

THE FT-IR SPECTROMETRIC STUDIES OF VIBRATIONAL BANDS OF *SEMECARPUS ANACARDIUM* LINN.F. LEAF, STEM POWDER AND EXTRACTS

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ABSTRACT

The present study was aimed to identify the functional groups present in the crude powder and extracts of *Semecarpus anacardium* Linn.f. leaves and stem through FT-IR spectrometry. 14 different polar and nonpolar organic solvents were used in the soxhlet extraction of the plant material. All the vibrational bands originated from different groups like C-H, C=C, C≡C, C-O, C=O, C-I, C-Cl, C-Br, C-F, >CH₂, C-N, C=C-C, S-S, N-H, NO₂, H-X, O-H, P-O-C etc., and may be termed as key bands and can be studied for their absorption characteristics to differentiate individual plant parts like leaves, stem etc. The FT-IR analysis of leaf powder of *Semecarpus anacardium* proved the presence of alcohols, phenols, alkanes, alkenes, carboxylic acids, ethers, esters, aliphatic iodo compounds and polysulfides. The FT-IR analysis results of stem powder of *Semecarpus anacardium* revealed the presence of alcohols, phenols, alkanes, alkenes, amines, amides, aldehydes, ketones, esters, ethers carboxylic acids, nitro compounds, aliphatic iodo compounds. The FT-IR studies revealed the different characteristic peak values with various functional groups. The results of the present study generated the FT-IR spectrum profile for the medicinally important plant *Semecarpus anacardium* and can be used to identify the plant in the pharmaceutical industry.

Keywords: *Semecarpus anacardium* Linn.f., FT-IR spectrometry, functional groups.

INTRODUCTION

Fourier transform infrared spectrometry (FT-IR) is one of the most widely used methods to identify the chemical constituents and elucidate the structures of compounds and has been used as a requisite method to identify medicines in Pharmacopoeia of many countries. FT-IR has played a vital role in pharmaceutical analysis in recent years¹. FT-IR spectrometry 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 time². 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 sample³. Infrared spectroscopy provides a useful method for herbal analysis as well as for quantitative analysis of drugs and with the help of FT-IR continuous monitoring of the spectral baseline and simultaneous analysis of different components of the same sample is possible⁴⁻⁶. Applying metabolomic techniques to pharmacognosy as a marker is a new approach, generally used to identify the functional groups⁷.

Semecarpus anacardium Linn.f. (Family- Anacardiaceae) commonly known as Bhallataka or marking nut is used in indigenous systems of medicine for the treatment of various diseases^{8,9}. It is a deciduous tree distributed in the sub-Himalayan tract and in tropical parts of India. Many compounds mainly biflavonoids, phenolics, bhilawanols, sterols, anacardic acid and glycosides have been identified as constituents of *Semecarpus anacardium* nut extract. On the basis of chemical and spectral data, several biflavonoids such as jeediflavanone, galluflavanone, nallaflavanone, semecarpetin and anacarduflavanone have been characterized¹⁰. Several monophenolic compounds known as semecarpol and bhilawanol were also isolated¹¹. Further analysis revealed the presence of iron, copper, sodium, calcium and aluminium in traces¹² and also the plant is good source of minerals like sulphur, magnesium, phosphorus¹³.

The present study was intended to resolve the functional constituents present in the leaves and stem of *Semecarpus anacardium* which will be useful for the proper identification of the active compounds and the chemical profiles will be used as a pharmacognostic marker to differentiate the adulterant from the commercial samples.

MATERIALS AND METHODS

Plant collection and authentication

The leaves and stem of *Semecarpus anacardium* were collected from an open field around Mumbai, Maharashtra. The identification of the

plant was done at the Blatter Herbarium, St. Xavier's College, Mumbai. The plant specimen matches with the Blatter Herbarium specimen no.T-472 of S. C. Tavakari. Leaves were shade dried and made into coarse powder with mechanical grinder and then passed through sieve, B.S.S Mesh No.60.

Apparatus

Bruker Alpha-T FTIR equipped with universal sampling module, equipped with a room temperature DTGS detector. The scan range was taken from 400 to 4000 cm⁻¹ with a resolution of 4 cm⁻¹.

Chemicals

Chloroform, Toluene, Carbon tetrachloride, Ethyl acetate, Hexane, Ethyl alcohol, Methanol, Acetone, 2-propanol, Petroleum ether (60-80°C), 2-butanone, Dichloromethane, Ethyl ether were all A.R. grade (Merck, India), Distilled water.

Preparation of the plant extract

The leaf powder of *Semecarpus anacardium* (20 gms) was extracted with 250 ml each of polar and nonpolar solvents by soxhlet extraction for 8 hrs. The extracts obtained were later kept for evaporation to remove the excess solvents. These extracts were then stored in plastic bottles in refrigerator for FT-IR analysis. Powdered leaf material was extracted using water, chloroform, toluene, carbon tetrachloride, ethyl acetate, hexane, ethyl alcohol, methanol, acetone, 2-propanol, petroleum ether (60-80°C), 2-butanone, dichloromethane, ethyl ether. The crude powder and dried extracts were mixed with KBr salt using mortar and pestle and compressed into a thin pellet.

RESULTS AND DISCUSSION

The FT-IR spectrum was used to identify the functional groups of the active components based on the peak value in the region of infrared radiation. The leaf and stem powder and extracts of *Semecarpus anacardium* were analysed by the FT-IR spectrometers and the functional groups of the components were separated based on its peak ratio. The FT-IR analysis of leaf powder and different leaf extracts of *Semecarpus anacardium* proved the presence of alcohols, phenols, alkanes, alkenes, carboxylic acids, ethers, esters, polysulfides and aliphatic iodo compounds etc., [Table 1-15, Fig 1-15]. The FT-IR analysis results of stem powder and stem extracts of *Semecarpus anacardium* revealed the presence of alcohols, phenols,

alkanes, alkenes, amines, amides, aldehydes, ketones, esters, ethers [Table 16-18, Fig 16-18].
 carboxylic acids, nitro compounds, aliphatic iodo compounds etc.,

Table 1: FT-IR Peak Values of *Semecarpus anacardium* Leaf Powder

| Wave number cm ⁻¹ | Bond | Functional Group Assignment | Group Frequency, cm ⁻¹ |
|------------------------------|-------------|--|-----------------------------------|
| 3310.05 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 |
| 2919.69 | C-H | Alkanes | 2850-2970 |
| 1616.85 | C=C | Alkenes | 1610-1680 |
| 1449.51 | C-H | Alkanes | 1340-1470 |
| 1102.52 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 534.25 | C-I stretch | Aliphatic iodo compounds | 500-600 |
| 472.39 | S-S stretch | Polysulfides | 470-500 |

Table 2: FT-IR Peak Values of *Semecarpus anacardium* Water Leaf Extract

| Wave number cm ⁻¹ | Bond | Functional Group Assignment | Group Frequency, cm ⁻¹ |
|------------------------------|------------------|-------------------------------------|-----------------------------------|
| 3432.66 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 |
| 2090.52 | Carbonyl stretch | Transition metal carbonyl compounds | 1800-2100 |
| 1645.21 | C=C | Alkenes | 1610-1680 |

