FTIR spectroscopy combined with chemometric: a versatile tool for quality evaluation of fried vermicelli

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Abstract

Keywords:

Fried vermicelli
Soxhlet extraction
Fatty acids
GC-MS
FTIR
Chemometrics

Article history:

Received 16.01.2017
Received in revised
form 19.03.2017
Accepted 30.03.2017

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DOI: 10.24263/2304-
974X-2017-6-1-8

Introduction. Snacks are common food throughout the world including subcontinent. Most of the snack foods are prepared in oil and fat. In current study, fried vermicelli (common snack food) was selected to evaluate the quality as it is largely consumed in many countries.

Materials and methods. Fried vermicelli was subjected for the extraction of total oil by applying Soxhlet extraction method using hexane as a solvent. Fatty acid composition of extracted fried vermicelli oil was checked on GC-MS. Similarly, FTIR spectroscopy was also used to record the spectra of same oil for the development of simple methodology to quantify fatty acid groups and ratios.

Results and discussion. High percentage of oil content was observed in all fried vermicelli samples (19.77–32.99%). Fatty acid composition exposed that palmitic (34.6–47.5%), stearic (4.76 to 10.6%), oleic (27.2–37.0%) and elaidic acid (12.0–24.3%) were predominant fatty acids among saturated and monounsaturated fatty acids. While polyunsaturated fatty acids were observed comparatively in less quantity in fried vermicelli (0.66 to 5.99 %). The presence of higher *trans* fatty acids indicated that fried vermicelli was prepared in hydrogenated oil. Fatty acid ratios of some important groups were observed in the range of 0.72–1.92 SFA/UFA, 0.013–0.130 cis PUFA/SFA, 0.1 to 1.81 *trans* FA/cis FA, 0.01 to 0.097 cis PUFA/SFA + TFA, 27.7–37.05 cis MUFA + cis PUFA/SFA + TFA. The obtained results of groups and ratios by GC-MS were used to develop different calibration models for the quantification of fatty acid groups and fatty acid ratios using PLS chemometric approach. The developed PLS models using selected wavelength regions showed higher correlations (>0.99) with GC-MS results.

Conclusions. It can be concluded that quality of fried vermicelli marketed locally is worrisome matter for the consumers and quality control authorities. FTIR provided complete profiling of groups and ratios in fried vermicelli very accurately with negligible difference in the results. The proposed methodology serves as a rapid and simple quantitative tool for quality evaluation of major groups and ratios.

Introduction

Nutritionists are interested in the fatty acid intake, as the oil and fats play an essential role in human nutrition as energy source and metabolic activities since it is a major research focus in nutritional sciences. They regulate the physiological process in human body structure and produce energy [1].

Currently, nutritionists recommend intake of saturated fatty acids (SFA), monounsaturated fatty acids (MUFA) and polyunsaturated fatty acids (PUFA) in a balanced amount for a nutritious diet because higher intake of SFA has been associated with cardiovascular diseases (CVD), whereas MUFA and PUFA consumption is related with beneficial health effects [2]. MUFA and PUFA substituted SFA [3] because MUFA lower the risk factors of CVD [4]. PUFA can be linked to negative or beneficial health effects [5]. The epidemiological research on clinical role of n-6/n-3 ratio of PUFA was studied and found an increased risk of cardiovascular and coronary heart diseases [6]. Conversely, PUFA/SFA ratio is associated with CVD which can be lower by replacing SFA with PUFA in a balanced diet [7] as the increased intake of PUFA has beneficial effects [8]. However, some detrimental properties are also there, unsaturated FA can be reacted with oxygen especially in air which makes them rancid [9]. The process of partial hydrogenation is used to avoid the rancidity of unsaturated FA [10]. Before hydrogenation process, unsaturated FA present in *cis* configuration, whereas partial hydrogenation converts some of the *cis* double bonds into its *trans* configuration and relocate the position of double bonds [11]. WHO scientific review committee on *trans* fat recommend daily intake of partially hydrogenated oil should be less than 1% [12]. FDA proposed nutritional facts labeling rules to separate the *trans* fat from total fat content, which was effective from 1st January 2006 [11]. FDA remove partially hydrogenated oil which is the primary source of *trans* fat, from the list of GRAS (Generally recognized as safe) and allow food companies to eliminate the partially hydrogenated oils by reformulating their products by 2018 [13].

In Pakistan, no any study has been reported on the fatty acids as well as *trans* fatty acid contents of fried vermicelli, as it is a very popular snack food in sub-continent. GC-MS is considered as an authentic technique for the quantification of fatty acid composition. The current study is conducted to investigate the main classes of fatty acid present in different fried vermicelli samples collected from different locations of Hyderabad, Sindh. The results of GC-MS correlated with the specific regions of FTIR spectra using PLS chemometric technique.

Materials and methods

Chemicals and reagents

Solvents and chemicals, such as hexane, methanol and potassium hydroxide (analytical grade) purchased from Merck (Darmstadt, Germany).

