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Functional Group Evaluation of Hydrogenated Vegetable Oil Using FTIR Method

Priya Subramanian Kalaimani^{1,2}, Suman Thamburaj¹, Suresh Kumar Kalakandan^{*1}, Akhila Etikala¹, Anju Mariam Johnson¹, Praveen Kumar Dubey¹

¹Department of Food Biotechnology, National Institute of Food Technology Entrepreneurship and Management, Thanjavur, TamilNadu, India-613005

²Affiliated to Bharathidasan University, Tiruchirappalli, Tamil Nadu, India-620024

Abstract: This study aimed to predict the functional group changes in the natural form to hydrogenated form of vegetable oils using FTIR spectroscopic method. The edible oil, which are palm oil, groundnut oil, sesame oil, and vanaspathi(hydrogenated vegetable oil) were observed with relative intensities of the peak and characteristic area percentage of peaks. It is found that trans fatty acids at the peak of 966.34cm^{-1} in the region of $980-960\text{cm}^{-1}$ strong C=C bending vibration due to the presence of alkene disubstituted (trans) observed in the hydrogenated form of vegetable oil. Because the nutritional composition of the vegetable oil is intensely reduced and long-term consumption will bring adversative health problems for humans.

Keywords: FTIR, Palm oil, Groundnut oil, Sesame oil, Vanaspathi, Transfats

I. INTRODUCTION

Edible vegetable oil is one of the primary fat compounds that are associated with daily intake and prepared by the seeds of specific plants. After the extraction, refining, and processing it is subjected to consumption. These edible vegetable oils vary depending on the producing areas, processing methods, and nutritional value. In India, vegetable oil has been considered the primary product for cooking. Likewise, Ghee is also used for frying, cooking, spreading various food items. It is especially for preparing snacks[1]. Because of the immense power and health benefits, ghee is considered a holy product in religious rituals[2]. For Siddha, Ayurveda, and Unani treatments, ghee has been prescribed as the medicine[3]

Vanaspathi is entirely or partly hydrogenated vegetable oil, which is habitually used as a cost-effective substitute for ghee. It is much cheaper than desi ghee[4]. Most of the hydrogenated vegetable oil is made from palm or palm olein oil[5]. Hydrogenation is the process, where manufacturers add hydrogen to a liquid fat, using nickel as a catalyst at room temperature. For food preparation purposes in various household and commercial places, vanaspathi is preferred. It enhances a nice aroma, taste, and flavor. In the Indian market, various kinds of edible oil are available. Vanaspathi plays a crucial role in the edible oil trade. The economic value increased by production is about 1.2 million tonnes annually[6]. In addition, it is responsible for a 10% share in the edible oil market. According to National Consumption Survey data by 2009, rural and urban populations in India took the fat around 20g and 30g per day, respectively. According to diet studies and FSSAI transfat tribune, the consumption of trans fat foods in 2017 around 1.5 million deaths occurred[7]. Vegetable oils had edible mere largely through vanaspathi route. In life, many consumers often use vanaspathi for softening the food items means of textural improvement and flavor enhancer[8]. During processing thermal decomposition with hydrogenation responds to the index of the oil quality and one of the sensory values.

People in India use vanaspathi and oil on daily routine for cooking food items. Vanaspathi were taken by all statuses of lower and middle-class people. Because it favors oils to vanaspathi ghee, there could be a reverse trend of giving up the use of vanaspathi in favor of refined oil[9]. By 2024, the market value of vanaspathi raised to INR 4653 billion. In India, trans fats from hydrogenated vegetable oil in the form of vanaspathi are consumed in greater quantity than in the united states[10]. Almost 3 million deaths occurred per year by cardiovascular diseases in India because of transfat dietary intake been recorded in 2017. The World Health Organization announced the contribution of high ischemic heart disease (IHD) risk in India due to high intakes of trans fatty acids[11]. The hydrogenated fat leads to the formation of Trans fatty acids, which cause many deleterious effects on human health. It may cause indigestion, cardiovascular disease, and obesity. There is a need to differentiate the functional group changes in the natural form from hydrogenated vegetable oil.

