].
Nowadays, sesame (Til) seed and oil have been used as a food due to their rich nutty flavour [11] and healing oil for hundreds of years [12]. It is a good source of protein 22% and fatty oil 54% [13]. Sesame oil contains Magnesium, Copper, Calcium, Iron, Zinc and Vitamin B6. Copper provides relief for rheumatoid arthritis. It is established that Magnesium supports vascular and respiratory health systems while Calcium helps prevent colon cancer, osteoporosis and migraine; zinc is known to promote health [14].

Materials and Methods
Collection of plant material
The fresh leaves, stems, and roots of the *Sesamum indicum* L. plant were collected from Terkheda village in Kalamb tehsil of the Dharashiv district in Maharashtra, India.
The samples were washed thoroughly in running tap water to remove soil particles and adhered debris, and finally washed with sterile distilled water. The leaves, stems and roots.

Extraction

The coarsely powdered plant material of *Sesamum indicum* L. leaves, stems, and roots were kept inside the bottles of different distilled water, ethanol, methanol, chloroform and ether extracts. The menstruum is poured on top until it completely covers the plant material. The bottles are kept closed for three days and shaken occasionally to ensure complete extraction. At the end of extraction, the micelle is separated from marc by Whatman filtration paper. Subsequently, the micelle is separated from the menstruum by evaporation on top of the water bath. It was then transferred to glass vials and kept at 4 °C for future use.

Preliminary phytochemical analysis

Qualitative phytochemical analysis was carried out, and the results observed were based on the colour change or precipitate formation after adding specific reagents.

Fourier transform infrared spectrophotometer (FTIR)

The Fourier Transform Infrared Spectrophotometer (FTIR) is the most powerful tool for identifying the types of chemical bonds and functional groups present in compounds.

The wavelength of light absorbed is characteristic of the chemical bond. The chemical bonds in a molecule can be determined by interpreting the infrared absorption spectrum. The dried powder of different parts of plant material were used for FTIR analysis. 10 mg of the dried powder was encapsulated in 100 mg of KBr pellet to prepare translucent sample discs. The powdered samples of plant material were loaded in an FTIR spectroscope (Shimadzu, IR Affinity 1, Japan), with a Scan range from 400 to 4000 cm^{-1} with a resolution of 4 cm^{-1}.

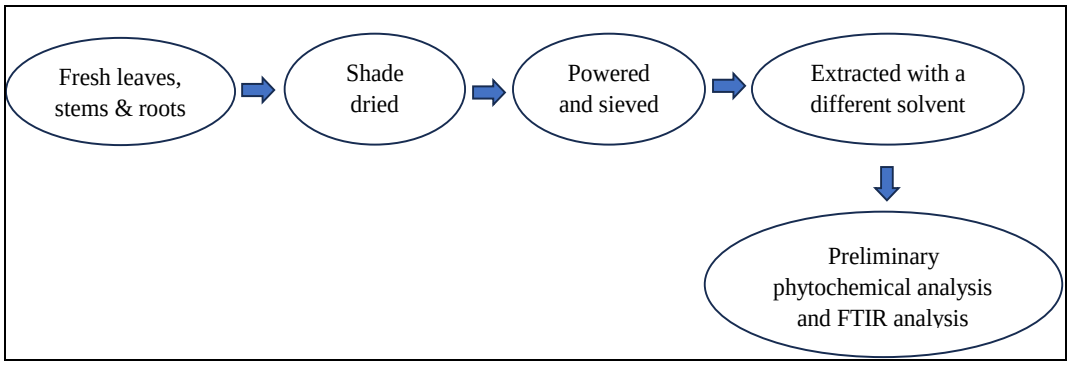

Fig 1: Schematic representation of extraction processes

Results

From the Preliminary Phytochemical Analysis of leaves, stems and roots of *Sesamum indicum* L. plants, the presence or absence of carbohydrates, alkaloids, proteins, flavonoids, phenols, tannin, phytosterol and carbohydrates were investigated. The results of this study are shown in Table 1.