Sample collection

18 samples of fried vermicelli were collected from different local shops of Hyderabad, Pakistan.

Oil extraction

Fried vermicelli samples were subjected for the extraction of total fat and oil by applying Soxhlet extraction method using hexane as a solvent [14]. Total oil content was calculated as percentage mass of the sample. Extracted fried vermicelli oil was transferred into vials and kept at -4 °C until further analysis.

Determination of fatty acid composition

Fatty acid composition of fried vermicelli was analyzed by preparing Fatty acid methyl ester (FAME) using IUPAC standard method [15]. GC-MS chromatograms of fried vermicelli were recorded via Agilent GC-MS. Obtained data was analyzed using ChemStation software. For identification of fatty acids in fried vermicelli, NIST and Wiley libraries were used to compare the fatty acids by matching >90% similarity.

Gas chromatography – mass spectrometry conditions

FAME were analyzed on gas chromatography (Agilent 6890 N) coupled with a mass selective detector (Agilent MS-5975) and an auto sampler injector (Agilent 7683-B) (Little Fall, NY, USA). For the separation of FAME, 5% phenyl methylsiloxane (HP-5MS) capillary column having 30 m length with internal diameter of 0.25 mm from Agilent Technologies (Palo Alto, CA, USA) was used. Initial oven temperature 150 oC was set for 2 min and ramped at 4 C/min up to 230 °C and hold for 5 min. Helium was used as a carrier gas with flow rate of 1ml/min and a split ratio 1:50. Temperature of injector and detector was set at 240 °C and 260 °C, respectively. Electron impact (EI) ionization source at 70 ev in mass spectrometer was used with the scan range of 50–550 m/z as reported in earlier study [16].

Statistical analyses and calculations

Peaks were identified by GC-MS libraries of NIST and Wiley and percentage of fatty acids were quantified by area percent method.

Fourier Transform Infrared spectroscopy

All the infrared spectra of Fried vermicelli samples were recorded using Nicolet 320 Fourier transform infrared (FTIR) spectrometer (Thermo Nicolet Analytical Instruments) Madison, WI, USA with ZnSe Single bounce ATR accessory (Spectra-Tech, Shelton, CT) with KBr beam splitter and deuterated triglycine sulphate (DTGS) detector. OMNIC software (version 7.3) was used for the instrumental control and acquisition of data. 24 accumulated scans with the resolution of 4 cm⁻¹ in the range of 4000–650 cm⁻¹ were set for recording spectra. Background spectrum was collected before acquiring each spectrum of sample. Soft tissue and hexane were used for the cleaning of ZnSe crystal after every sample.

Results and discussion

Snack food products are of wider interest for food researchers because of its high consumption. Fried vermicelli is one of the common snack food in sub-continent especially in Pakistan. It is a type of pasta, round in section and somewhat thinner than

spaghetti. It is prepared using different recipes and looks like thin vermicelli usually roasted/fried in oil/fat until light brown color appears. Initially, the samples were subjected to oil extraction using Soxhlet extractor to know the exact oil content. High percentage of oil content was observed in all fried vermicelli samples (19.77 and 32.99%). The highest amount of oil was extracted from fried vermicelli-14 and minimum quantity was found in fried vermicelli-18. Table 1 shows the fatty acids composition of fried vermicelli expressed in percentage. In analyzed samples, palmitic (C-16:0) and stearic acid (C-18:0) were present in higher amounts, whereas dodecanoic (C-12:0), myristic (C-14:0) and arachidic acid (C-20:0) found in relatively low quantities. Among SFA, palmitic acid in fried vermicelli was present in the range of 34.6–47.5%. The stearic acid in fried vermicelli was present in the range of 4.76–10.6%. Oleic acid was observed as main contributor among MUFA in fried vermicelli samples. The percentage of oleic acid was found between 27.2–37.0% in fried vermicelli. Among MUFA, elaidic acid (*trans* fatty acid) was also detected in all fried vermicelli samples. The *trans* fatty acids in fried vermicelli was quantified in the range of 12.0–24.3%, highest and lowest value was found in fried vermicelli-17 and vermicelli-2, respectively, which indicated that fried vermicelli prepared in hydrogenated oil. Nutritional values of PUFA are very important because of essential FAs. The amount of PUFA in fried vermicelli samples was observed comparatively in less quantity (0.66–5.99 %). Linoleic acid (C18:2) was the main fatty acid in PUFA group.

