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Analysis of *Tabebuia rosea* oil and *Tabebuia rosea* oil methyl esters using Fourier transform infrared (FTIR) spectroscopy

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Abstract

Fourier transform infrared (FTIR) spectroscopy method was used for the analysis of phytochemicals present in *Tabebuia rosea* seed oil and its biodiesel. FT-IR spectra of *Tabebuia rosea* seed oil and its biodiesel have been recorded in the region 2925 - 604 Cm^{-1} . FT-IR is a vibrational spectroscopy that records absorptions of IR light by chemical bonds in all molecules including polymers. The different frequency ranges and their different functional groups were analyzed during the study period. FT-IR spectroscopy of the *Tabebuia rosea* seed oil reveals diverse functional groups and there by confirmed the possible presence of phytochemicals such as Terpenoids, Steriods, Flavonoids, Tannins, Coumarins, etc.

Keywords: Fourier transform infrared (FTIR) spectroscopy, *Tabebuia rosea*, botanical origin, biofuel

Introduction

FT-IR is one of the most extensively used methods to classify the chemical constituents and elucidate the compounds structures, and has been used as an essential method to identify medicines in Pharmacopoeia of many countries. Owing to the fingerprint characters and extensive applicability to the samples, FT-IR has played an important role in pharmaceutical analysis in recent years ^[1].

Fourier transform infrared (FTIR) spectroscopy has received great attention in quantitative analysis of fats and oils over the years. It has a major advantage over the conventional grating instruments, having more energy throughput (the Jacquinot advantage), excellent reproducibility, and accuracy from the laser source. With increasing use of the microcomputer, FTIR is capable of manipulating spectral information (subtraction, rationing, derivative spectra, and deconvolution) and advanced chemometric software to handle calibration development ^[2].

In the search for products derived from plants with potential biological activity, it has been described that some species belonging to the Bignoniaceae family have anti-inflammatory, anti-microbial, and anti-tumoral potential, due to its empirical use in rural areas in Colombia, Bolivia, Brazil, and other Latin American countries. Within this family, *Tabebuia rosea* (Bertol.) DC. Has been known to be used in traditional medicine in the Northern Coast of Colombia for the treatment of skin conditions such as pruritic diseases and infections with fungi and yeast.

T. rosea is a tree that reaches 30 m height and has a 1 m diameter trunk, its bark is flaky and is recognized by bell-shaped ornate purple and pink flowers³. Few studies have evaluated the biological activity of *T. rosea* extracts; therefore, the aim of this work was to determine the antioxidant, anti-inflammatory, and antiproliferative potential of the leaf and inner bark extracts obtained from *T. rosea* ^[3]. Based on the review of literature there is no study recorded in *Tabebuia rosea*. Hence, in the current study an attempt had been made to identify phytochemicals present in *Tabebuia rosea* seed oil and its biodiesel by FTIR methods.

Methods and Materials

The *Tabebuia rosea* seeds were collected and segregated from the campus of University of Mysore. The seeds were randomly selected according to the amount needed for the experimental work in the month of January and February.

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Prior to the extraction process, the seeds were dried at 60 °C for 7 hrs till weight remains constant, in order to reduce the moisture content. The separation of the outer cover from the seeds (cotyledon) was carried out by hand removal in order to achieve very high yield. Mortar and pestle were used to pulverise the seeds into coarse powder [4].

Extraction and conversion of oil

The oil was extracted using Soxhlet extractor with Petroleum ether as the solvent at 40-60 °C. This was allowed to continue for 2-3 hours. At the end of extraction, the resulting mixture containing the oil was heated to recover solvent from the oil. The experiment was repeated by placing fresh seed powder sample for further extraction of oil.

Conversion of the oil to biodiesel/TOME (*T.rosea* oil methyl esters) was carried out according S. Sirigeri *et al.* (2019) [5].

FT-IR analysis

The FT-IR studies have been followed by the method described by Yang, H *et al.* (2005) [6]. The sample was completely dried to remove the solvent and the surface adhered film was scratched carefully and its FT IR spectra were recorded using a PerkinElmer (Instrument Serial Number 94012) double beam spectrometer in the spectral range of 4000–400 cm⁻¹. FT IR spectra were recorded to identify the functional groups of the extracted oil and TOME.

Results

Analysis of the oil

The obtained FT IR spectrum for the *Tabebuia rosea* seed oil to identify the functional groups is given below (figure. 01). The peaks obtained for the oil sample is given in the Table 1. The analytical evaluation of the oil was carried out by the comparison of the peaks with the previous similar works of Hong yang *et al.* (2005) [7], Lerma-garcia *et al.* (2010) [8] and Pugazhendy (2012) [9]. The analytical evaluation of the oil spectra is given in Table 02.

