

FTIR SPECTROSCOPIC STUDIES ON *AERVA LANATA* (L.) JUSS. EX SCHULT.YAMUNADEVI MARISWAMY<sup>1</sup>, WESELY EDWARD GNANARAJ<sup>2</sup>, JOHNSON MARIMUTHU@ANTONISAMY<sup>3\*</sup>

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## ABSTRACT

Aim: The present study was aimed to identify the functional groups present in the crude powder of *Aerva lanata* (L.) Juss. ex Schult. stem, leaves, root and flower through FT-IR spectroscopy. Methods: FTIR method was performed on a Thermo Scientific Spectrophotometer system which was used to detect the characteristic peak values and their functional groups. Results: The results of *A. lanata* flower FTIR analysis confirmed the presence of amide, alcohols, phenols, alkanes, carboxylic acids, aldehydes, ketones, alkenes, primary amines, aromatics, esters, ethers, alkyl halides and aliphatic amines compounds which shows major peaks at 3675.36, 3618.49, 3587.12, 2918.08, 2849.76, 1771.81, 1733.59, 1652.96, 1636.03, 1457.06, 1318.57, 1243.66, 1053.77 and 510.63 respectively. The leaves of *A. lanata* FTIR analysis results proved the presence of alcohols, phenols, alkanes, carboxylic acids, aldehydes, alkenes, nitro compounds, alcohols, carboxylic acids, esters, ethers, aliphatic amines and alkyl halides compounds. The FTIR analysis results of *A. lanata* root revealed the presence of amines, amides, alkanes, aldehydes, ketones, esters, carboxylic acids, carbonyls, alkenes, primary amines, nitro compounds, aromatics, alcohols, esters, ethers and alkyl halides compounds. The FTIR analysis results of *A. lanata* stem validated the presence of amide, alcohols, phenols, amines, alkanes, ketones, primary amines, nitro compounds, alcohols, carboxylic acids, esters, ethers, alkyl halides and aliphatic amines. The FTIR spectroscopic studies revealed the different characteristic peak values with various functional compounds. Conclusion: The results of the present study generated the FTIR spectrum profile for the medicinally important plant *A. lanata* and can be used to identify the plant in the pharmaceutical industry.

**Key words:** *Aerva lanata*, FTIR, Spectroscopy, Functional groups

## INTRODUCTION

Chemotaxonomy has strongly inclined the entire field of biology, which is also useful for plant systematics. Fourier Transform Infrared (FTIR) Spectroscopy is a rapid, noninvasive, high-resolution analytical tool for identifying types of chemical bonds in a molecule by producing an infrared absorption spectrum that is like a molecular fingerprint<sup>1</sup>. FTIR has been shown to be a valuable tool for differentiating, classifying and discriminating closely related microbial strains, plants and other organisms<sup>2-13</sup>. It is one of the most widely used methods to identify the chemical constituents and elucidate the structural compounds and has been used as a requisite method to identify medicines in Pharmacopoeia of many countries. However, some adulterants come out in the medicinal market along with the high value medicinal materials. At present, the chromatography is the main tool used to identify the adulterants from the medicinal materials and extract products based on the chemical profile. It is well known that the medicinal materials comprise hundreds of components, and produce their curative effects through mutual effects of many ingredients, so the limited numbers of specific components cannot availablely reflect the real qualities of the herbal medicines. Therefore, an effective and inexpensive analysis method to entirely monitor the whole constituents of the medicinal materials and their corresponding extract products is required<sup>14</sup>. FT-IR has played a vital role in pharmaceutical analysis in recent years<sup>15, 16</sup>. FT-IR spectroscopy is a physico-chemical analytical technique that does not determine concentrations of individual metabolites but provides a snapshot of the metabolic composition of a tissue at a given time<sup>1</sup>. The FT-IR method measures predominantly the vibrations of bonds within chemical functional groups and generates a spectrum that can be regarded as a biochemical or metabolic "fingerprint" of the sample.