Table 1: Preliminary Phytochemical Analysis of leaves, stem and root of *Sesamum indicum* L.

***Sesamum indicum* L.**																
Sr. No.	**Test**	**Aqueous Extract**			**Ethanolic Extract**			**Methanolic Extract**			**Chloroform Extract**			**Ether Extract**		
		L	S	R	L	S	R	L	S	R	L	S	R	L	S	R
1.	Alkaloids	+	+	+	+	+	-	+	+	-	+	-	-	+	-	-
2.	Proteins	+	+	-	-	+	+	+	-	+	-	+	-	-	-	-
3.	Flavonoids	+	+	-	+	-	-	-	-	+	-	-	-	-	+	-
4.	Phenols & Tannins	-	+	-	-	-	+	+	-	-	-	-	-	-	-	-
5.	Phytosterol	+	+	-	+	+	-	+	-	+	-	-	-	-	-	-
6.	Carbohydrates	+	-	+	+	+	+	+	+	+	+	-	+	+	+	+

'+' indicates presence; '-' indicates an absence & L-leaf, S-stem, R-root.

Functional groups identification

The FTIR spectrum was used to identify the functional groups of the active components present in the Extract based on the peak values in the region of IR radiation. When the Extract was passed into the FTIR, the functional groups of the components were separated based on the ratio of their peaks. The results of FTIR analysis confirmed the presence of alcohol, phenol, alkanes, aldehyde, aromatic compounds, secondary alcohol, aromatic amines, and halogen compounds.

Table 2: FTIR peak values and functional groups in the leaf of *Sesamum indicum* L.

Wave No. (cm-1)	Bond type	Functional group
3738.05	O-H	Alcohol
3662.82	O-H	Alcohol
3537.45	O-H	Alcohol
2918.30	N-H	Amine salt
2223.92	C≡N	Nitrile
156.42	N=N=N	Azide
2046.47	N=C=S	Isothiocyanate
1905.67	C-H	Aromatic Compound
1255.66	C-O	Aromatic Ester
1020.34	C-N	Amine

The FTIR spectrum of the leaf of the *Sesamum indicum* L. plant shows the absorption at 3738.05, 3662.82 and 3537.45 cm-1 is due to the O-H stretching of alcohol in the extract. The band at 2918.17 cm-1 is due to the N-H stretching of the amine salt. The absorption at 2223.92 cm-1 is due to the C≡N stretching of nitrile in the extract. The band at 2156.42 cm-1 is due to N=N=N stretching associated with the azide mode of the extracts. The vibrational absorption band at 2046.47 cm^{-1} was assigned to N=C=S stretching of isothiocyanate. The band at 1905.67 cm-1 is due to C-H stretching associated with the aromatic compound of the extracts. A band at 1255.66 cm-1 represents the C-O stretching of aromatic ester in the extract. A band at 1020.34 cm-1 represent the C-N stretching of amine in the extract.