Table 2 shows the fatty acid ratios and nutritive values of the fried vermicelli. SFA/UFA ratio showed co-relation of two main fatty acid groups. The value of this ratio was found between 0.72 – 1.92, indicated that SFA proportion present in higher amount. It has been reported that high ratio increases plasma very low density lipoprotein (VLDL) lipids and reduces the hepatic hypertriglyceridemic effect [17]. The minimum value of cis PUFA/SFA ratio set as 0.45 by British Department of Health, UK [18]. In this study, cis PUFA/SFA ratio were found lower than recommended limits in fried vermicelli samples which are not good for health in terms of CVD. Highest value of cis PUFA/SFA was found in fried vermicelli-12 (0.103) and minimum in fried vermicelli-3 (0.013). Trans FA/cis FA ratio is also a very important parameter which shows the degree of conversion of cis to *trans* configuration. In current study the ratio was found between 0.1 and 1.81. Higher values of this ratio indicated higher proportion of hydrogenated oil. cis PUFA/SFA + TFA and cis MUFA + cis PUFA/SFA + TFA are commonly used to express nutritional value of edible oils and fats [19]. In this study the values of cis PUFA/SFA + TFA were found between 0.01 and 0.097, whereas cis MUFA + cis PUFA/SFA + TFA ratio were found in the range of 27.7 to 37.05 in fried-vermicelli.

Table 1

Fatty acid composition of fried vermicelli

Fried vermicelli Sample No.	C 12:0	C 14:0	C 16:0	C18:2	C18:1 Cis	C18:1 trans	C18:0	C 20:0
1	-	0.14 ±0.01	41.5 ±0.00	2.73 ±0.00	37.0 ±0.01	12.2 ±0.00	6.38 ±0.00	-
2	-	0.54 ±0.01	41.7 ±0.01	2.14 ±0.02	35.1 ±0.07	12.0 ±0.01	8.49 ±0.01	-
3	0.03 ±0.01	0.25 ±0.03	41.6 ±0.01	0.66 ±0.01	33.0 ±0.04	13.8 ±0.01	10.6 ±0.07	0.07 ±0.00
4	-	0.52 ±0.02	37.3 ±0.01	3.22 ±0.05	30.6 ±0.01	19.4 ±0.01	8.91 ±0.02	-
5	-	0.66 ±0.01	38.8 ±0.02	5.99 ±0.02	32.5 ±0.00	14.5 ±0.01	7.54 ±0.01	-
6	0.02 ±0.01	0.26 ±0.05	34.6 ±0.01	1.97 ±0.01	32.0 ±0.01	23.4 ±0.05	7.60 ±0.01	0.12 ±0.01
7	0.18 ±0.01	0.86 ±0.00	40.6 ±0.00	3.92 ±0.00	30.2 ±0.01	15.4 ±0.01	8.58 ±0.00	0.24 ±0.05
8	0.16 ±0.01	0.89 ±0.01	42.1 ±0.00	3.90 ±0.01	28.8 ±0.03	17.2 ±0.01	6.73 ±0.00	0.27 ±0.01
9	0.30 ±0.01	0.79 ±0.01	40.8 ±0.06	3.58 ±0.04	29.3 ±0.00	16.7 ±0.06	8.60 ±0.02	-
10	0.55 ±0.01	-	47.5 ±0.00	1.56 ±0.01	27.2 ±0.01	18.4 ±0.01	4.76 ±0.05	-
11	-	0.68 ±0.02	39.6 ±0.01	2.81 ±0.03	28.3 ±0.05	22.9 ±0.01	5.78 ±0.01	-
12	-	0.40 ±0.02	38.5 ±0.01	4.74 ±0.01	30.0 ±0.01	19.3 ±0.03	6.94 ±0.00	0.15 ±0.04
13	-	0.48 ±0.01	38.8 ±0.04	2.86 ±0.01	28.5 ±0.00	23.9 ±0.01	5.43 ±0.01	-
14	-	0.15 ±0.05	40.4 ±0.05	1.40 ±0.00	31.6 ±0.05	20.5 ±0.02	5.88 ±0.01	-
15	-	0.37 ±0.01	37.0 ±0.00	2.15 ±0.01	31.6 ±0.01	22.0 ±0.00	6.74 ±0.05	0.18 ±0.05
16	0.02 ±0.01	0.26 ±0.06	37.3 ±0.02	1.91 ±0.05	33.6 ±0.02	20.4 ±0.01	6.49 ±0.01	0.06 ±0.00
17	0.03 ±0.01	0.38 ±0.01	39.1 ±0.01	1.30 ±0.02	28.5 ±0.02	24.3 ±0.04	6.38 ±0.06	0.07 ±0.01
18	-	0.69 ±0.01	41.9 ±0.00	2.48 ±0.02	29.4 ±0.01	16.5 ±0.01	9.06 ±0.01	-

Table 2

Fatty acid groups and fatty acids ratios of fried vermicelli (SFA, cis MUFA, trans MUFA, total MUFA, cis PUFA, SFA+TFA, MUFA+PUFA, cis MUFA+PUFA, SFA/PUFA, cis PUFA/SFA, trans MUFA+ cis MUFA, cis PUFA / SFA+TFA, cis MUFA+PUFA/SFA+TFA)