*Aerva lanata* (L.) Juss. ex Schult. is an important medicinal plant, found throughout tropical India as a common weed in fields and wasteland<sup>17</sup>. Even now, wild collection of the species continues to be a source of raw drug in Ayurvedic preparations. Because of its popularity in folk medicine, *A. lanata* has become the subject of intense pharmacological and chemical studies for the last 30 years. Numerous studies have proven its versatile pharmacological activities: anthelmintic, demulcent, anti-inflammatory, diuretic, expectorant, hepatoprotective<sup>18</sup>, nephroprotective<sup>19</sup>, anti-diabetic activity, anti-hyperglycaemic activity in rats<sup>20</sup>, anti-microbial, cytotoxic, urolithiatic, hypoglycemic, anti-hyperlipidaemic<sup>21</sup>, anti-parasitic and anti-helminthic activities<sup>22</sup>. In order to identify the

bioactive compounds responsible for the above pharmacological activities, phytochemical studies have been carried out by several workers with the report of different kinds of bioactive compounds particularly alkaloids such as Canthin-6-one and beta-carboline, aervine [10-hydroxycanthin-6-one], methylaervine [10-methoxycanthin-6-one], aervoside [10-β-Dglucopyranosyloxycanthin-6-one] and aervolanine [3-(6-methoxy-β-carboline-1-yl)propionic acid] from leaves of *Aerva lanata*.

The main limitation in the use of traditional remedies is the lack of standardization of raw material, manufacturing process and the final product. A biomarker on the other hand is a group of chemical compounds which are in addition to being unique for that plant material also correlates with biological efficacy. So the need arises to lay standards by which the right material could be selected and incorporated into the formulation. A detailed exo-morphology, histo-morphology and physicochemical studies on the leaf and stem and micro-morphological studies of *A. lanata* have been carried out<sup>23</sup>. However, more work needs to be undertaken to fully characterize these compounds, to identify the active molecules with bioactive roles. To fulfill the requirement, the present study was intended to resolve the functional constituents present in the stem, leaves, root and flower of *Aerva lanata* L which will be useful for the proper identification of the active compounds and the chemical profile will be used as a pharmacognostic marker to differentiate the adulterant from the commercial samples. Applying metabolomic techniques to pharmacognosy as a marker is a new approach, generally used to identify as functional groups. With this knowledge the present study was aimed to identify the functional groups present in crude powder of *Aerva lanata* stem, leaves, root and flower through FT-IR spectroscopy.

## MATERIALS AND METHODS

## Collection and processing of plant material

*Aerva lanata* (L.) Juss. ex Schult. was collected by handpicking from the natural habitats of Coimbatore district, Tamil Nadu, India authenticated by Dr. E.G. Wesely and the voucher specimens were deposited in the St. Xavier's College Herbarium (XCH 28077) for further reference. The whole plant samples were washed thoroughly in running tap water to remove soil particles and adhered debris followed by sterile distilled water. The washed plants were blotted

on the blotting paper and spread out at room temperature in shade. Shade dried samples were grounded to fine powder using tissue blender. The powdered samples were then stored in a refrigerator for further use.

#### FTIR SPECTROSCOPIC ANALYSIS

All spectra were obtained with the aid of an OMNI-sampler attenuated total reflectance (ATR) accessory on a Nicolet FTIR spectrophotometer (Thermoscientific Nicolet is10, USA) followed by previous methods with some modifications<sup>10,14</sup>. A small amount of powdered leaves was respectively placed directly on the germanium piece of the infrared spectrometer with constant pressure applied and data of infrared absorbance, collected over the wave number ranged from 4000 cm<sup>-1</sup> to 675 cm<sup>-1</sup> and computerized for analyses by using the Omnic software (version 5.2). The reference spectra were acquired from the cleaned blank crystal prior to the presentation of each sample replicate. All spectra were collected with a resolution of 4-1 cm and to improve the signal-to-noise ratio, 256 scans were co-added and averaged. Samples were run in triplicate and all of them were undertaken within a day period.