Table 3: FT-IR Peak Values of *Semecarpus anacardium* Chloroform Leaf Extract

| Wave number cm ⁻¹ | Bond | Functional Group Assignment | Group Frequency, cm ⁻¹ | Wave number cm ⁻¹ | Bond | Functional Group Assignment | Group Frequency, cm ⁻¹ |
|------------------------------|------|-----------------------------------|-----------------------------------|------------------------------|-----------------|--|-----------------------------------|
| 3817.83 | - | Unknown | - | 1718.36 | C=O | Aldehydes, Ketones, Carboxylic acids, Esters | 1690-1760 |
| 3733.70 | - | Unknown | - | 1421.28 | C-H | Alkanes | 1340-1470 |
| 3584.20 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 | 1363.89 | NO ₂ | Nitro compounds | 1300-1370 |
| 3524.53 | O-H | Monomeric Carboxylic acids | 3500-3650 | 1222.85 | C-N | Amines, Amides | 1180-1360 |
| 3413.62 | N-H | Amines, Amides | 3300-3500 | 1092.80 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 3004.74 | H-C | Aromatic H-X group | 3000- 3050 | 953.73 | C-H | Alkenes | 675-995 |
| 2969.80 | C-H | Alkanes | 2850-2970 | 903.19 | C-H | Alkenes | 675-995 |
| 2925.15 | C-H | Alkanes | 2850-2970 | 773.00 | C-Cl stretch | Aliphatic chloro compounds | 700-800 |
| 2145.11 | C≡C | Alkynes | 2100-2260 | 529.91 | C-I | Aliphatic iodo compounds | 500-600 |

Table 4: FT-IR Peak Values of *Semecarpus anacardium* Toluene Leaf Extract

| Wave number cm ⁻¹ | Bond | Functional Group Assignment | Group Frequency, cm ⁻¹ |
|------------------------------|-----------------|--|-----------------------------------|
| 3839.61 | - | Unknown | - |
| 3649.93 | O-H | Monomeric Carboxylic acids | 3500-3650 |
| 2918.66 | C-H | Alkanes | 2850-2970 |
| 2364.60 | - | Unknown | - |
| 1726.17 | C=O | Aldehydes, Ketones, Carboxylic acids, Esters | 1690-1760 |
| 1315.02 | NO ₂ | Nitro compounds | 1300-1370 |
| 1188.34 | C-N stretch | Secondary amine | 1130-1190 |
| 970.09 | C-H | Alkenes | 675-995 |
| 472.00 | S-S stretch | Polysulfides | 470-500 |

Table 5: FT-IR Peak Values of *Semecarpus anacardium* CCl₄ Leaf Extract

| Wave number cm ⁻¹ | Bond | Functional Group Assignment | Group Frequency, cm ⁻¹ | Wave number cm ⁻¹ | Bond | Functional Group Assignment | Group Frequency, cm ⁻¹ |
|------------------------------|-----------------|--|-----------------------------------|------------------------------|-------------|-----------------------------|-----------------------------------|
| 3439.44 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 | 970.81 | C-H | Alkenes | 675-995 |
| 2954.89 | C-H | Alkanes | 2850-2970 | 894.07 | C-H | Alkenes | 675-995 |
| 2917.37 | C-H | Alkanes | 2850-2970 | 829.73 | C-H | Alkenes | 675-995 |
| 2849.26 | C-H | Alkanes | 2850-2970 | 729.82 | C-H | Aromatic rings | 690-900 |
| 2329.08 | - | Unknown | - | 719.51 | C-H | Aromatic rings | 690-900 |
| 1736.08 | C=O | Aldehydes, Ketones, Carboxylic acids, Esters | 1690-1760 | 646.63 | C-Br | Aliphatic bromo compounds | 600-700 |
| 1541.19 | NO ₂ | Nitro compounds | 1500-1570 | 605.98 | C-Br | Aliphatic bromo compounds | 600-700 |
| 1494.30 | C=C-C | Aromatic ring Aryl Stretch | 1510-1450 | 578.55 | C-I stretch | Aliphatic iodo compounds | 500-600 |
| 1462.86 | C-H | Alkanes | 1340-1470 | 515.61 | C-I stretch | Aliphatic iodo compounds | 500-600 |
| 1377.66 | C-H | Alkanes | 1340-1470 | 493.23 | S-S stretch | Polysulfides | 470-500 |
| 1363.92 | NO ₂ | Nitro compounds | 1300-1370 | 483.02 | S-S stretch | Polysulfides | 470-500 |
| 1275.76 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050- 1300 | 473.97 | S-S stretch | Polysulfides | 470-500 |

| | | | | | | | |
|----------------|----------------|---|------------|---------------|----------------|-----------------|---------|
| 1247.76 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050- 1300 | 464.05 | S-S stretch | Aryl disulfides | 430-500 |
| 1187.96 | C-N | Amines, Amides | 1180-1360 | 454.10 | S-S stretch | Aryl disulfides | 430-500 |
| 1081.51 | C-O stretch | Alcohols, Ethers, Carboxylic acids, Esters | 1050- 1300 | - | - | - | - |

Table 6: FT-IR Peak Values of *Semecarpus anacardium* Ethyl acetate Leaf Extract

| Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} | Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} |
|------------------------------|---------------------|---|-----------------------------------|------------------------------|-----------------|---|-----------------------------------|
| 3630.55 | O-H | Monomeric Alcohols, Phenols | 3590-3650 | 1555.18 | C=C | Aromatic rings | 1500-1600 |
| 3548.02 | O-H | Monomeric Carboxylic acids | 3500-3650 | 1465.86 | C-H | Alkanes | 1340-1470 |
| 3464.77 | N-H | Amines, Amides | 3300-3500 | 1447.87 | C-H | Alkanes | 1340-1470 |
| 2985.53 | H-O | H-bonded H-X group | 2500-3500 | 1373.22 | C-H | Alkanes | 1340-1470 |
| 2942.10 | C-H | Alkanes | 2850-2970 | 1300.66 | NO ₂ | Nitro compounds | 1300-1370 |
| 2909.19 | C-H | Alkanes | 2850-2970 | 1240.00 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2878.16 | C-H | Alkanes | 2850-2970 | 1160.39 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2674.36 | O-H | Hydrogen bonded Carboxylic acids | 2500-2700 | 1098.11 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2473.39 | - | Unknown | - | 1047.65 | C-N stretch | Primary amines | 1020-1090 |
| 2307.39 | - | Unknown | - | 1004.65 | C-F stretch | Aliphatic fluoro compounds | 1000-1150 |
| 2155.10 | C≡C | Alkynes | 2100-2260 | 938.53 | C-H | Alkenes | 675-995 |
| 2086.45 | Carbonyl stretch | Transition metal carbonyl compounds | 1800-2100 | 917.93 | C-H | Alkenes | 675-995 |
| 2009.89 | Carbonyl stretch | Transition metal carbonyl compounds | 1800-2100 | 847.54 | C-H | Aromatic rings | 690-900 |
| 1889.93 | Carbonyl stretch | Transition metal carbonyl compounds | 1800-2100 | 786.62 | C-H | Aromatic rings | 690-900 |
| 1743.93 | C=O | Aldehydes, Ketones, Carboxylic acids, Esters | 1690-1760 | 634.55 | C-Br stretch | Aliphatic bromo compounds | 600-700 |
| 1655.17 | C=C | Alkenes | 1610-1680 | 608.11 | C-Br stretch | Aliphatic bromo compounds | 600-700 |

