Fourier transform infrared spectroscopy and chemometrics for chemical property prediction of chemically interesterified lipids with butterfat and vegetable oils during storage

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ABSTRACT

The storage stability of structured lipids has a great importance for food industry and should be defined clearly. The aim of the study is to manufacture structured lipids by chemical interesterification of butterfat with different vegetable oils, to determine some chemical properties of interesterified lipids throughout storage and to predict free fatty acid, peroxide value, malondialdehyde and mono-di-triacylglycerol contents of these lipids by using middle infrared spectroscopy (FT-MIR). Prediction models were constructed by using partial least square (PLS) regression with an external cross-validation. The PLS model for TAG with FT-MIR data showed an excellent predictive potential with higher R^2_{cal}=0.98, R^2_{cv}=0.99 and lower RMSE values. The model for monoacylglycerol content (MAG) showed a good predictive ability with higher R^2_{cal}=0.88, R^2_{cv}=0.90 and lower RMSE values. The PLS model constructed with FT-IR spectra for diacylglycerol (DAG) content have good capability of prediction due to higher R^2 and lower RMSE values. For the prediction of malondialdehyde (MAD) of interesterified lipids by FT-MIR spectra, regression coefficient of calibration set was found as 0.84. For the prediction of peroxide value (PV) of interesterified lipids with FT-MIR spectra, R^2_{CV}=0.76 and RMSEC=1.52 and RMSECV=1.15. Infrared spectroscopy technique could be used for analyzing the chemical changes of fats during storage and also suggests a rapid and non-destructive techniques as good alternatives to the traditional analytical methods.

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1. Introduction

Butterfat contains a wide range of lipid components and has been used as an ingredient in different food applications. The recent advances in technologies for fat modification have improved its uses in food industry. There are several mechanisms available for the modification of butterfat including fractionation, crystallization, short-path distillation, ultrasound processing and interesterification [1].

Interesterification reactions catalyze positional rearrangement of fatty acids on the glycerol backbone of triacylglycerols. The chemical catalysts snatch the fatty acids from their original location and randomly distribute on the glycerol backbone. The interesterification of binary blend of butterfat with different vegetable oils results in increases of unsaturated fatty acid ratio, reduction in hardness, better melting profiles, lower consistency and improved nutritional properties [2,3,4]. The chemical interesterification of butterfat with corn oil significantly reduced trisaturated and triunsaturated triacylglycerol contents [5]. The binary blends of butterfat-canola oils showed better melting behaviour, microstructure and rheological properties after chemical interesterification [6].

Infrared (IR) radiation is the region of the electromagnetic spectrum between the visible and the microwave wavelengths [7]. The infrared region is subdivided into three (near-, mid- and far-infrared) sections. The nominal range of wavelengths for mid-infrared (MIR) is from 2500 to 25.000 nm (4000 to 400 cm^{-1}). The samples in different phases (solid, liquid and gase) have the ability of absorbing IR radiation at specific wavelengths known as 'fingerprint region (1500–800 cm^{-1})'. In general, the spectral signatures in the MIR region are based on the fundamental stretching, bending, and rotating vibrations of the molecules. The spectral peaks of MIR region are quite sharper and better resolved. An MIR spectrum consists of a series of absorbance peaks belong to O–H, N–H, C–H, and S–H bands arranged in order of decreasing wavenumber [8,9].

IR spectroscopy techniques provide useful informations about food processing and storage for controlling some quality parameters of the products [10]. The IR spectra determines types and number of chemical bonds present in different food samples that can be used to analyze chemical changes occurring in both processing and storage. There are several studies related to IR spectroscopy applications to determine some properties of fats and oils [11,12,13].

It is well known that the combination of chemometrics with analytical methods could enhance the information generated in order to increase their use for applications in food industry including composition measurement, process monitoring, traceability and authenticity. Moreover, the attachment of chemometrics with MIR spectroscopic methods provide the ability to determine more than one component at a time. The engagements have also the capability of detecting patterns in a data set and to develop mathematical models to predict or monitor composition of food samples [10,13,14].

The chemical alterations in fats and oils that could occur during storage has a great attention due to food safety, food quality, economic loses and consumers demands. Therefore, it is highly needed to adjust both process parameters and conditions suitable for long-term storage. The MIR spectroscopy combined with chemometrics have been extensively used to measure chemical composition of fats and oils. However, a few studies can be found on the use of this methods for storage of interesterified lipids. In this study, it was aimed to characterize some chemical properties of structured lipids produced by chemical interesterification of butterfat with different vegetable oils during storage and to investigate the capability of MIR spectroscopy coupled to chemometrics to predict some chemical properties including peroxide value, malondialdehyde, free fatty acid and mono-di-triacylglycerol contents of these lipids.