#### RESULTS AND DISCUSSION

The FTIR spectrum was used to identify the functional group of the active components based on the peak value in the region of infrared radiation. The leaves powder of *A. lanata* was passed into the FTIR and the functional groups of the components were separated based on its peak ratio. The results of *A. lanata* flower FTIR analysis confirmed the presence of amide, alcohols, phenols, alkanes, carboxylic acids, aldehydes, ketones, alkenes, primary amines, aromatics, esters, ethers, alkyl halides and aliphatic amines compounds which shows major peaks at 3675.36, 3618.49, 3587.12, 2918.08, 2849.76, 1771.81, 1733.59, 1652.96, 1636.03, 1457.06, 1318.57, 1243.66, 1053.77 and 510.63 respectively (Fig-1A; Table-1). The leaves of *A. lanata* FTIR analysis results proved the presence of alcohols, phenols, alkanes, carboxylic acids, aldehydes, alkenes, nitro compounds, alcohols, carboxylic acids, esters, ethers, aliphatic amines and alkyl halides compounds (Fig-1B; Table-2). The FTIR analysis results of *A. lanata* root revealed the presence of amines, amides, alkanes, aldehydes, ketones, esters, carboxylic acids, carbonyls, alkenes, primary amines, nitro compounds, aromatics, alcohols, esters, ethers and alkyl halides compounds (Fig-1C; Table-3). The FTIR analysis results of *A. lanata* stem validated the presence of amide, alcohols, phenols, amines, alkanes, ketones, primary amines, nitro compounds, alcohols, carboxylic acids, esters, ethers, alkyl halides and aliphatic amines (Fig-1D; Table-4).

Table - 1: FTIR Peak Values of *Aerva lanata* Flower

FLOWER AB WITH VALUE		FLOWER TR WITH VALUE	
Peak values	Functional group	Peak values	Functional group
3852.01	Unknown	3852.01	Unknown
3734.32	Unknown	3819.86	Unknown
2917.09	Alkanes	3800.19	Unknown
2849.57	Carboxylic acids	3734.32	Unknown
2361.45	Unknown	3647.99	Amide
1732.83	Ketones	2917.09	Alkanes
1652.18	Alkenes	2849.57	Carboxylic acids
1372.88	Unknown	2361.45	Unknown
1243.66	Alkyl halides	1732.83	Ketones
1052.85	Aliphatic amines	1652.18	Alkenes
502.76	Alkyl halides	1506.18	Nitro compounds
475.77	Unknown	1372.88	Unknown
467.43	Unknown	1243.66	Alkyl halides
452.89	Unknown	1052.85	Aliphatic amines
		502.76	Alkyl halides
		486.59	Alkyl halides
		475.77	Unknown
		467.43	Unknown
		452.89	Unknown

Table - 2: FTIR Peak Values of *Aerva lanata* Leaves

LEAF AB WITH VALUE		LEAF TR WITH VALUE	
Peak values	Functional group	Peak values	Functional group
3891.43	Unknown	3903.12	Unknown
3881.26	Unknown	3881.26	Unknown
3820.59	Unknown	3701.43	Unknown
3701.43	Unknown	3628.57	Alcohols, phenols
3628.57	Alcohols, phenols	3618.49	Alcohols, phenols
3618.49	Alcohols, phenols	3587.12	Unknown
3587.12	Unknown	3566.55	Unknown
3566.55	Unknown	3545.36	Unknown
3545.36	Unknown	3392.46	Amines, amides
2917.66	Alkanes	2917.66	Alkanes
2849.76	Carboxylic acids	2849.76	Carboxylic acids
2360.84	Unknown	2360.84	Unknown
1733.68	Aldehydes	2343.20	Unknown
1652.96	Alkenes	1733.68	Aldehydes
1558.73	Unknown	1716.99	Esters
1540.76	Nitro compounds	1652.96	Alkenes
1374.18	Unknown	1558.73	Unknown
1319.44	Alcohols, carboxylic acids, esters, ethers	1540.76	Nitro compounds
1049.64	Aliphatic amines	1374.18	Unknown
467.38	Unknown	1319.44	Alcohols, carboxylic acids, esters, ethers
443.36	Unknown	1049.64	Aliphatic amines
		502.57	Alkyl halides
		467.38	Unknown
		443.36	Unknown