Table 7: FT-IR Peak Values of *Semecarpus anacardium* Hexane Leaf Extract

| Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} | Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} |
|------------------------------|-----------------|---|-----------------------------------|------------------------------|----------------|--|-----------------------------------|
| 3411.66 | N-H | Amines, Amides | 3300-3500 | 1187.53 | C-N | Amines, Amides | 1180-1360 |
| 2954.63 | C-H | Alkanes | 2850-2970 | 1158.43 | C-O stretch | Alcohols, Ethers, Carboxylic acids, Esters | 1050- 1300 |
| 2924.63 | C-H | Alkanes | 2850-2970 | 1080.94 | C-O stretch | Alcohols, Ethers, Carboxylic acids, Esters | 1050- 1300 |
| 2869.31 | C-H | Alkanes | 2850-2970 | 1026.43 | C-F stretch | Aliphatic fluoro compounds | 1000-1150 |
| 1742.55 | C=O | Aldehydes, Ketones, Carboxylic acids, Esters | 1690-1760 | 967.76 | C-H | Alkenes | 675-995 |
| 1626.28 | C=C | Alkenes | 1610-1680 | 893.83 | C-H | Alkenes | 675-995 |
| 1492.33 | NO ₂ | Aromatic nitro compounds in simple Hetero-oxy compounds | 1485-1555 | 818.51 | C-H | Alkenes | 675-995 |
| 1459.07 | C-H | Alkanes | 1340-1470 | 700.15 | C-H | Aromatic rings | 690-900 |
| 1377.02 | C-H | Alkanes | 1340-1470 | 646.17 | C-Br | Aliphatic bromo compounds | 600-700 |
| 1363.17 | C-H | Alkanes | 1340-1470 | 607.60 | C-Br | Aliphatic bromo compounds | 600-700 |
| 1313.23 | NO ₂ | Nitro Compounds | 1300-1370 | 497.39 | S-S stretch | Polysulfides | 470-500 |
| 1248.70 | C-O stretch | Alcohols, Ethers, Carboxylic acids, Esters | 1050- 1300 | - | - | - | - |

Table 8: FT-IR Peak Values of *Semecarpus anacardium* Ethyl alcohol Leaf extract

| Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} | Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} |
|------------------------------|------------------|-------------------------------------|-----------------------------------|------------------------------|-----------------|--|-----------------------------------|
| 3338.16 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 | 1380.57 | C-H | Alkanes | 1340-1470 |
| 2974.40 | H-O | H- bonded H-X group | 2500-3500 | 1330.73 | NO ₂ | Nitro compounds | 1300-1370 |
| 2927.67 | C-H | Alkanes | 2850-2970 | 1274.67 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2885.41 | C-H | Alkanes | 2850-2970 | 1090.48 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2541.90 | O-H | Hydrogen bonded Carboxylic acids | 2500-2700 | 1050.43 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2256.37 | C≡C | Alkynes | 2100-2260 | 881.27 | C-H | Aromatic rings | 690-900 |
| 1925.32 | Carbonyl stretch | Transition metal carbonyl compounds | 1800-2100 | 803.71 | C-H | Alkenes | 675-995 |
| 1654.85 | C=C | Alkenes | 1610-1680 | 771.19 | C-H | Alkenes | 675-995 |
| 1455.62 | C-H | Alkanes | 1340-1470 | - | - | - | - |
| 1422.86 | C-H | Alkanes | 1340-1470 | - | - | - | - |

Table 9: FT-IR Peak Values of *Semecarpus anacardium* Methanol Leaf Extract

| Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} |
|------------------------------|------------------------------------|--|-----------------------------------|
| 3855.39 | - | Unknown | - |
| 3366.30 | N-H | Amines, Amides | 3300-3500 |
| 2946.08 | C-H | Alkanes | 2850-2970 |
| 2833.75 | C-H stretch | Methoxy, Methyl ether O-CH ₃ | 2850-2815 |
| 2522.92 | O-H | Hydrogen bonded Carboxylic acids | 2500-2700 |
| 2223.33 | C≡C | Alkynes | 2100-2260 |
| 2044.45 | Carbonyl stretch | Transition metal carbonyl compounds | 1800-2100 |
| 1651.62 | C=C | Alkenes | 1610-1680 |
| 1449.68 | C-H | Alkanes | 1340-1470 |
| 1219.47 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 1114.64 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 1031.99 | Methylene >CH ₂ stretch | Cyclohexane ring vibrations | 1000-1055 |

Table 10: FT-IR Peak Values of *Semecarpus anacardium* Acetone Leaf Extract

| Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} |
|------------------------------|------------------------------------|--|-----------------------------------|
| 3421.46 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 |
| 2978.67 | H-O | H- bonded H-X group | 2500-3500 |
| 2103.29 | C≡C | Alkynes | 2100-2260 |
| 1701.17 | C=O | Aldehydes, Ketones, Carboxylic acids, Esters | 1690-1760 |
| 1645.75 | C=C | Alkenes | 1610-1680 |
| 1421.11 | C-H | Alkanes | 1340-1470 |
| 1368.65 | NO ₂ | Nitro compounds | 1300-1370 |
| 1232.40 | C-N | Amines, Amides | 1180-1360 |
| 1163.09 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 1093.66 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 1022.61 | Methylene >CH ₂ stretch | Cyclohexane ring vibrations | 1000-1055 |
| 950.41 | C-H | Alkenes | 675-995 |

Table 11: FT-IR Peak Values of *Semecarpus anacardium* 2-propanol Leaf Extract

| Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} | Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} |
|------------------------------|------------------|----------------------------------|-----------------------------------|------------------------------|-----------------|--|-----------------------------------|
| 3818.10 | - | Unknown | - | 1768.93 | C=O stretch | Open chain Acid anhydrides | 1740-1790 |
| 3798.55 | - | Unknown | - | 1646.13 | C=C | Alkenes | 1610-1680 |
| 3734.19 | - | Unknown | - | 1467.73 | C-H | Alkanes | 1340-1470 |
| 3365.96 | N-H | Amines, Amides | 3300-3500 | 1409.17 | C-H | Alkanes | 1340-1470 |
| 2971.53 | H-O | H- bonded H-X group | 2500-3500 | 1379.58 | C-H | Alkanes | 1340-1470 |
| 2932.69 | C-H | Alkanes | 2850-2970 | 1341.03 | C-H | Alkanes | 1340-1470 |
| 2884.32 | C-H | Alkanes | 2850-2970 | 1309.51 | NO ₂ | Nitro compounds | 1300-1370 |
| 2721.64 | C-H stretch | Aldehyde | 2700-2800 | 1161.90 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2659.32 | O-H | Hydrogen bonded Carboxylic acids | 2500-2700 | 1129.90 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2409.24 | - | Unknown | - | 1110.44 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2195.69 | C≡C | Alkynes | 2100-2260 | 953.02 | C-H | Alkenes | 675-995 |
| 1903.12 | Carbonyl stretch | Transition metal carbonyls | 1800-2100 | 817.31 | C-H | Alkenes | 675-995 |