Fried vermicelli Sample No.	cis MUFA+PUFA/ SFA+TFA	cis PUFA/ (SFA+TFA)	trans / cis	cis PUFA/SFA	SFA/PUFA	cis MUFA+PUFA	MUFA+PUFA	SFA+TFA	cis PUFA	Total MUFA	trans MUFA	cis MUFA	SFA
1	37.05	0.045	0.308	0.057	0.923	39.74	51.99	60.26	2.73	49.30	12.26	37.01	48.00
2	35.15	0.034	0.322	0.042	1.030	37.26	49.25	62.72	2.14	47.1	11.99	35.12	50.73
3	33.04	0.010	0.410	0.013	1.105	33.69	47.50	66.31	0.66	46.8	13.81	33.03	52.50
4	30.70	0.049	0.571	0.069	0.878	33.87	53.23	66.12	3.22	50.0	19.36	30.65	46.76
5	32.59	0.097	0.377	0.128	0.887	38.48	53.00	61.51	5.99	47.0	14.52	32.49	46.99
6	32.05	0.030	0.688	0.046	0.743	33.99	57.36	66.01	1.97	55.4	23.37	32.02	42.64
7	30.22	0.059	0.452	0.078	1.020	34.08	49.49	65.92	3.92	45.6	15.41	30.16	50.51
8	28.81	0.058	0.528	0.078	1.004	32.66	49.89	67.34	3.90	46.0	17.23	28.75	50.11
9	29.36	0.053	0.507	0.071	1.018	32.89	49.55	67.11	3.58	46.0	16.67	29.31	50.45
10	27.27	0.022	0.638	0.030	1.118	28.81	47.20	71.19	1.56	45.6	18.39	27.25	52.80
11	28.30	0.041	0.736	0.061	0.854	31.08	53.94	68.92	2.81	51.1	22.86	28.26	46.06
12	30.04	0.072	0.557	0.103	0.850	34.71	54.05	65.29	4.74	49.3	19.34	29.97	45.95
13	28.52	0.042	0.764	0.064	0.809	31.34	55.28	68.66	2.86	52.4	23.94	28.49	44.72
14	31.67	0.021	0.619	0.030	0.868	33.05	53.53	66.95	1.41	52.1	20.47	31.64	46.47
15	31.60	0.032	0.652	0.048	0.795	33.72	55.71	66.28	2.15	53.6	21.98	31.57	44.29
16	33.64	0.030	0.573	0.043	0.790	35.52	55.88	64.48	1.91	53.9	20.35	33.61	44.12
17	28.50	0.018	0.814	0.028	0.850	29.78	54.04	70.22	1.30	52.7	24.26	28.48	45.95
18	29.43	0.036	0.518	0.048	1.067	31.87	48.37	68.13	2.48	45.9	16.50	29.40	51.63

ATR-FTIR spectra of fried vermicelli

The representative FTIR spectra of extracted oil of fried vermicelli are shown in Figure 1A. The assignments of the bands corresponding to the stretching vibration modes are usually easier than the assignments of the bands corresponding to the bending vibration modes due to overlap [20]. The stretching vibration band at 3004 cm^{-1} and two intense bands at 2920 cm^{-1} and 2851 cm^{-1} correspond to the cis double-bonds and asymmetric and symmetric stretching vibration of aliphatic C-H_2 functional groups, respectively.

Intense band of carbonyl functional group of triglycerides appear at 1742 cm^{-1} , the aliphatic groups of the CH_2 and CH_3 shows a band near 1465 cm^{-1} because of the bending vibrations, whereas the rocking vibrations of CH band at 1418 cm^{-1} appeared due to the cis-olefins and 1377 cm^{-1} band is due to bending vibrations of CH_2 groups. Stretching vibrations of C-O ester group typically shows four bands at 1235 , 1161 , 1116 and 1097 cm^{-1} along with CH_2 group associated with bending vibrations at first two frequencies i.e.

1235 cm^{-1} and 1161 cm^{-1} . Characteristic band of isolated *trans* olefins at 966 cm^{-1} appears due to the bending vibrations of C-H out of plane deformation, while the band at 721 cm^{-1} is due to the rocking vibration of out of plane *cis* olefins overlapping of CH_2 .

FTIR spectral pre-treatment and data correction

For the FTIR quantification of various fatty acid groups and their ratios, different regions of the mid IR range were used to construct suitable model using 1st and 2nd derivative spectra in order to improve regression values as compare to the pure absorbance signal. Figure 1A, 1B and 1C shows normal, 1st derivative and 2nd derivative spectra of extracted fried vermicelli oil, respectively.

PLS models

Table 3A and Table 3B illustrates the quality parameters based on Fig 2A and Fig 2B including selected spectral region, baseline type, factors, R^2 value and RMSEC of models to predict groups such as SFA, MUFA, *cis*-MUFA, PUFA, TFA and fatty acid ratios. The number of factors used in PLS models were auto selected by TQ software in regression analysis based on attaining minimum predicted residual error of sum of squares (PRESS) value. For the development of calibration model partial least square (PLS) regression was applied, whereas the obtained GC-MS values of SFA, MUFA, *cis*-MUFA, PUFA, TFA and their ratios were used as reference to establish correlation between actual GC-MS and predicted FTIR values. For each PLS model 18 samples were used as calibration points. It was found that difference between actual and predicted values of SFA, MUFA, *cis*-MUFA, PUFA, TFA and their ratios were very small which indicates successfulness of developed PLS models.