II. MATERIALS AND METHODS

A. Sample Preparation and Sources

The selected samples such as palm oil, groundnut oil, sesame oil, and hydrogenated vegetable oil, and Ghee were procured from the local market, Thanjavur, TamilNadu, India.

B. FTIR Spectrum Analysis

The collected samples subjected to analysis were kept in a sample holder. Using ATR-FTIR spectrometer Shimadzu IR tracer-100 scanned with 4cm^{-1} resolution in the range of $4500\text{--}500\text{ cm}^{-1}$ region. Before the analysis, the instrument was calibrated of all vegetable oil, fat samples. On a sequential basis, the samples were taken by dropper and were analyzed at the rate of 45 scans/minute. Before and after analyzing the sample, the sample holder of the instrument was cleaned using tissue paper with chloroform thoroughly to avoid contamination from one sample to another sample. The spectrogram data projected been saved after the analysis and functional group studied for discrimination of samples [12].

III. RESULTS AND DISCUSSION

The FTIR analysis was carried out for five samples and the spectrogram was analysed in the region between $4500\text{--}500\text{ cm}^{-1}$ were measured in figure 1-5. Among all the samples, some major peaks been identified are 721.38 cm^{-1} , 1377.17 cm^{-1} , 1463.97 cm^{-1} , 2852.72 cm^{-1} , 922.16 cm^{-1} , 2953.02 cm^{-1} . The spectrum of ghee 582.5 cm^{-1} , 721.38 cm^{-1} , 966.34 cm^{-1} , 1099.43 cm^{-1} , 1112.93 cm^{-1} , 1159.22 cm^{-1} , 1236.37 cm^{-1} , 1298.09 cm^{-1} , 1377.17 cm^{-1} , 1417.68 cm^{-1} , 1463.97 cm^{-1} , 1743.65 cm^{-1} , 2852.72 cm^{-1} , 2922.16 cm^{-1} and 2953.02 cm^{-1} was recorded in FTIR region [13]. For groundnut oil, unique ester at 1712.79 cm^{-1} , whereas for the entire sample have shown the presence of ester at 1159.22 cm^{-1} . At 1097.5 cm^{-1} stretching observed for ether in sample at C-O stretch. Only vanaspathi have shown wave number at 966 cm^{-1} for anhydride related to trans fatty acid, which is present in ghee and vanaspathi.