Table 12: FT-IR Peak Values of *Semecarpus anacardium* Petroleum ether Leaf Extract

| Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} |
|------------------------------|---------------|--|-----------------------------------|
| 3438.97 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 |
| 2917.95 | C-H | Alkanes | 2850-2970 |
| 2849.53 | C-H | Alkanes | 2850-2970 |
| 1737.22 | C=O | Aldehydes, Ketones, Carboxylic acids, Esters | 1690-1760 |
| 1463.08 | C-H | Alkanes | 1340-1470 |
| 1384.31 | NO_2 | Nitro compounds | 1300-1370 |
| 1275.17 | C-N | Amines, Amides | 1180-1360 |
| 1187.83 | C-N | Amines, Amides | 1180-1360 |
| 1081.91 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 971.02 | C-H | Alkenes | 675-995 |
| 894.90 | C-H | Alkenes | 675-995 |
| 473.41 | S-S stretch | Polysulfides | 500-470 |

Table 13: FT-IR Peak Values of *Semecarpus anacardium* 2- butanone Leaf Extract

| Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} | Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} |
|------------------------------|--------------------------|--|-----------------------------------|------------------------------|---------------|--|-----------------------------------|
| 3584.29 | O-H | Monomeric Carboxylic acids | 3500-3650 | 1417.12 | C-H | Alkanes | 1340-1470 |
| 3524.31 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 | 1366.25 | C-H | Alkanes | 1340-1470 |
| 3416.21 | N-H | Amines, Amides | 3300-3500 | 1257.24 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2980.19 | H-O | H-bonded H-X group | 2500-3500 | 1206.41 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2940.34 | C-H | Alkanes | 2850-2970 | 1172.93 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2910.06 | C-H | Alkanes | 2850-2970 | 1086.89 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2883.10 | C-H | Alkanes | 2850-2970 | 996.12 | P-O-C stretch | Aliphatic Phosphates | 990-1050 |
| 2122.95 | $\text{C}\equiv\text{C}$ | Alkynes | 2100-2260 | 945.67 | C-H | Alkenes | 675-995 |
| 1718.83 | C=O | Aldehydes, Ketones, Carboxylic acids, Esters | 1690-1760 | 760.62 | C-H | Aromatic rings | 690-900 |
| 1459.54 | C-H | Alkanes | 1340-1470 | 588.57 | C-I stretch | Aliphatic iodo compounds | 500-600 |

Table 14: FT-IR Peak Values of *Semecarpus anacardium* Dichloromethane Leaf Extract

| Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} |
|------------------------------|------|--|-----------------------------------|
| 3438.08 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 |
| 2923.26 | C-H | Alkanes | 2850-2970 |
| 2852.31 | C-H | Alkanes | 2850-2970 |
| 1736.00 | C=O | Aldehydes, Ketones, Carboxylic acids, Esters | 1690-1760 |
| 1455.92 | C-H | Alkanes | 1340-1470 |
| 1379.03 | C-H | Alkanes | 1340-1470 |
| 1162.94 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 971.96 | C-H | Alkenes | 675-995 |
| 731.50 | C-H | Alkenes | 675-995 |

Table 15: FT-IR Peak Values of *Semecarpus anacardium* Ethyl ether Leaf extract

| Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} |
|------------------------------|---------------|--|-----------------------------------|
| 3332.53 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 |
| 2924.66 | C-H | Alkanes | 2850-2970 |
| 2853.66 | C-H | Alkanes | 2850-2970 |
| 1706.21 | C=O | Aldehydes, Ketones, Carboxylic acids, Esters | 1690-1760 |
| 1616.46 | C=C | Alkenes | 1610-1680 |
| 1511.38 | NO_2 | Nitro compounds | 1500-1570 |
| 1458.58 | C-H | Alkanes | 1340-1470 |
| 1377.60 | C-H | Alkanes | 1340-1470 |
| 1216.68 | C-N | Amines, Amides | 1180-1360 |
| 971.69 | C-H | Alkenes | 675-995 |
| 829.59 | C-H | Alkenes | 675-995 |
| 758.78 | C-H | Alkenes | 675-995 |

Table 16: FT-IR Peak Values of *Semecarpus anacardium* Stem Powder

| Wave number cm^{-1} | Bond | Functional Group Assignment | Group Frequency, cm^{-1} |
|------------------------------|------|--|-----------------------------------|
| 3330.15 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 |
| 2918.66 | C-H | Alkanes | 2850-2970 |
| 1734.07 | C=O | Aldehydes, Ketones, Carboxylic acids, Esters | 1690-1760 |

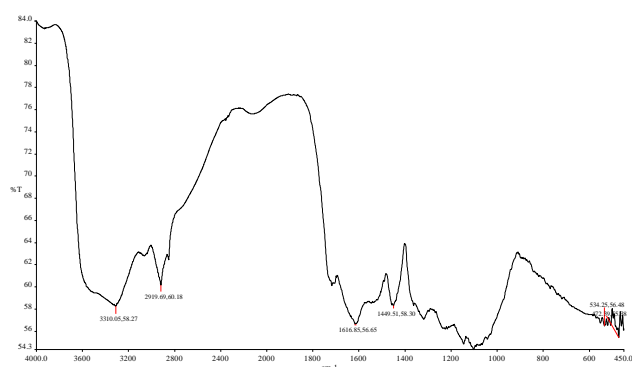
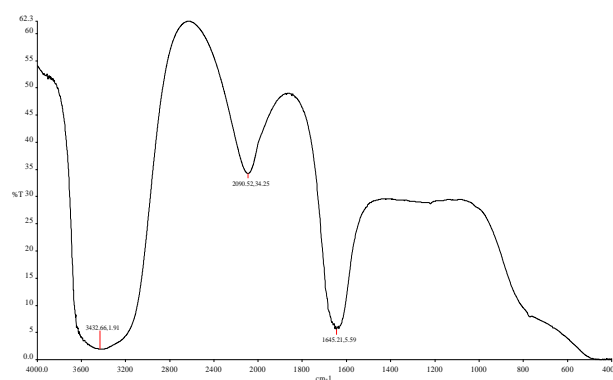
| | | | |
|---------|-----------------|--|-----------|
| 1617.17 | C=C | Alkenes | 1610-1680 |
| 1459.06 | C-H | Alkanes | 1340-1470 |
| 1319.17 | NO ₂ | Nitro Compounds | 1300-1370 |
| 1240.91 | C-N | Amines, Amides | 1180-1360 |
| 1063.94 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 533.90 | C-I stretch | Aliphatic iodo compounds | 500-600 |