Minimum three models were developed by selecting different spectral regions for each fatty acids groups and ratios. For SFA model best results were achieved in the regions of 2970–2820 & 1400–1200 cm^{-1} with R^2 and RMSEC value of 0.999 and 0.112, respectively. Model developed for total MUFA showed higher R^2 value 0.99916 in the region of 3000–3050 cm^{-1} using linear removed baseline with RMSEC 0.132. On the other hand, individually *cis* and *trans* MUFA models demonstrated good results with linear removed baseline in the region of 3050–2850 cm^{-1} and 2nd derivative in the spectral range of 980–945 cm^{-1} . The high R^2 values were achieved in both models 0.999 and 0.991 with minimum RMSEC value 0.00984 and 0.504, respectively. For the quantification of *cis* PUFA in fried vermicelli, best model was developed in the range of 2989–2869 cm^{-1} using linear removed baseline type with R^2 and RMSEC values of 0.999 and 0.031, respectively. The developed PLS model for fatty acid ratios including SFA+TFA (2880–2815 & 980–945), MUFA+PUFA (3010–2880), *cis* MUFA+PUFA (3050–2650 & 1650–1800), SFA/UFA (3010–2880), *cis* PUFA/SFA (2950–2800 & 679–786), *trans* MUFA/*cis* MUFA (2950–2880 & 980–945) and *cis* MUFA+PUFA/SFA+TFA (3050–2800 & 1520–1000) showed R^2 values of 0.999 except in *cis* PUFA/(SFA+TFA) (2950–2800 & 980–945) model which has R^2 value of 0.997 with the maximum RMSEC value of 0.092 in SFA+TFA model and minimum RMSEC was found to be 0.11e-3 in *cis* PUFA/ SFA model. Table 4A and Table 4B show the results of fatty acids groups and fatty acids ratios respectively, obtained from GC-MS and FTIR with difference between them. In all the developed FTIR models, there is very little difference compared to GC-MS results.

Figure 1.
 A - Normal FTIR spectra of fried vermicelli; B - 1st derivative spectra;
 C - 2nd derivative spectra of all the samples

Table 3A

FTIR PLS correlation model of fatty acid groups

Fatty acid	Spectral region cm⁻¹	Baseline type	Factors	R²	RMSEC
SFA	3050–650	None	2	0.818	1.74
	2950–2820&1125–1080	None	4	0.956	0.888
	2970–2820&1400–1200	None	7	0.999	0.112
cis MUFA	3050–2950	None	8	0.999	0.0357
	3020–650	None	3	0.885	1.15
	3050–2850	Linear removed	10	0.999	0.009
<i>trans</i> MUFA	980–945	None	4	0.984	0.674
	980–945	1 st Derivative	4	0.988	0.605
	980–945	2nd Derivative	5	0.991	0.504
Total MUFA	3050–650	None	3	0.958	1.04
	4000–650	None	2	0.959	1.03
	3050–3000	Linear Removed	9	0.999	0.132
cis PUFA	2989–2869	None	5	0.984	0.229
	4000–650	None	1	0.759	0.839
	2989–2869	Linear Removed	8	0.999	0.031

Table 3B

FTIR PLS correlation model of fatty acid ratios

Fatty acid ratios	Spectral region cm ⁻¹	Baseline type	Factors	R ²	RMSEC
SFA+TFA	2880–2815 &	None	9	0.999	0.092
	980–945	None	2	0.808	1.570
	3010–750 &	None	7	0.999	0.101
	990–945 3050–2950				
MUFA+PUFA	3010–2880	None	7	0.999	0.091
	3015–2835	None	6	0.999	0.122
	3040–2830	None	4	0.992	0.383
Cis MUFA+PUFA	3050–2700 &	None	3	0.984	0.480
	1650–1800	None	3	0.839	1.480
	3050–2870 &	1st	4	0.999	0.060
	1650–1800 3050–2650 & 1650–1800	Derivative			
SFA/UFA	3030–2880	None	6	0.999	0.006
	3040–2880	None	6	0.998	0.006
	3010–2880	None	7	0.999	0.003
cis PUFA/ SFA	2950–2800 &	None	8	0.999	0.11e⁻³
	679–786	None	5	0.992	0.003
	2950–2800 3000–2800	None	3	0.929	0.009
trans MUFA/ cis MUFA	2950–2830 &	None	5	0.994	0.015
	980–945	None	3	0.975	0.031
	3050–2950 &	Linear	7	0.999	0.006
	980–945 2950–2880 & 980–945	removed			
cis PUFA/(SFA+TFA)	3050–2800 &	None	4	0.980	0.003
	980–945	None	5	0.992	0.002
	2950–2800	Linear	6	0.997	0.001
	2950–2800 & 980–945	removed			
Cis MUFA+PUFA/ SFA+TFA	3050–2800 &	None	7	0.998	0.053
	1000–900	None	8	0.999	0.006
	3050–2800 & 1520–1000	None	4	0.961	0.681
	3050–2800 & 1830–920

Figure 2A. PLS models for SFA, cis-MUFA, *trans*-MUFA, total-MUFA and total PUFA.