Table - 3: FTIR Peak Values of *Aerva lanata* Root

ROOT AB WITH VA		ROOT TR WITH VALUE	
Peak values	Functional group	Peak values	Functional group
3789.14	Unknown	3948.48	Unknown
3758.35	Unknown	3820.56	Unknown
3502.57	Amide	3502.57	Amide
3336.52	Amines, amides	3336.52	Amines, amides
2917.24	Alkanes	2917.24	Alkanes
2359.83	Unknown	2359.83	Unknown
2343.06	Unknown	2343.06	Unknown
1868.33	Unknown	1868.33	Unknown
1844.18	Unknown	1844.18	Unknown
1791.99	Unknown	1791.99	Unknown
1771.81	Aldehydes	1771.81	Aldehydes
1733.59	Ketones	1733.59	Ketones
1716.04	Esters	1716.04	Esters
1698.87	Carboxylic acids	1698.87	Carboxylic acids
1683.69	Carbonyls	1683.69	Carbonyls
1652.93	Alkenes	1652.93	Alkenes
1646.74	Primary amines	1646.74	Primary amines
1635.86	Primary amines	1635.86	Primary amines
1558.67	Unknown	1521.46	Nitro compounds
1489.35	Aromatics	1472.61	Aromatics
1472.61	Aromatics	1457.06	Aromatics
1457.06	Aromatics	1418.50	Aromatics
1418.50	Aromatics	1374.09	Unknown
1374.09	Unknown	1318.57	Alcohols, carboxylic acids, esters, ethers
1318.57	Alcohols, carboxylic acids, esters, ethers	1032.23	Aliphatic amines
1032.23	Aliphatic amines	510.63	Alkyl halides
510.63	Alkyl halides	502.64	Alkyl halides
502.64	Alkyl halides	487.01	Alkyl halides
475.46	Unknown	475.46	Unknown
467.43	Unknown	467.43	Unknown
452.72	Unknown	452.72	Unknown
437.78	Unknown	437.78	Unknown
432.32	Unknown	432.32	Unknown
425.87	Unknown	425.87	Unknown