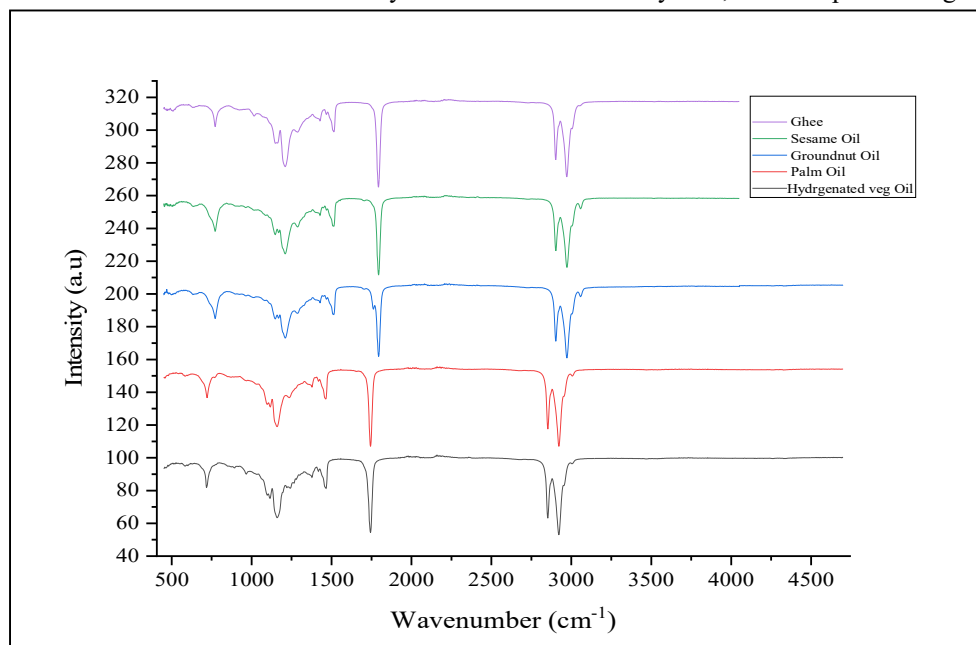


Fig. 1 FTIR spectrum of Ghee, Sesame oil, Groundnut Oil, Palm Oil, hydrogenated veg oil

The common functional group is depicted in Figure 6. The peak 721.38 cm^{-1} , the functional group obtained may be aliphatic chloro compound, CH_2 , CH_3 symmetric bending vibration 9 aliphatic groups, corresponding to 1377.17 cm^{-1} peak. Bending vibration of CH_2 and CH_3 aliphatic groups, nitrosamines at 1463.97 cm^{-1} at C-H stretch. Aromatics and ketones were found at all tested samples with C-H stretch at 1236.37 cm^{-1} and 1145 cm^{-1} . The band at 966 cm^{-1} , responding C=C vibrations, specific Trans fats acts as marker present in vanaspathi has not been found in the ghee samples. Hydrogenated fat has the highest trans content associated with a rich hardness index [14]. These $\text{HC}=\text{CH}$ functional groups are responsible for the complex form in vanaspathi so it leads to unhealthy issues like indigestion, cancer, obesity-related diseases [15]. Many researchers stated that the Trans fatty acids intake leads to cardiovascular diseases, breast cancer, nervous disorder, pregnancy duration reduced, preeclampsia risks, and vision problems for infants, colon cancer and causes allergy [6].

Table 1 Peaks Intensity and Area Percentage of Palm Oil

No.	Peak	Intensity	Correlation Intensity	Base (H)	Base (L)	Area	Corr. Area
1	721.38	82.33	13.22	761.88	642.3	947.072	450.39
2	1097.5	78.38	2.29	1105.21	1041.56	936.581	-17.041
3	1116.78	76.8	3.59	1128.36	1105.21	494.417	40.597
4	1159.22	64.76	17.56	1215.15	1128.36	2236.457	730.479
5	1236.37	82.45	2.9	1330.88	1215.15	1442.516	61.161
6	1377.17	88.82	3.82	1396.46	1357.89	335.508	51.662
7	1463.97	81.66	14.41	1508.33	1425.4	686.89	377.426
8	1743.65	52.69	46.14	1830.45	1683.86	1459.02	1301.394
9	2852.72	63.25	26.94	2879.72	2763.99	1134.196	349.818
10	2922.16	52.73	32.23	2951.09	2879.72	1977.785	933.691
11	2953.02	83.18	0.63	2993.52	2951.09	373.01	-50.543