Table 17: FT-IR Peak Values of *Semecarpus anacardium* Methanol Stem Bark Extract

| Wave number cm ⁻¹ | Bond | Functional Group Assignment | Group Frequency, cm ⁻¹ |
|------------------------------|------------------------------------|--|-----------------------------------|
| 3857.06 | - | Unknown | - |
| 3366.50 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 |
| 2945.34 | C-H | Alkanes | 2850-2970 |
| 2833.57 | C-H stretch | Methoxy, Methyl ether O-CH ₃ | 2850-2815 |
| 2522.84 | O-H | Hydrogen bonded Carboxylic acids | 2500-2700 |
| 2226.61 | C≡C | Alkynes | 2100-2260 |
| 2044.45 | Carbonyl stretch | Transition metal carbonyl compounds | 1800-2100 |
| 1654.75 | C=C | Alkenes | 1610-1680 |
| 1450.06 | C-H | Alkanes | 1340-1470 |
| 1114.90 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 1032.44 | Methylene >CH ₂ stretch | Cyclohexane ring vibrations | 1000-1055 |

Table 18: FT-IR Peak Values of *Semecarpus anacardium* 2- butanone Stem Bark Extract

| Wave number cm ⁻¹ | Bond | Functional Group Assignment | Group Frequency, cm ⁻¹ | Wave number cm ⁻¹ | Bond | Functional Group Assignment | Group Frequency, cm ⁻¹ |
|------------------------------|------------------|--|-----------------------------------|------------------------------|-----------------|--|-----------------------------------|
| 3529.95 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 | 1459.53 | C-H | Alkanes | 1340-1470 |
| 3416.79 | O-H | Hydrogen bonded Alcohols, Phenols | 3200-3600 | 1416.78 | C-H | Alkanes | 1340-1470 |
| 2980.23 | H-O | H-bonded H-X group | 2500-3500 | 1365.37 | NO ₂ | Nitro compounds | 1300-1370 |
| 2940.51 | C-H | Alkanes | 2850-2970 | 1257.53 | C-N | Amines, Amides | 1180-1360 |
| 2910.07 | C-H | Alkanes | 2850-2970 | 1206.43 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2883.27 | C-H | Alkanes | 2850-2970 | 1172.63 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2830.86 | C-H stretch | Methoxy, Methyl ether O-CH ₃ | 2815-2850 | 1086.89 | C-O | Alcohols, Ethers, Carboxylic acids, Esters | 1050-1300 |
| 2516.77 | O-H | Hydrogen bonded Carboxylic acids | 2500-2700 | 1033.84 | C-N stretch | Primary amine | 1020-1090 |
| 2302.49 | - | Unknown | - | 996.44 | P-O-C stretch | Aliphatic Phosphates | 990-1050 |
| 2122.90 | C≡C | Alkynes | 2100-2260 | 945.37 | C-H | Alkenes | 675-995 |
| 1887.21 | Carbonyl stretch | Transition metal carbonyl compounds | 1800-2100 | 760.89 | C-H | Aromatic rings | 690-900 |
| 1718.77 | C=O | Aldehydes, Ketones, Carboxylic acids, Esters | 1690-1760 | 589.32 | C-I stretch | Aliphatic iodo compounds | 500-600 |

Fig 1: FT-IR Spectrum of *Semecarpus anacardium* Leaf PowderFig 2: FT-IR Spectrum of Water *Semecarpus anacardium* Leaf Extract