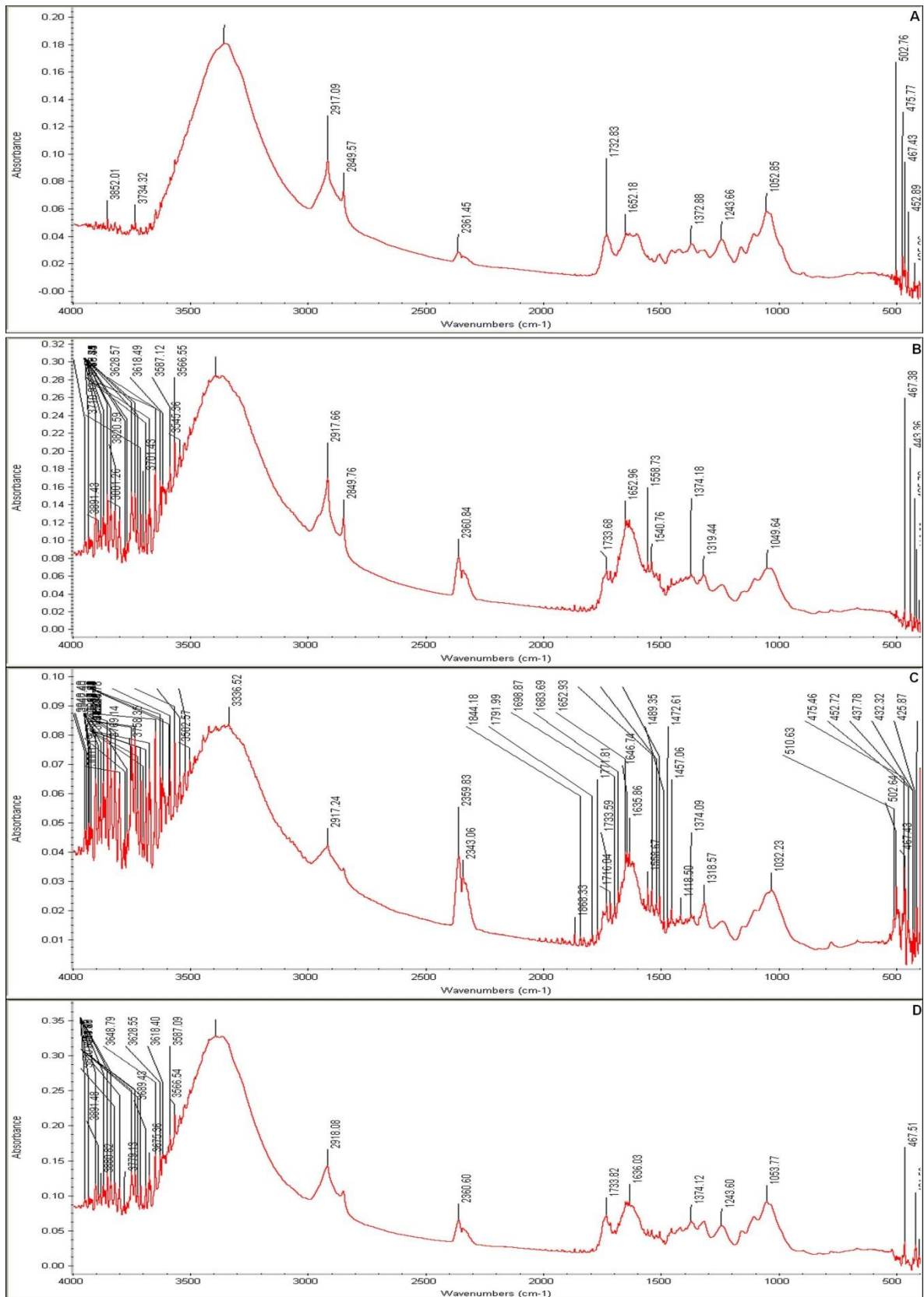


Fig. 1. FTIR Spectrum of *Aerva lanata* (L.) Juss. ex Schult.

- A. FTIR Spectrum of *A. lanata* – Flower
- B. FTIR Spectrum of *A. lanata* – Leaves
- C. FTIR Spectrum of *A. lanata* – Root
- D. FTIR Spectrum of *A. lanata* – Stem

Table - 4: FTIR Peak Values of *Aerva lanata* Stem

STEM AB WITH VALUE		STEM TR WITH VALUE	
Peak values	Functional group	Peak values	Functional group
3891.48	Unknown	3948.55	Unknown
3880.82	Unknown	3903.12	Unknown
3770.13	Unknown	3820.62	Unknown
3689.43	Amide	3801.27	Unknown
3675.36	Amide	3724.68	Unknown
3648.79	Amide	3710.89	Unknown
3628.55	Alcohols, phenols	3648.79	Amide
3618.40	Alcohols, phenols	3628.55	Alcohols, phenols
3587.09	Unknown	3618.40	Alcohols, phenols
3566.54	Unknown	3587.09	Unknown
2918.08	Alkanes	3392.60	Amines, amides
2360.60	Unknown	2918.09	Alkanes
1733.82	Ketones	1733.82	Ketones
1636.03	Primary amines	1636.03	Primary amines
1374.12	Unknown	1507.24	Nitro compounds
1243.60	Alkyl halides	1374.12	Unknown
1053.77	Aliphatic amines	1319.56	Alcohols, carboxylic acids, esters, ethers
467.51	Unknown	1243.60	Alkyl halides
		1053.76	Aliphatic amines
		467.51	Unknown

The crude powder subjected to FTIR analysis is used for the identification of functional constituents present in *A. lanata*. The FTIR analysis revealed the similarity and variation between the various parts of *A. lanata* based on the functional group presence and absorption spectrum. From the spectra 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.

Spectral differences are the objective reflection of componential differences. By using the macroscopic fingerprint characters of FT-IR spectrum, we can judge the origin of different extracts accurately and effectively, trace the constituents in the extracts, identify the medicinal materials true or false and even evaluate the qualities of medicinal materials. So, FT-IR spectrum reflecting objectively the panorama of chemical constituents in complex system is a most credible method to validate and identify the mix-substance systems such as traditional medicine and herbal medicine<sup>14</sup>. The results of the present study spectrum also revealed the functional constituents present in the crude powder of *A. lanata*. Many workers applied the FTIR spectrum as a tool for differentiating, classifying and discriminating closely related plants and other organisms<sup>2-15</sup>. The results of the present study also supplemented the previous observations and provided the similarity and variation in functional groups at parts (leaves, stem, root and flower) level also. Therefore, the present work on *A. lanata* displayed novel phytochemical markers as useful analytical tool to check not only the quality of the powder but also to identify the medicinally important plant. Further advanced spectroscopic studies are required for the structural elucidation and identification of compounds.

## CONCLUSION

The results of the present study confirmed that *A. lanata* may be wealthy resource of phyto-constituents which can be isolated and examined for bio-efficacies and pharmacological activities.

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