Peak intensity and peak area analysis are given in Table.5. The Peak is 721.38, for palm oil, intensity and area (82.33; 947.072) for groundnut oil intensity and the area is (79.46; 1427.919). For sesame oil (79.15; 1505.396) and vanaspathi intensity and area (81.81; 921.02). As such the peak intensity, area of ghee (84.63; 772.562). Then corresponding to (CH₂) stretching vibration peak 1463.97cm⁻¹. C-H stretching vibrations peak intensity and area (88.82; 335.508) for palm oil. Likewise, (88.97; 315.857) for groundnut oil. However, sesame oil (88.81; 555.808). For vansapathi intensity reduced to (88.05; 477.53) comparing groundnut oil. Especially for ghee the intensity (88.12; 618.905 at peak 1463.97cm⁻¹ the intensity increased from (81.66; 686.89) for palm oil. Groundnut oil showed (81.92; 717.864). Sesame oil peak intensity is (82.16; 688.182). Vanaspathi has been shown the peak of (81.31; 711.464). The most acceptable ghee showed (81.47; 687.39). The peak 1743.65 cm⁻¹, stretching vibrations of the C=O stretch of aldehydes the intensity and peak area for palm oil (52.69; 1459.02), Groundnut oil (56.28; 1270.833), sesame oil (52.38; 1499.046), vansapathi (54.34; 1565.658) ghee (47.61; 1666.64)[16]. The peak 2852.72cm showing the intensity and area of palm (63.25; 1134.196), groundnut (65.61; 1157.222), sesame (67.18; 1110.156), vansapathi is (63.14; 1161.621), and ghee (64.22; 1094.961). At 2922.16cm⁻¹ peaks for palm oil (52.73; 1977.785), groundnut (55.31; 1936.267), sesame oil (57.03; 1872.441), vansapathi intensity of peak and area (52.94; 2009.352), ghee intensity of peak and area is (53.38; 1937.157). For the corresponding peak 2953.02cm⁻¹, the peak intensity and area for palm oil are (83.18; 373.01, groundnut oil intensity is (82.27; 410.235), sesame oil peak intensity is (82.35; 400.424), vansapathi (83; 376.099), for ghee the peak intensity and area is (83.04; 388.435). Similarly, various researches found some trans fats in the hydrogenated fats[17]. Although vegetable oil has saturated fatty acids, total fat in cookies did not increase significantly. However, the partially hydrogenated vegetable oil used in bakery products is rich in TFA. The replacement of vansapathi with butter or tropical oils high in saturated fatty acids could reasonably be expected to coronary heart disease risks. Thus the specific effect on cardiovascular risk is dependent on the original content of TFA in the food product[10].

Table 2 Peaks Intensity And Area Percentage Of Sesame Oil

No.	Peak	Intensity	Correlation Intensity	Base (H)	Base (L)	Area	Corr. Area
1	721.38	79.15	16.87	792.74	636.51	1505.396	879.921
2	1039.63	88.79	0.69	1047.35	989.48	556.036	14.044
3	1097.5	77.14	4.82	1109.07	1047.35	1022.143	77.333
4	1118.71	78.3	1.71	1126.43	1109.07	360.974	14.532
5	1159.22	65.34	16.04	1215.15	1126.43	2276.245	674.717
6	1238.3	81.8	4.01	1311.59	1215.15	1302.229	109.486
7	1377.17	88.81	4.58	1392.61	1330.88	555.808	124.743
8	1463.97	82.16	13.36	1485.19	1423.47	688.182	370.784
9	1743.65	52.38	46.25	1824.66	1670.35	1499.046	1291.811
10	2852.72	67.18	22.73	2879.72	2752.42	1110.156	235.998
11	2922.16	57.03	27.45	2951.09	2879.72	1872.441	799.761
12	2953.02	82.35	0.69	2991.59	2951.09	400.424	-36.158

Table 3
Peaks intensity and area percentage of groundnut oil

No.	Peak	Intensity	Correlation. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	721.38	79.46	16.03	781.17	636.51	1427.919	771.552
2	1097.5	79.28	3.81	1109.07	1041.56	979.618	39.723
3	1118.71	79.74	1.85	1126.43	1109.07	336.519	16.685
4	1159.22	67.6	14.92	1217.08	1126.43	2177.641	624.049
5	1236.37	82.68	2.79	1330.88	1217.08	1442.268	93.68
6	1377.17	88.97	3.29	1392.61	1357.89	315.857	42.162
7	1463.97	81.92	13.21	1508.33	1425.4	717.864	332.43
8	1712.79	85.27	3.58	1720.5	1666.5	380.828	-22.285
9	1743.65	56.28	33.52	1832.38	1720.5	1270.833	516.582
10	2852.72	65.61	24.11	2879.72	2767.85	1157.222	332.456
11	2922.16	55.31	28.91	2951.09	2879.72	1936.267	841.788
12	2953.02	82.27	0.67	2991.59	2951.09	410.235	-36.35