Figure 2B. PLS models for SFA+TFA, MUFA+PUFA, cis-MUFA+PUFA, SFA/TFA, cis PUFA/SFA, trans MUFA/ cis MUFA, cis PUFA/SFA+TFA and Cis MUFA+PUFA/ SFA+TFA.

Table 4A

Comparative results of FTIR and GC methods for fatty acid groups

Fried vermicelli Sample No	SFA			cis MUFA			trans MUFA		
	GC	FTIR	Diff	GC	FTIR	Diff	GC	FTIR	Diff
1	48.003	47.769	-0.234	37.010	37.017	0.007	12.255	12.235	-0.020
2	50.730	50.860	0.130	35.120	35.116	-0.004	11.990	12.596	0.606
3	52.498	52.504	0.006	33.030	33.024	-0.006	13.808	13.075	-0.733
4	46.760	46.921	0.161	30.650	30.634	-0.016	19.360	19.597	0.237
5	46.999	47.006	0.006	32.492	32.493	0.001	14.516	14.696	0.180
6	42.641	42.606	-0.036	32.016	32.022	0.006	23.369	23.222	-0.147
7	50.508	50.492	-0.016	30.165	30.156	-0.008	15.412	14.737	-0.675
8	50.113	50.051	-0.062	28.755	28.758	0.003	17.228	17.927	0.699
9	50.447	50.450	0.002	29.310	29.303	-0.007	16.666	16.838	0.172
10	52.798	52.803	-0.017	27.248	27.264	0.016	18.392	18.465	0.073
11	46.062	45.915	-0.147	28.265	28.255	-0.009	22.859	22.747	-0.112
12	45.950	45.845	-0.105	29.970	29.963	-0.007	19.340	19.428	0.088
13	44.721	44.683	-0.037	28.487	28.495	0.009	23.935	23.659	-0.276
14	44.293	44.327	0.034	31.573	31.579	0.006	21.984	22.679	0.695
15	44.124	44.319	0.195	33.614	33.606	-0.008	20.354	21.051	0.698
16	45.955	45.867	-0.088	28.480	28.467	-0.013	24.262	23.108	-1.154
17	46.473	46.675	0.202	31.646	31.663	0.018	20.474	20.562	0.089
18	51.627	51.611	0.005	29.398	29.409	0.012	16.499	16.081	-0.418

Fried vermicelli Sample No	Total MUFA			cis PUFA		
	GC	FTIR	Diff	GC	FTIR	Diff
1	49.265	49.281	0.016	2.730	2.713	-0.017
2	47.110	47.131	0.021	2.140	2.077	-0.063
3	46.838	46.867	0.029	0.663	0.698	0.035
4	50.010	49.810	-0.200	3.220	3.236	0.016
5	47.007	46.735	-0.272	5.993	5.962	-0.031
6	55.386	55.595	0.209	1.973	2.011	0.038
7	45.576	45.791	0.215	3.916	3.920	0.004
8	45.983	46.093	0.110	3.905	3.910	0.005
9	45.976	46.091	0.115	3.576	3.598	0.023
10	45.640	45.476	-0.164	1.561	1.539	-0.022
11	51.124	51.237	0.113	2.814	2.767	-0.047
12	49.310	49.317	0.007	4.740	4.803	0.063
13	52.422	52.288	-0.134	2.858	2.823	-0.034
14	53.557	53.612	0.055	2.149	2.162	0.013
15	53.968	53.884	-0.084	1.908	1.927	0.019
16	52.742	52.706	-0.035	1.304	1.294	-0.010
17	52.119	52.037	-0.082	1.407	1.431	0.024
18	45.897	45.978	0.081	2.476	2.459	-0.016