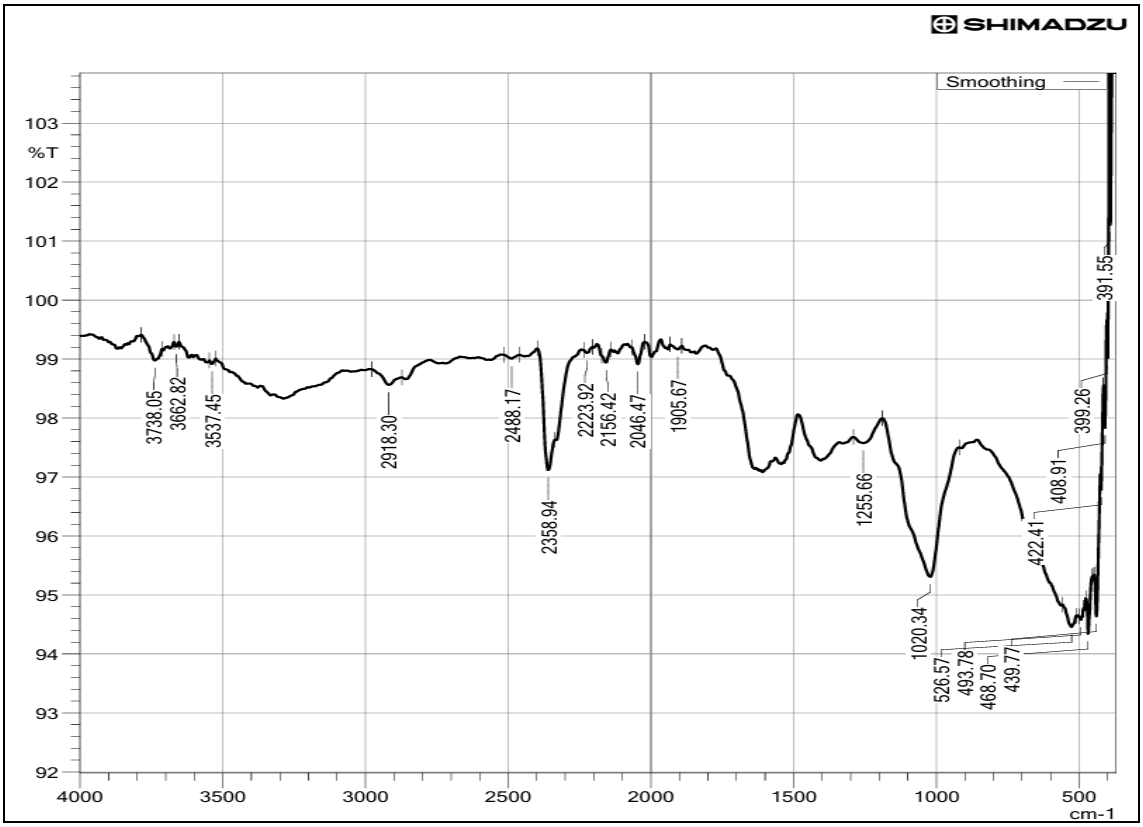

Fig 2: FTIR spectrum of *Sesamum indicum* L. leaf

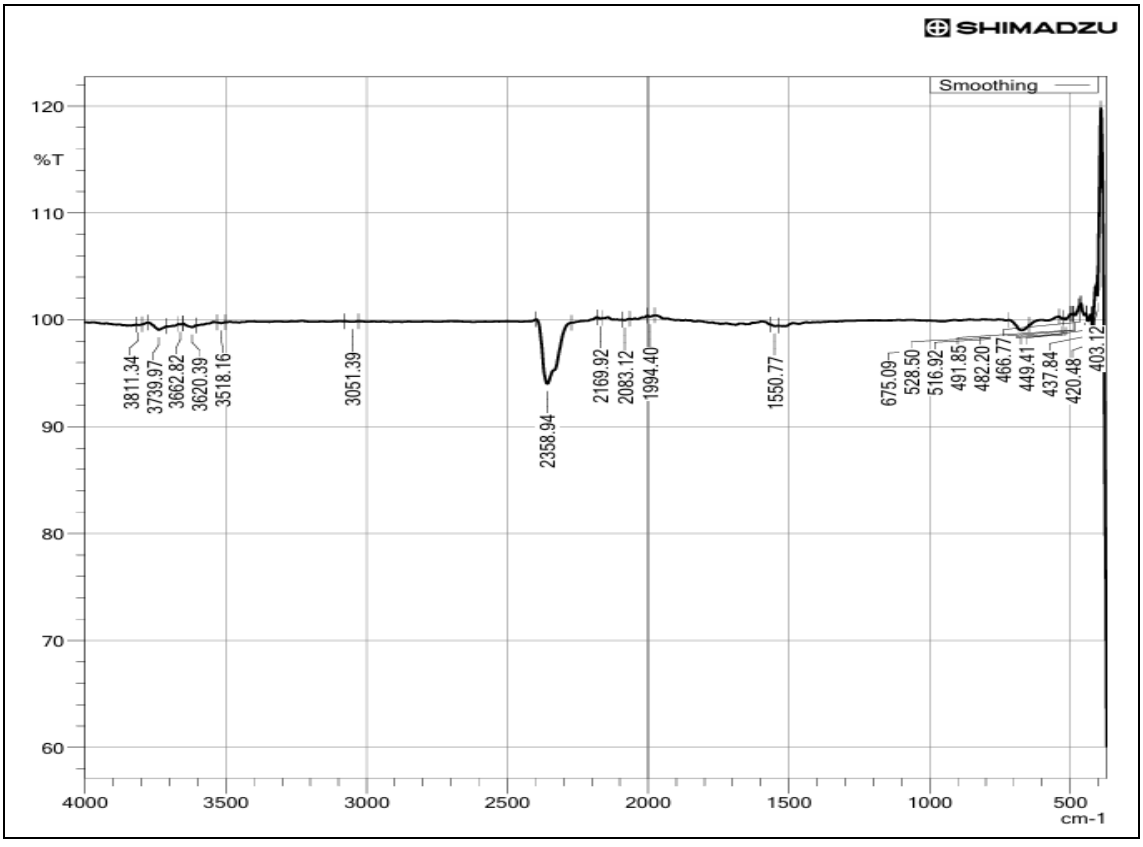

Fig 3: FTIR spectrum of *Sesamum indicum* L. stem

Table 3: FTIR peak values and functional groups in the stem of *Sesamum indicum* L.

Wave No. (cm-1)	Bond type	Functional group
3811.34	O-H	Alcohol
3739.97	O-H	Alcohol
3662.82	O-H	Alcohol
3620.39	O-H	Alcohol
3518.16	O-H	Alcohol
3051.39	O-H	Carboxylic Acid
2169.92	N=N=N	Azide
2083.12	N=C=S	Isothiocyanate
1994.40	N=C=S	Isothiocyanate
1550.77	N-O	Nitro compound

The FTIR spectrum of the stem of the *Sesamum indicum* L. plant shows the absorption at 3811.34, 3739.97, 3662.82, 3620.39 and 3518.16 cm-1 is due to the O-H stretching of alcohol in the extract. The band at 3051.39 cm-1 is due to the O-H stretching of carboxylic acid. The absorption at 2169.92 cm-1 is due to the N=N=N stretching of azide in the extract. The band at 2083.12 and 1994.40 cm-1 is due to N=C=S stretching associated with the isothiocyanate mode of the extracts. The band at 1550.77 cm-1 is due to N-O stretching associated with the nitro compound of the extracts.