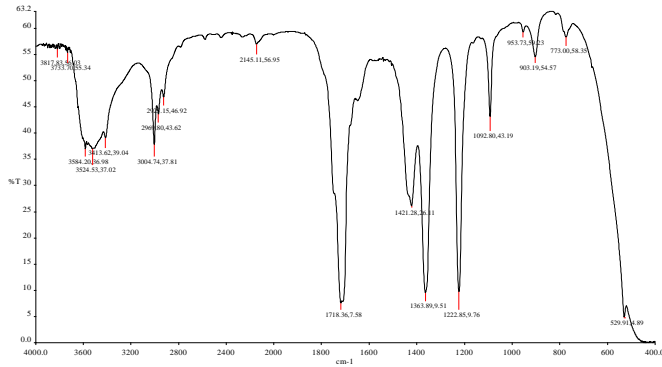


Fig 3: FT-IR Spectrum of Chloroform *Semecarpus anacardium* Leaf Extract

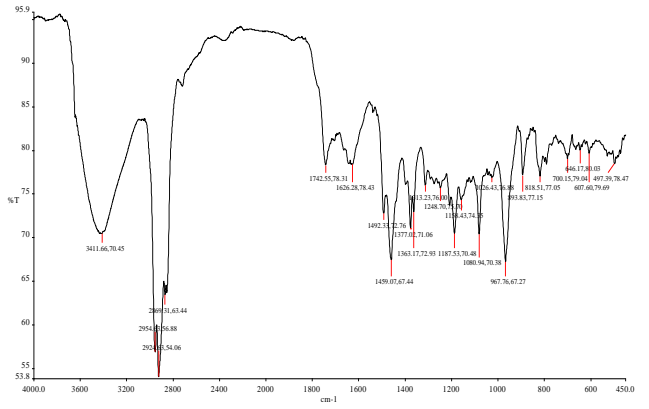


Fig 7: FT-IR Spectrum of Hexane *Semecarpus anacardium* Leaf Extract

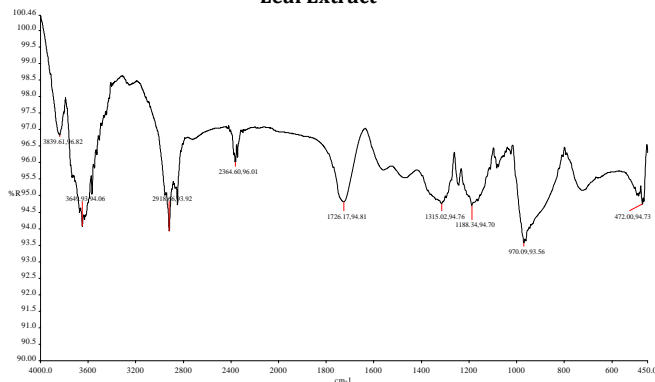


Fig 4: FT-IR Spectrum of Toluene *Semecarpus anacardium* Leaf Extract

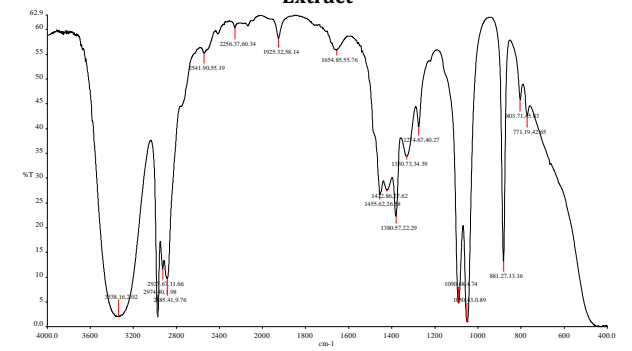


Fig 8: FT-IR Spectrum of Ethyl alcohol *Semecarpus anacardium* Leaf Extract

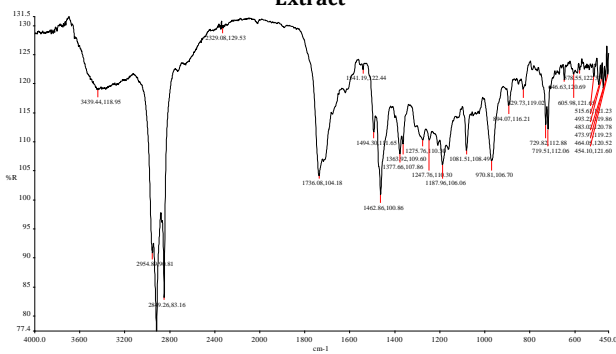


Fig 5: FT-IR Spectrum of CCl₄ *Semecarpus anacardium* Leaf Extract

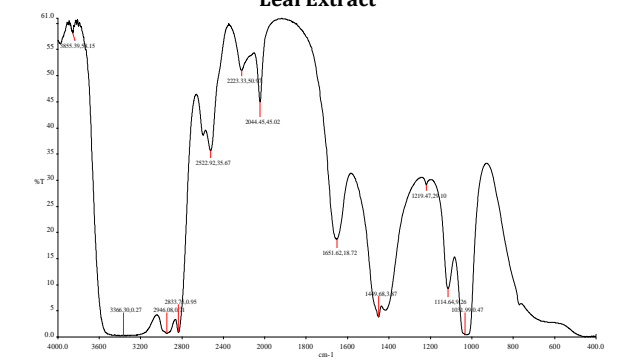


Fig 9: FT-IR Spectrum of Methanol *Semecarpus anacardium* Leaf Extract

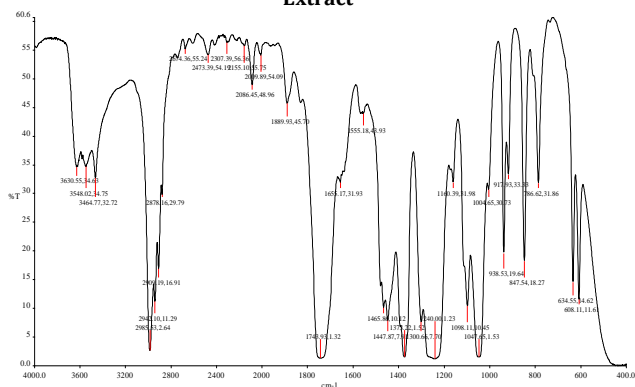


Fig 6: FT-IR Spectrum of Ethyl acetate *Semecarpus anacardium* Leaf Extract

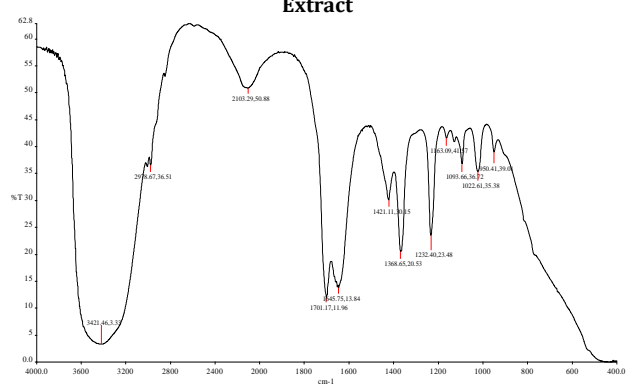


Fig 10: FT-IR Spectrum of Acetone *Semecarpus anacardium* Leaf Extract

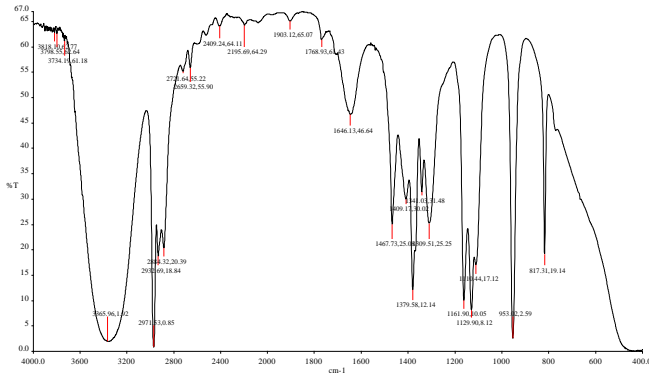


Fig 11:FT-IR Spectrum of 2-propanol *Semecarpus anacardium* Leaf Extract

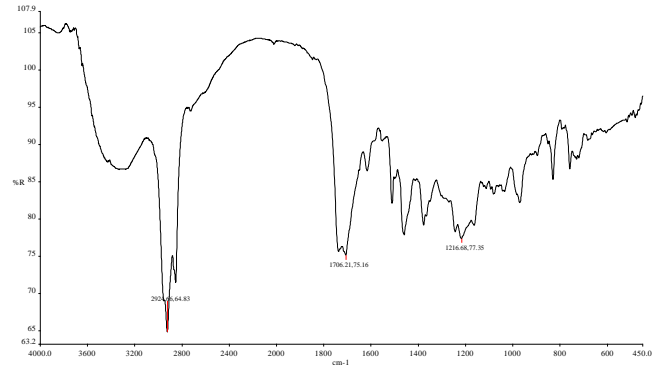


Fig 15:FT-IR Spectrum of Ethyl ether *Semecarpus anacardium* Leaf Extract

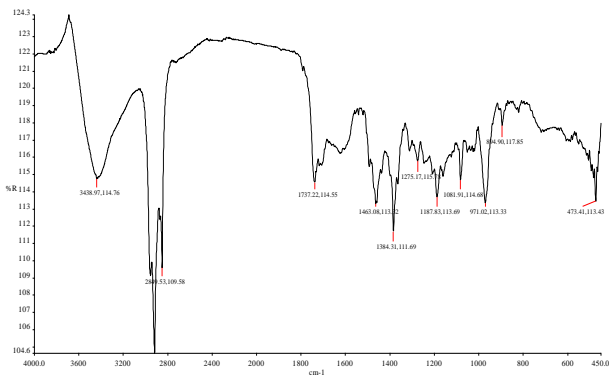


Fig 12:FT-IR Spectrum of Petroleum ether *Semecarpus anacardium* leaf Extract

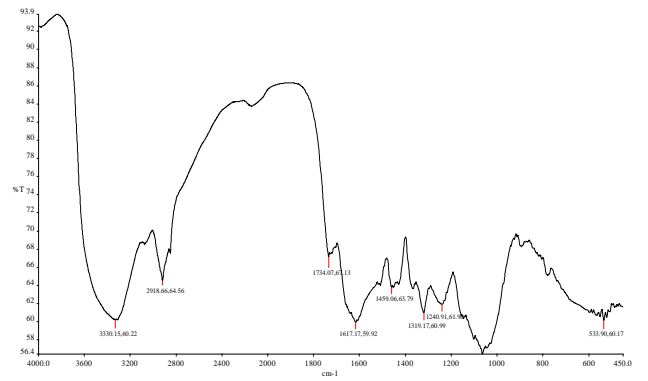


Fig 16:FT-IR Spectrum of *Semecarpus anacardium* Stem Powder

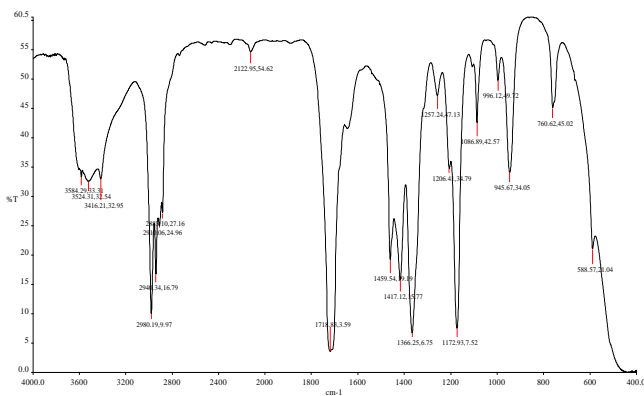


Fig 13:FT-IR Spectrum of 2-butanone *Semecarpus anacardium* leaf Extract

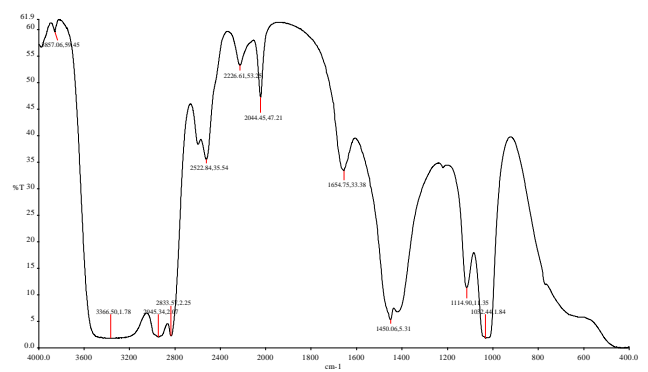


Fig 17:FT-IR Spectrum of Methanol *Semecarpus anacardium* Stem Bark Extract

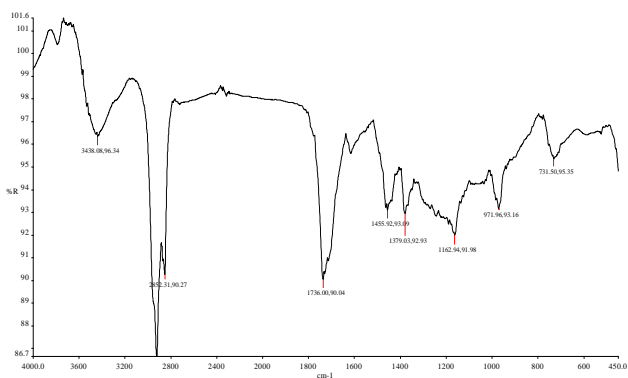


Fig 14:FT-IR Spectrum of Dichloromethane *Semecarpus anacardium* Leaf Extract

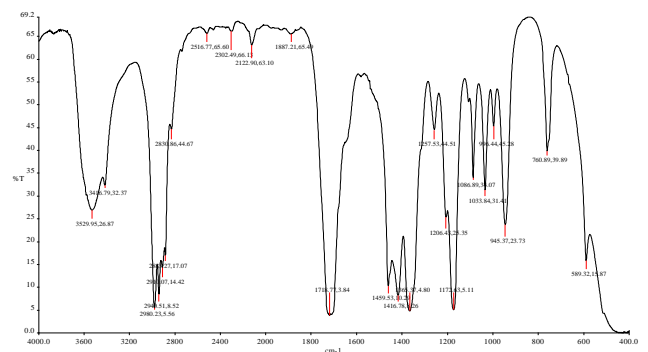


Fig 18:FT-IR Spectrum of 2-butanone *Semecarpus anacardium* Stem Bark Extract

The functional groups which are present in the samples are further described in details. C-H bond of Alkane (2850-2970 cm^{-1}) group frequency are only present only in crude leaf powder of *Semecarpus anacardium* and in chloroform, toluene, carbon tetrachloride and

hexane leaf extracts. C-H bond of Alkane (1340-1470 cm^{-1}) group frequency were found to be present only in *Semecarpus anacardium* acetone leaf extract. Both the group frequencies of the C-H bond of Alkane (2850-2970 cm^{-1}) and (1340-1470 cm^{-1}) were present in ethyl acetate, ethyl alcohol, methanol, 2-propanol, petroleum ether, 2-butanone, dichloromethane, ethyl ether leaf extracts, stem powder and methanol, 2-butanone stem bark extracts.