Table 4B

Comparative results of FTIR and GC methods for fatty acid ratios

Sample No	SFA+TFA			MUFA+PUFA			Cis UFA+ PUFA			cis PUFA/ (SFA+TFA)		
	GC	FTIR	Diff	GC	FTIR	Diff	GC	FTIR	Diff	GC	FTIR	Diff
1	60.258	60.345	0.087	51.995	52.093	0.098	39.740	39.752	0.012	0.045	0.045	-0.000
2	62.720	62.770	0.050	49.250	49.225	-0.025	37.260	37.219	-0.041	0.034	0.034	0.000
3	66.306	66.257	-0.049	47.501	47.419	-0.082	33.693	33.733	0.040	0.010	0.009	-0.001
4	66.120	66.173	0.053	53.230	53.171	-0.059	33.870	33.864	-0.006	0.049	0.048	-0.001
5	61.515	61.469	-0.046	53.000	53.071	0.071	38.485	38.549	0.064	0.097	0.097	0.000
6	66.011	66.035	0.024	57.358	57.466	0.108	33.989	34.060	0.071	0.030	0.031	0.001
7	65.920	65.759	-0.161	49.492	49.334	-0.158	34.080	34.069	-0.011	0.059	0.059	0.000
8	67.341	67.464	0.123	49.888	49.936	0.048	32.659	32.632	-0.027	0.058	0.059	0.001
9	67.114	67.062	-0.051	49.552	49.583	0.031	32.886	33.034	0.148	0.053	0.056	0.003
10	71.190	71.178	-0.012	47.201	47.333	0.132	28.809	28.797	-0.012	0.022	0.021	-0.001
11	68.921	69.090	0.169	53.938	53.941	0.003	31.079	31.162	0.083	0.041	0.037	-0.004
12	65.290	65.258	-0.032	54.050	54.153	0.103	34.710	34.666	-0.044	0.072	0.070	-0.002
13	68.656	68.530	-0.125	55.279	55.301	0.022	31.344	31.357	0.013	0.042	0.042	-0.000
14	66.277	66.446	0.169	55.707	55.578	-0.128	33.723	33.647	-0.076	0.032	0.031	-0.001
15	64.478	64.372	-0.106	55.876	55.735	-0.141	35.522	35.443	-0.079	0.030	0.032	0.002
16	70.216	70.202	-0.014	54.045	54.129	0.083	29.784	29.758	-0.026	0.018	0.020	0.002
17	66.947	66.874	-0.073	53.527	53.417	-0.110	33.053	32.930	-0.123	0.021	0.023	0.002
18	68.127	68.122	-0.005	48.373	48.378	0.006	31.873	31.889	0.015	0.036	0.035	-0.001

Sample No	SFA/UFA			Cis PUFA / SFA			Trans MUFA/ cis MUFA			Cis MUFA+PUFA/ SFA+TFA		
	GC	FTIR	Diff	GC	FTIR	Diff	GC	FTIR	Diff	GC	FTIR	Diff
1	0.920	0.917	-0.003	0.057	0.057	-0.000	0.308	0.311	0.003	37.050	37.057	0.007
2	1.030	1.027	-0.003	0.042	0.042	0.000	0.322	0.313	-0.009	35.150	35.151	0.001
3	1.100	1.104	0.004	0.013	0.013	-0.000	0.410	0.405	-0.005	33.040	33.039	-0.001
4	0.880	0.883	0.003	0.069	0.069	0.000	0.572	0.581	0.009	30.700	30.696	-0.004
5	0.890	0.883	-0.007	0.128	0.128	-0.000	0.377	0.379	0.002	32.590	32.589	-0.001
6	0.740	0.738	-0.002	0.046	0.046	-0.000	0.688	0.675	-0.013	32.050	32.049	-0.001
7	1.020	1.027	0.007	0.078	0.078	0.000	0.452	0.456	0.004	30.220	30.215	-0.005
8	1.000	0.996	-0.004	0.078	0.078	-0.000	0.528	0.536	0.008	28.810	28.800	-0.010
9	1.020	1.019	-0.001	0.071	0.071	0.000	0.507	0.513	0.006	29.360	29.360	-0.000
10	1.120	1.119	-0.001	0.030	0.030	-0.000	0.638	0.651	0.013	27.270	27.270	0.000
11	0.850	0.850	-0.000	0.061	0.061	-0.000	0.736	0.734	-0.002	28.300	28.316	0.016
12	0.850	0.855	0.005	0.103	0.103	-0.000	0.557	0.556	-0.001	30.040	30.044	0.004
13	0.810	0.810	0.000	0.064	0.064	0.000	0.764	0.768	0.004	28.520	28.516	-0.004
14	0.730	0.730	0.000	0.048	0.048	-0.000	0.652	0.656	0.004	31.600	31.596	-0.004
15	0.800	0.805	0.005	0.043	0.043	-0.000	0.573	0.564	-0.009	33.640	33.640	-0.000
16	0.790	0.793	0.003	0.028	0.028	0.000	0.814	0.809	-0.005	28.500	28.509	0.009
17	0.850	0.843	-0.007	0.030	0.030	0.000	0.619	0.610	-0.009	31.670	31.663	-0.007
18	0.870	0.871	0.001	0.048	0.048	-0.000	0.518	0.519	0.001	29.430	29.431	0.001

Conclusion

In the present study, fried vermicelli was completely analyzed for their fatty acid profile including various groups and ratios by GC-MS. Based on results, it was concluded that fried vermicelli contain high percentage of oil ranging from 19.77 and 32.99%. Fatty acid composition revealed that SFA and MUFA present in higher amount as compare to PUFA in fried vermicelli. All fried vermicelli samples showed higher *trans* fatty acids which indicated that samples were prepared in hydrogenated oil. Furthermore, fried vermicelli also showed less nutritional values in comparison to recommended values of *trans* fat and cis PUFA/SFA ratio set as 0.5% and 0.45, respectively. FTIR spectroscopy successfully applied to quantify fatty acid groups and ratios in fried vermicelli using chemometric. The developed PLS models showed higher correlations (>0.99) with less calibration error. The selected wavelength regions can be used to quantify the fatty acid group and their ratios using FTIR with least analysis time without using organic solvents.