Table 4
Peaks intensity and area percentage of hydrogenated vegetable oil

No.	Peak	Intensity	Correlation Intensity	Base (H)	Base (L)	Area	Corr. Area
1	717.52	81.81	14.35	777.31	653.87	921.024	447.223
2	966.34	90.09	2.34	979.84	925.83	401.279	36.506
3	1031.92	89.9	0.5	1041.56	987.55	499.163	10.485
4	1099.43	77.18	1.86	1105.21	1041.56	994.932	-22.224
5	1114.86	75.27	4.06	1128.36	1105.21	519.203	47.154
6	1159.22	63.46	18.49	1211.3	1128.36	2297.686	820.937
7	1220.94	81.81	0.66	1224.8	1211.3	237.8	3.789
8	1226.73	82.19	0.03	1230.58	1224.8	102.944	0.093
9	1242.16	81.45	1.88	1257.59	1230.58	468.844	23.88
10	1265.3	84.59	1.28	1274.95	1257.59	251.619	8.569
11	1278.81	86.8	0.88	1294.24	1274.95	231.134	7.307
12	1300.02	89.39	0.52	1328.95	1294.24	337.652	8.28
13	1377.17	88.05	3.91	1406.11	1354.03	477.53	71.019
14	1465.9	81.31	14.68	1508.33	1425.4	711.464	384.519
15	1743.65	54.34	44.1	1824.66	1683.86	1565.658	1361.396
16	2852.72	63.14	26.77	2879.72	2762.06	1161.621	345.133
17	2922.16	52.94	31.83	2951.09	2879.72	2009.352	950.293
18	2953.02	83	0.7	2993.52	2951.09	376.099	-49.005

Table 5
Peaks Intensity and Area Percentage of Ghee

No.	Peak	Intensity	Correlation Intensity	Base (H)	Base (L)	Area	Corr. Area
1	582.5	96.08	0.45	588.29	557.43	100.259	7.636
2	721.38	84.35	12.25	781.17	671.23	738.891	365.251
4	1099.43	74.23	1.43	1107.14	985.62	1627.686	-386.901
5	1112.93	74.38	2.2	1128.36	1107.14	489.58	29.172
6	1159.22	59.97	22.23	1213.23	1128.36	2445.66	940.139
7	1236.37	81.02	3.36	1296.16	1213.23	1279.626	110.846
8	1298.09	89.34	0.16	1330.88	1296.16	332.368	6.172
9	1377.17	87.87	5.75	1406.11	1330.88	679.379	174.574
10	1417.68	91.82	2.03	1425.4	1406.11	133.587	17.838
11	1463.97	81.26	14.59	1508.33	1425.4	701.529	373.106
12	1743.65	47.61	51.3	1832.38	1662.64	1666.64	1483.855
13	2852.72	64.09	26.28	2881.65	2762.06	1128.092	323.516
14	2922.16	53.65	31.48	2951.09	2881.65	1909.643	901.77
15	2954.95	83.16	1.32	2997.38	2951.09	394.491	-56.064

Table 6
Functional Group Organization of Palm Oil, Groundnut Oil, Sesame Oil, Vanaspathi, and Ghee.