C=C bond of Alkene (1610-1680 cm^{-1}) group frequency were present in the crude *Semecarpus anacardium* leaf powder and water, ethyl acetate, ethyl alcohol, methanol, acetone, 2-propanol, ethyl ether leaf extracts, stem powder and methanol extract of stem bark. C-H bond of Alkene (675-995 cm^{-1}) group frequency occurred in chloroform, toluene, carbon tetrachloride, ethyl acetate, hexane, ethyl alcohol, acetone, 2-propanol, petroleum ether, 2-butanone, dichloromethane, ethyl ether leaf extracts and 2-butanone stem bark extract. C \equiv C bond of Alkyne (2100-2260 cm^{-1}) group frequency was present in chloroform, ethyl acetate, ethyl alcohol, methanol, acetone, 2-propanol, 2-butanone leaf extracts and methanol and 2-butanone stem bark extracts.

C-H bond of Aromatic ring (690-900 cm^{-1}) group frequency were present in carbon tetrachloride, ethyl acetate, hexane, ethyl alcohol, 2-butanone leaf extracts and 2-butanone stem bark extract.

C=C bond of Aromatic ring (1500-1600 cm^{-1}) group frequency were present only in ethyl acetate leaf extract.

O-H bond of Monomeric Alcohols, Phenols (3590-3650 cm^{-1}) group frequency were present only in ethyl acetate leaf extract. O-H bond of Hydrogen bonded Alcohols, Phenols (3200-3600 cm^{-1}) group frequency were present in leaf powder and water, chloroform, carbon tetrachloride, ethyl alcohol, acetone, petroleum ether, 2-butanone, dichloromethane, ethyl ether leaf extracts, stem powder and methanol, 2-butanone stem bark extracts. O-H bond of Monomeric Carboxylic acid (3500-3650 cm^{-1}) group frequency was present in chloroform, toluene and 2-butanone leaf extracts. O-H bond of Hydrogen bonded Carboxylic acid (2500-2700 cm^{-1}) group frequency were present in ethyl acetate, ethyl alcohol, methanol, 2-propanol leaf extracts and methanol, 2-butanone stem bark extracts.

N-H bond of Amines, Amides (3300-3500 cm^{-1}) group frequency were present in chloroform, ethyl acetate, hexane, methanol, 2-propanol and 2-butanone leaf extracts. C-N bond of Amines, Amides (1180-1360 cm^{-1}) group frequency were present in chloroform, carbon tetrachloride, acetone, petroleum ether and ethyl ether leaf extracts, stem powder and 2-butanone stem bark extract.