Acknowledgements

The National Centre of Excellence in Analytical Chemistry, University of Sindh, Jamshoro, Pakistan is gratefully acknowledged for providing the financial support and laboratory facilities.

References

1. Burlingame B., Nishida C., Uauy R., Weisell R. (2009), Fats and fatty acids in human nutrition: introduction, *Annals of Nutrition and Metabolism*, 55(1–3), pp. 5–7.
2. Simopoulos, A. P. (2002), The importance of the ratio of omega-6/omega-3 essential fatty acids, *Biomedicine & pharmacotherapy*, 56(8), pp. 365–379.
3. Mozaffarian D., Micha R., Wallace S. (2010), Effects on coronary heart disease of increasing polyunsaturated fat in place of saturated fat: a systematic review and meta-analysis of randomized controlled trials, *PLoS Medicine*, 7(3), e1000252, DOI: 10.1371/journal.pmed.1000252
4. Gillingham L G., Harris-Janzen S., Jones P J. (2011), Dietary monounsaturated fatty acids are protective against metabolic syndrome and cardiovascular disease risk factors, *Lipids*, 46(3), pp. 209–228.
5. Poudyal H., Panchal S K., Diwan V., Brown L. (2011), Omega-3 fatty acids and metabolic syndrome: Effects and emerging mechanisms of action, *Progress in Lipid Research*, 50(4), pp. 372–387.
6. Erkkila A., de Mello V D., Risérus U., Laaksonen D E. (2008), Dietary fatty acids and cardiovascular disease: an epidemiological approach, *Progress in Lipid Research*, 47(3), pp. 172–187.
7. Oh K., Hu FB., Manson J E., Stampfer M J., Willett W C. (2005), Dietary fat intake and risk of coronary heart disease in women: 20 years of follow-up of the nurses' health study, *American Journal of Epidemiology*, 161(7), pp. 672–679.
8. Czernichow S., Thomas D., Buckert E. (2010), n-6 Fatty acids and cardiovascular health: A review of the evidence for dietary intake recommendations, *British Journal of Nutrition*, 104(06), pp. 788–796.

9. Shahidi F., Wanasundara U N. (2002), Methods for measuring oxidative rancidity in fats and oils, *Food lipids: Chemistry, Nutrition and Biotechnology*, pp. 387–403.
10. Eckel R H., Borra S., Lichtenstein A H., Yin-Piazza S Y. (2007), Understanding the complexity of trans fatty acid reduction in the American Diet American Heart Association *trans Fat conference 2006: report of the trans fat conference planning group*, *Circulation*, 115(16), pp. 2231–2246.
11. Food and Drug Administration F.D.A. (2003), Food labeling: trans fatty acids in nutrition labeling, nutrient content claims, and health claims. Final rule, *Federal Register*, 68(133), pp. 41433.
12. Uauy R., Aro A., Clarke R., L'abbé M R., Mozaffarian D., Skeaff C M., Stender S., Tavella M. (2009), WHO Scientific Update on trans fatty acids: summary and conclusions, *European Journal of Clinical Nutrition*, 63, pp. S68–S75.
13. Food and Drug Administration F.D.A. (2015), *The FDA takes step to remove artificial trans fats in processed foods*, Available at: <http://www.fda.gov/NewsEvents/Newsroom/PressAnnouncements/ucm451237.html> accessed 12.02.2016.
14. AOAC (1997), *Official methods of analysis. 16th ed*, Gaithersburg, Maryland.
15. IUPAC (1979), *Standard methods for the analysis of oils, fats and derivatives* (6th ed.), Pergamon Press, Oxford, pp. 96–98.
16. Kandhro A., Sherazi S T H., Mahesar S A., Bhanger M I., Talpur M Y., Arain S. (2008), Monitoring of fat content, free fatty acid and fatty acid profile including trans fat in Pakistani biscuits, *Journal of the American Oil Chemists' Society*, 85(11), pp. 1057–1061.
17. Chang N W., Ten Wu C., Chen F N., Huang P C. (2004), High polyunsaturated and monounsaturated fatty acid to saturated fatty acid ratio increases plasma very low density lipoprotein lipids and reduces the hepatic hypertriglyceridemic effect of dietary cholesterol in rats, *Nutrition research*, 24(1), pp. 73–83.
18. HMSO, UK Department of Health. (1994), Nutritional aspects of cardiovascular disease. London, *Report on Health and Social Subjects*, 46, pp. 37–46
19. Alonso L., Fraga M J., Juarez M. (2000), Determination of trans fatty acids and fatty acid profile in margarines marketed in Spain, *American Oil Chemists' Society*, 77(2), pp. 131–136.
20. Guillen M D., Cabo N. (1997), Infrared spectroscopy in the study of edible oils and fats, *Journal of the Science of Food and Agriculture*, 75(1), pp. 1–11.