Analysis of the Biodiesel

The obtained FT IR spectrum for the *Tabebuia rosea* oil methyl esters (TOME) to identify the functional groups is given below (figure. 02). The peaks obtained for the TOME is given in the Table 3.

The analytical evaluation of the oil was carried out by the comparison of the peaks. The peaks observed were similar to

that of the oil (table 2) with few other additional peaks which were classified to the functional groups as listed in the table 4.

Discussion

FT-IR technique was used for evaluation the type of organic and inorganic complexes in plant extract. From the spectra (Fig. 1 and 2), we can see clearly that although they show substantial overlap of each absorption spectrum of various components, each band represents an overall overlap of some characteristic absorption peaks of functional groups in the samples. The FTIR spectra of *Tabebuia rosea* seed oil and its biodiesel are rather similar. The FT-IR analyzes of *Tabebuia rosea* seed oil and TOME represents the following functional groups. The infra-red spectrum shows a frequency ranges from 3000–2850 cm⁻¹ peaks represent the C-H stretching vibration presence of alkenes [1]. The frequency ranges from 3300–2500 cm⁻¹ peak display the characteristic absorptions of groups representing aliphatic O-H stretching vibration which indicate the presence of carboxylic acids. The frequency ranges from 2260–2100 cm⁻¹ peak correspond to –C (triple bond) C– stretching vibration (ester alkynes) [10]. The frequency ranges from 1750-1735 cm⁻¹ peak represent C=O stretching vibration (ester and amino acid) [11]. The following peaks 1680–1640 cm⁻¹ are mainly attributed to the –C=C– stretching vibration present in the alkenes. The frequency ranges from 1550–1475 cm⁻¹ peak are assigned to the N–O asymmetric stretching vibration present in the nitro compounds. The particular frequency ranges from 1320–1000 cm⁻¹ C-O stretching, O-H bending vibration indicate presence of alcohols, carboxylic acids, esters, ethers. The following frequency ranges from 1300–1150 cm⁻¹, are assigned to the C–H wag (–CH₂X) stretching presence of alkyl halides, the peak range 1250–1020 cm⁻¹ present in C–N stretching, presence of aliphatic amines, the peak value representing 910–665 cm⁻¹ appears in N–H symmetric stretching vibration primary, secondary amines. The frequency ranges from 700-610 cm⁻¹ peaks represent the –C (triple bond) C–H: C–H bend stretching vibration of alkynes components. The frequency ranges from 690–515 cm⁻¹ peaks characterize C–Br stretching vibration presence of alkyl halides compounds [10]. However, their tiny differences make it difficult to identify unambiguously them by utilizing the conventional FT-IR technique only. So, depending on the fingerprint characters of the peaks positions, shapes and intensities, the fundamental components indwell in the materials can be seen clearly [1].