C-O bond of Alcohols, Ethers, Carboxylic acids, Esters (1050-1300 cm^{-1}) group frequency were present in leaf powder and chloroform, carbon tetrachloride, ethyl acetate, hexane, ethyl alcohol, methanol, acetone, 2-propanol, petroleum ether, 2-butanone and dichloromethane leaf extracts, stem powder and methanol, 2-butanone stem bark extracts. C=O bond of Aldehydes, Ketones, Carboxylic acids, Esters (1690-1760 cm^{-1}) group frequency were present in chloroform, toluene, carbon tetrachloride, ethyl acetate, hexane, acetone, petroleum ether, 2-butanone, dichloromethane and ethyl ether leaf extracts, stem powder and 2-butanone stem bark extract.

NO_2 bond of Nitro compounds (1500-1570 cm^{-1}) group frequency were present only in carbon tetrachloride and ethyl ether leaf extracts. NO_2 bond of Nitro compounds (1300-1370 cm^{-1}) group frequency were present in chloroform, toluene, carbon tetrachloride, ethyl acetate, hexane, ethyl alcohol, acetone, 2-propanol and petroleum ether leaf extracts, stem powder and 2-butanone stem bark extract.

The C-H stretch vibrations for methyl and methylene are the most characteristic in terms of recognizing the compound as an organic compound containing at least one aliphatic fragment. In this functional groups from Saturated Aliphatic and Alicyclic compounds like Cyclohexane ring vibrations (1000-1055 cm^{-1}) were present in methanol and acetone leaf extracts and methanol stem bark extract. Special methyl ($-\text{CH}_3$) frequencies like Methoxy, methyl ether O-CH $_3$, C-H stretch (2815-2850 cm^{-1}) were present only in 2-butanone stem bark extract. The existence of one or more aromatic rings in a

structure is normally readily determined from the C-H and C=C ring-related vibrations. The other most important set of bands are the aromatic ring vibrations centered around 1600 and 1500 cm^{-1} , which usually appear as a pair of band structures, often with some splitting. The appearance and ratio of these band structures is strongly dependent on the position and nature of substituents on the ring. Aromatic ring (aryl) group C=C-C (1450-1510 cm^{-1}) was present only in carbon tetrachloride leaf extract.

In Halogenated aliphatic compounds, the C-X bond typically possesses a unique group frequency, which may be assigned to the halogen-carbon stretching. Aliphatic fluoro compounds (1000-1150 cm^{-1}) C-F stretch were present in ethyl acetate and hexane leaf extracts. Aliphatic chloro compounds (700-800 cm^{-1}) C-Cl stretch were present only in chloroform leaf extract. Aliphatic bromo compounds (600-700 cm^{-1}) C-Br stretch were present in carbon tetrachloride, ethyl acetate and hexane leaf extracts. Aliphatic iodo compounds (500-600 cm^{-1}) C-I stretch were present in leaf powder and chloroform, carbon tetrachloride, 2-butanone leaf extracts, stem powder and 2-butanone stem bark extract.

In Amino Compounds with some respects, the infrared spectra and the characteristic group frequencies of amines tend to parallel those of alcohols and ethers. The terms primary, secondary, and tertiary are used to describe amines, but the substitution relates to the nitrogen, not the adjoining carbon (as with alcohols). Only the primary and secondary amines exhibit the most characteristic group frequencies, which are associated with the N-H bond. Primary amine (1020-1090 cm^{-1}) CN stretch were present in ethyl acetate leaf extract and 2-butanone stem bark extract. Secondary amine (1130-1190 cm^{-1}) CN stretch were present only in toluene leaf extract.

The Carbonyl group compounds are not only chemically important, but are also important in the interpretation of infrared spectra. The C=O absorption is almost always one of the most characteristic in the entire spectrum, and it is also most likely to be the most intense spectral feature. Aldehyde (2700-2800 cm^{-1}) group frequencies were present only in 2-propanol leaf extract. Open-chain acid anhydride (1740-1790 cm^{-1}) group frequencies were present in only in 2-propanol leaf extract. Transition metal carbonyls (1800-2100 cm^{-1}) group frequencies were present water, ethyl acetate, ethyl alcohol, 2-propanol leaf extracts and methanol, 2-butanone stem bark extracts.

The group of Hetero-oxy compounds features X-O (where X= nitrogen, sulfur, phosphorus, and silicon) and X=O vibrations. In general, the stretching frequencies is observed within the main fingerprint spectral region (1500-400 cm^{-1}). Many of the compounds can be considered to be analogs of ethers, especially when an alkoxy group is present, featuring the X-O-C linkage. Aromatic nitro compounds (1485-1555 cm^{-1}) group frequencies were present only in hexane leaf extract. Aliphatic phosphates (990-1050 cm^{-1}) P-O-C stretch were present in 2-butanone leaf extract and 2-butanone stem bark extract.

Thiols and Thio-substituted compounds by definition, can be considered to be the direct analogs of the equivalent oxygenated compounds such as alcohols and ethers. Catenation is a unique chemical characteristic of sulfur, where the formation of S-S bonds in extended chains is common, hence the inclusion here of the S-S stretching frequencies. Aryl disulfides (430-500 cm^{-1}) S-S stretch was present only in CCl_4 leaf extract. Polysulfides (470-500 cm^{-1}) S-S stretch was present in leaf powder and toluene, carbon tetrachloride, hexane, petroleum ether leaf extracts.

In H-X group, the stretching of bonds between heavier atom and hydrogen (H-X-) occurs in the region between 2000 and 4000 cm^{-1} . The X-atoms and the structure to which they are attached determines the exact frequency. H-C (aromatic) (3000-3050 cm^{-1}) group frequency was present only in chloroform leaf extract. H-bonded (H-O): (2500-3500 cm^{-1}) group frequencies were present in ethyl acetate, ethyl alcohol, acetone, 2-propanol, 2-butanone soxhlet leaf extracts and 2-butanone stem bark extract.

The above listed infrared functional group absorptions characteristic were cited from the literature¹⁴⁻¹⁶. The FT-IR analysis

revealed the similarity and variation between the leaf and stem parts of *Semecarpus anacardium*. From the spectra we can clearly see 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. 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 and even evaluate the qualities of medicinal materials⁷.

CONCLUSION

The FT-IR analysis of *Semecarpus anacardium* clearly reveals the differences of categories of chemical constituents in crude powder and 14 different polar and nonpolar organic solvent extracts of leaf and stem bark. The crude plant material when extracted by organic solvents, shows more characteristic features in the FT-IR spectrum as the chemical compositions become more concentrated. Due to the similarity of the extraction method i.e. soxhlet extraction, the chemical constituents in the concentrated extracts are relatively consistent and therefore they show higher repeatability and comparability in FT-IR spectra. So, FT-IR spectrum reflecting objectively the panorama of chemical composition in complex plant material is a most appropriate method to validate and identify the mixed substance products such as traditional herbal medicine as well as their corresponding extracts. The results of the present study confirms that leaf and stem bark of *Semecarpus anacardium* is rich in the resources of phytoconstituents.

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