Peak List	Palm oil	Groundnut oil	Sesame oil	Vanaspathi	Ghee	Wavenumber (cm ⁻¹)	Functional group assignment	Chemical constituents
1	--	--	--	--	582.50	600-500	C-I stretch	Halogen (iodo compound)
2	721.38	721.38	721.38	--	721.38	500-738	C-Cl	Halogen compound (Chlorocompound)
3	--	--	1039.63	966.34	--	650-1000	PO3 stretch	Phosphate ion, alkene bends
4	1097.5	1097.5	1097.5	1031.92, 1099.43	1099.43	1100-1000	C-O stretch	Ether
5	1116.78	1118.71	1118.71	1114.86	1112.93	1020-1250	C-N stretch	Aliphatic amines
6	1159.22	1159.22	1159.22	1159.22	1159.22	1000-1200	C-O stretch	Ester
7	1236.37	1236.37	1238.3	1242.16,	1236.37	1200-1280	C-H stretch	Aromatics
8	--	--	--	1300.02	1298.09	1000-1320	C-O stretch	Alcohol, carboxylic acids, esters, ethers
9	1377.17	1377.17,	1377.17	1377.17	1377.17	1410-1310	O-H bend	Phenol or tertiary alcohol
10	--	--	--	--	1417.68	1600-1400	C=C_C, Aromatic ring	Aromatic
11	1463.97	1463.97	1463.97	1465.9	1463.97	1440-1470	C-H stretch	Bending vibration of CH ₂ and CH ₃ aliphatic groups, nitrosamines
12	--	1712.79	--	--	--		C=O stretching,	ester phospholipids
13	1743.65	1743.65	1743.65	1743.65	1750	1740-1725	C=O stretch	Aldehyde
14	2852.72	2852.72	2852.72	2852.72	2852.72	2850-2815	C-H symmetric stretch	Methoxy methyl ether
15	2922.16	2922.16	2922.16	2922.16	2922.16	2935-2915	Asymmetric stretching of -CH (CH ₂) vibration,	Lipids, protein
16	2953.02	2953.02	2953.02	2953.02	2954.95	2850-2975	C-H	Alkane

Table 7
Peak Area and Intensity of Palm, Groundnut, Sesame oil, Hydrogenated Vegetable oil, and Ghee.

Peak values	Palm oil		Groundnut oil		Sesame oil		Vanaspathi		Ghee	
	Intensity (a.u.)	Area (%)	Intensity (a.u.)	Area (%)	Intensity (a.u.)	Area (%)	Intensity (a.u.)	Area (%)	Intensity (a.u.)	Area (%)
721.38	82.33	947.072	79.46	1427.919	79.15	1505.396	81.81	921.024	84.63	772.562
1377.17	88.82	335.508	88.97	315.857	88.81	555.808	88.05	477.53	88.12	618.905
1463.97	81.66	686.89	81.92	717.864	82.16	688.182	81.31	711.464	81.47	687.39
1743.65	52.69	1459.02	56.28	1270.833	52.38	1499.046	54.34	1565.658	47.61	1666.64
2852.72	63.25	1134.196	65.61	1157.222	67.18	1110.156	63.14	1161.621	64.22	1094.961
2922.16	52.73	1977.785	55.31	1936.267	57.03	1872.441	52.94	2009.352	53.38	1937.157
2953.02	83.18	373.01	82.27	410.235	82.35	400.424	83	376.099	83.04	388.435

From this experiment, we found that so many variations were observed in the active functional group of vegetable oils from the liquid to hydrogenated form at room temperature. In addition, we identified a transfat functional group, and the area intensity was high compared to other oils[18].

IV. CONCLUSION

This work concluded that prepared hydrogenated form of vegetable oils containing Trans fats been detected using the FTIR spectroscopic method. The vegetable oils such as palm oil, groundnut oil, sesame oil, and vanaspathi (hydrogenated vegetable oil) were observed with relative intensities of the peak and characteristic area percentage of peaks. It is seen that trans fatty acids at the peak of 966.34cm^{-1} at strong C=C bending vibration in the region of $980\text{-}960\text{cm}^{-1}$ due to the presence of alkene disubstituted (trans) observed in the hydrogenated form of vegetable oil. Hence, it is advisable to consume a non-hydrogenated dietary intake to lead a healthy life.

V. CONFLICT OF INTEREST

The authors have no conflicts of interest regarding this investigation.

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