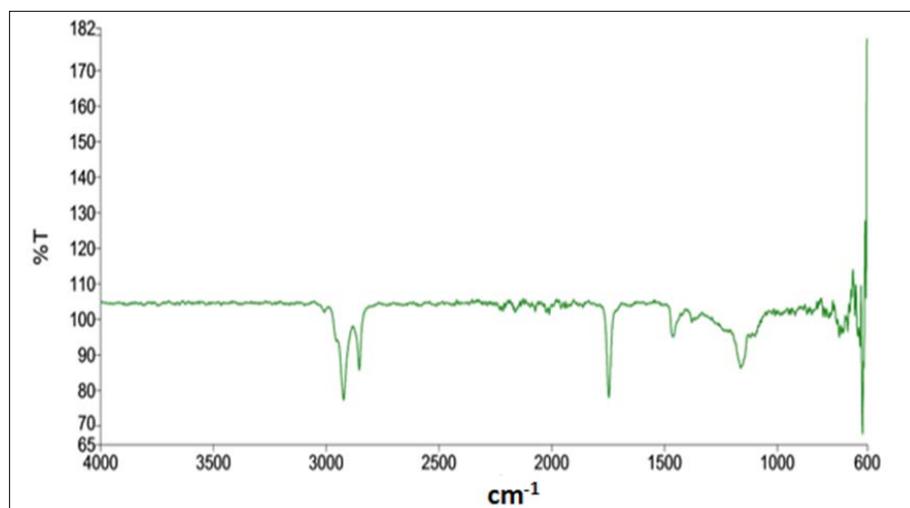


Fig 1: IR peaks of *Tabebuia rosea* seed oil

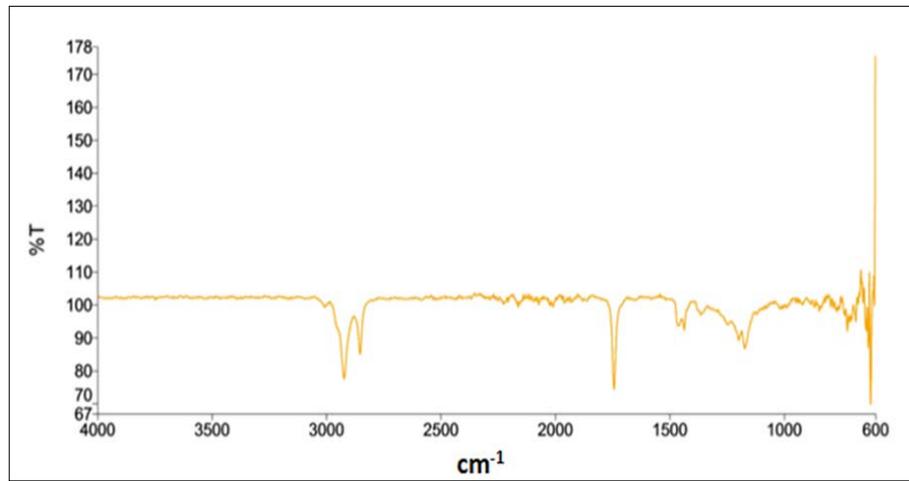


Fig 2: IR peaks of Tome

Table 1: IR peaks obtained for the oil sample

Peak	X(cm ⁻¹)	Y(%T)	Peak	X(cm ⁻¹)	Y(%T)	Peak	X(cm ⁻¹)	Y(%T)	Peak	X(cm ⁻¹)	Y(%T)
1	2924.3	76.56	2	2854.48	84.6	3	2215.5	100.25	4	2162.53	99.91
5	2073.14	100	6	2010.17	99.33	7	1958.53	100.88	8	1746	77.28
9	1462.26	93.44	10	1377.58	97.25	11	1161.71	85.12	12	844.43	99.2
13	794.11	98.8	14	782.91	98.64	15	768.42	98.39	16	722.2	93.35
17	710.87	94.22	18	685.12	94.83	19	653.32	99.01	20	640.82	93.57
21	629.61	90.71	22	619.41	67.58	23	603.44	103.61			

Table 2: Assessment of spectral range of FT IR to functional groups of *T. rosea* Oil

Sl. No	Range(cm ⁻¹)	Functional group
1.	2946–2881	–C–H (CH ₂)
2.	2881–2782	–C–H (CH ₂)
3.	2260–2100	–C(triple bond)C–, presence of alkynes
4.	1795–1677	–C=O (ester)
5.	1486–1446	–C–H (CH ₂)
6.	1382–1371	–C–H (CH ₃)
7.	1211–1147	–C–O
8.	885–802	=CH ₂
9.	802–754	–C–H
10.	754–701	–(CH ₂) _n –, –HC=CH– (cis)
11.	700–610	–C(triple bond)C–H: C–H, presence of alkynes
12.	709	C–H
13.	690–515	C–Br, presence of alkyl halides

Table 3: IR peaks obtained for the TOME sample

Peak	X(cm ⁻¹)	Y(%T)	Peak	X(cm ⁻¹)	Y(%T)	Peak	X(cm ⁻¹)	Y(%T)	Peak	X(cm ⁻¹)	Y(%T)
1	2924.58	77.4	2	2854.47	85.03	3	2226.96	100.2	4	2162.56	99.44
5	2072.65	100.08	6	2009.75	99.4	7	1959.59	100.52	8	742.85	74.32
9	1462.5	93.59	10	1435.93	92.41	11	1363.47	96.86	12	1197.81	89.23
13	1171.03	86.68	14	1007.23	98.64	15	918.77	100.02	16	865.81	99.21
17	844.89	98.05	18	794.23	99.42	19	768.11	97.93	20	721.87	92.06
21	711	94.75	22	685.12	94.95	23	653.27	100.7	24	639.05	92.12
25	630.4	86.93	26	620.43	69.6	27	603.57	99.79			

Table 4: Assessment of spectral range of FT IR to functional groups of TOME

Sl. No	Range(cm ⁻¹)	Functional group
1.	1446–1425	–C–H (CH ₃)
2.	1043–1006	–C–O
3.	929–885	–HC=CH– (cis)

Conclusion

Based on the systematically analysis of *Tabebuia rosea* seed oil and *Tabebuia rosea* oil methyl esters (TOME) contains important phytochemicals like reducing sugar, flavonoids, glycosides, tannins and terpenoid, which may contribute to its biological activities. The present results clearly indicate that

Tabebuia rosea seed extracts possess significant phenolic acids and therefore capable of antioxidant activities like synthetic drug ascorbate. FT-IR spectroscopy of the *Tabebuia rosea* seed oil reveals diverse functional groups and there by confirm the possible potential antioxidant activity and free radical scavenging properties.

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