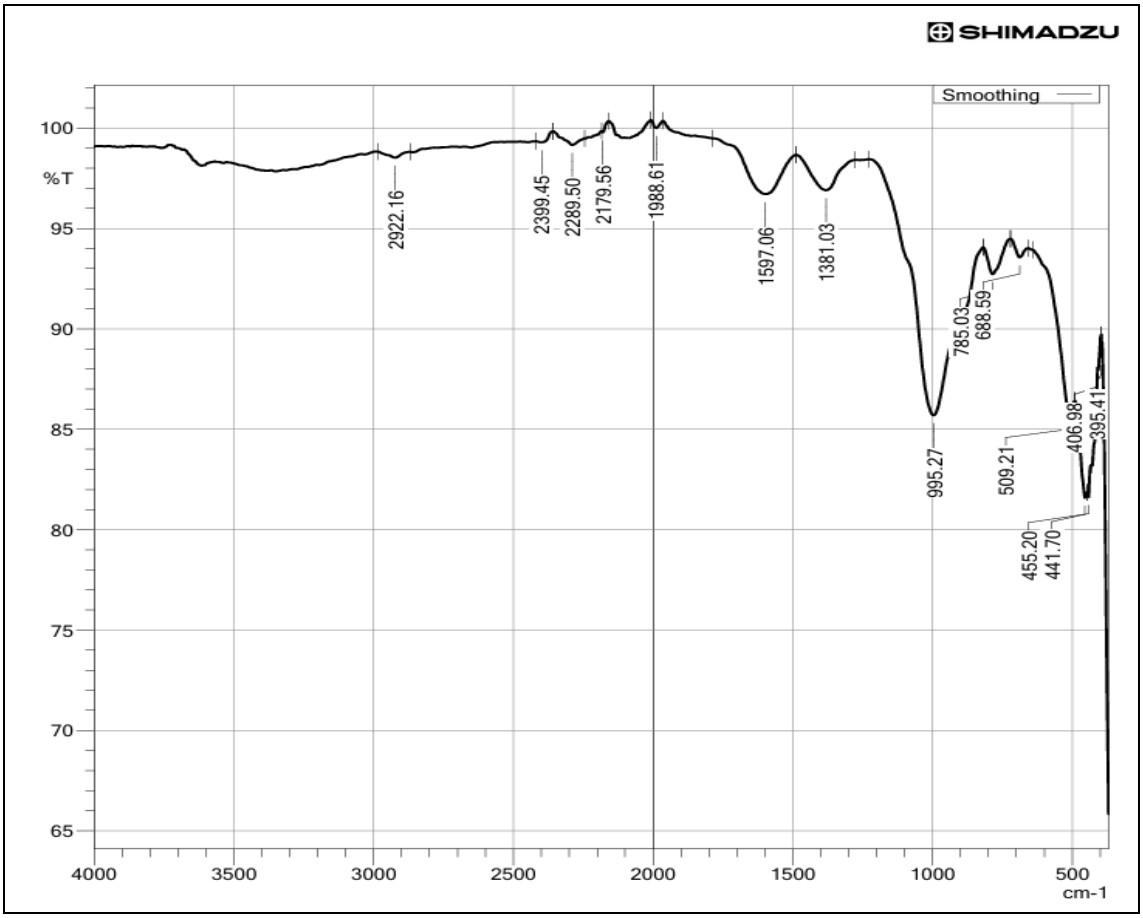

Fig 4: FTIR spectrum of *Sesamum indicum* L. root

Table 4: FTIR peak values and functional groups in the root of *Sesamum indicum* L.

Wave No. (cm-1)	Bond type	Functional group
2922.16	C-H	Alkane
1988.61	C=C=C	Allene
1597.06	N-H	Amine
1381.03	C-H	Aldehyde
995.27	C=C	Alkene

The FTIR spectrum of the root of the *Sesamum indicum* L. plant shows the absorption at 2922.16 cm-1 is due to the C-H stretching of the alkane in the extract. The band at 1988.61 cm-1 is due to the C=C=C stretching of allene. The absorption at 1597.06 cm-1 is due to the N-H stretching of the amine in the extract. The band at 1381.03 cm-1 is due to C-H stretching associated with the aldehyde mode of the extracts. A band at 995.27 cm-1 represents the C=C bending of alkene in the extract.

Conclusion

The present study results are a way to predict and compare the phytoconstituents present in this plant with other bioactive, medicinally important plants. It could be concluded that *Sesamum indicum* L. contain various bioactive compounds. So, it is recommended as a plant of phytopharmaceutical importance. However, further studies will need to be undertaken to ascertain its bioactivity, toxicity profile, and full effect on the ecosystem and agricultural products. It will also useful for identification of crude drugs obtained from this plant and pharmacological studies in future. The presence of

characteristic functional groups, such as Carboxylic acids, amines, amides, sulphur derivatives, polysaccharides, organic hydrocarbons, and halogens, is responsible for various medicinal properties of *Sesamum indicum* L.

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