2. Materials and methods

2.1. Production of Interesterified Lipids

The butterfat, refined corn and nut oils used for interesterification reactions were obtained from a local market. Sodium methoxide was used as chemical catalyst (Solem Kimya, Turkey). All binary blends were prepared at three different butterfat/oil blend ratios (5:5, 6:4, and 7:3 w/w) and chemically interesterified lipids were produced by adding 0.75 g catalyst/100 g sample. Fourty-two different structured lipids were manufactured by chemical interesterification [15]. Moreover, thirty-six non-interesterified blends were also prepared and all samples were stored at 7 °C for 10-20-30 days in a refrigerator (Arçelik, Turkey).

2.2. Determination of free fatty acid content

Titrimetric method specified in AOCS standard official method Ca 5a-40 was used in free fatty acid (FFA) determination of the products [16]. The analyses were performed twice. Acidity was expressed as percentage of oleic acid.

2.3. Determination of peroxide value

The peroxide value (PV) of samples were determined titrimetrically by the AOCS standard official method Cd 8-53 [17]. The analyses were performed twice. The PV expressed in terms of milliequivalents (meq) of oxygen per kilogramme of sample.

2.4. Determination of Mono-di-triacylglycerol Content

Mono- (MAG), di- (DAG) and triacylglycerol (TAG) contents of structured lipids were analyzed according to AOCS Cd11C-93

method by column chromatography [18]. Samples were dissolved in chloroform and transferred to the column by washing with chloroform three times. Then, 250 mL of 10, 25 and 100% (v/v) diethyl ether in petroleum ether were used for the elution of TAG, DAG and MAG fractions, respectively. The fractions were collected separately in a flask and solvents were evaporated in a rotary evaporator (Laborato 4000 Heidolph, Germany) at 50 °C. The flasks were dried until constant weight. Percentages of mass fractions were calculated for each part.

2.5. Malondialdehyde determination

For the malondialdehyde (MDA) analysis spectrophotometric method given in published procedure was used [19]. The absorbance was measured at 532 nm by using an UV−vis spectrophotometer (Optima SP3000, Japan). The MDA content of interesterified lipids were expressed as μg MDA per gram sample.

2.6. FT-MIR spectroscopy analyses

The FT-MIR spectra were collected by a spectrometer (Bruker Tensor II, Bruker Inc., Billerica, MA, USA) on structured lipids as well as on butterfat, and non-interesterified blends during storage. Spectra were collected over the range of 4000-400 cm^{-1}, at 4 cm^{-1} resolution, by using a single reflection ZnSe ATR cell and 32 scans for both samples and background. The measurements were dublicated on samples.

2.7. Data analysis

The FT-MIR spectral data are inexplicable and the analytical methods are not sufficient, more comprehensive multivariate analysis techniques should be accomplished. Therefore, raw FT-MIR spectral data were transferred to a multivariate data analysis software (SIMCA 14.1, MKS Umetrics, Umea, Sweeden) for multivariate quantitative analysis. The data matrice with 82 different lipid samples including butterfat (4), interesterified lipids (42), and non-esterified blends (36) were constructed with FT-MIR spectra of these samples. The capability of predicting chemical properties of interesterified fats from infrared spectra was investigated by Partial Least Square Analysis (PLS). All regression models were developed by using FT-MIR spectra of samples individually. The replicated spectra were averaged prior to the application of various preprocessing techniques including; standard normal variate (SNV), multiplicative scatter correction (MSC), first (d1) and second-order (d2) derivatives. The partial least square regression (PLS) analysis was applied to each pre-treated data matrices in order to predict the chemical properties of interesterified lipids throughout storage. Moreover, the models were also validated by an external cross-validation procedure. The PLS results are explained in terms of significant components (PCs), coefficients of determination in calibration (R^2_{cal}), cross-validation (R^2_{cv}), root mean square errors of calibration (RMSEC), and validation (RMSECV).

3. Results and discussions

3.1. Chemical properties of interesterified lipids during storage

The FFA content of interesterified samples and blends was determined in order to obtain a measure about the hydrolytic rancidity during storage. The FFA% of structured lipids ranged from 0.46 to 2.09 as reported in Table 1. The initial FFA% of butterfat is 1.34% while binary blends have an acidity range of 0.54-1.62%. Generally, FFA% of interesterified lipids decreased compared to initial blends after chemical interesterification as seen in another study [20]. The

Table 1

Minimum and maximum values of chemical parameters for interesterified lipids, binary blends and butterfat throughout storage.

Response	Butterfat (min-max value)	Interesterified Lipids (min-max value)	Binary Blends (min-max value)
FFA%	0.81-1.34	0.46-2.09	0.54-1.62
TAG%	63.96-66.59	55.21-80.48	57.22-83.90
DAG%	18.06-23.06	8.76-21.60	5.50-28.51
MAG%	3.40-5.70	1.35-6.86	1.13-10.68
PV meq (O_2/kg)	4.00-9.68	0.85-9.66	2.64-11.38
MDA (μg MDA/g)	12.15-23.40	0.12-0.90	1.26-16.09

*FFA, Free Fatty Acid Content; TAG, Triacylglycerol content; DAG, Diacylglycerol content; MAG, monoacylglycerol content; PV, Peroxide Value; MDA, Malondialdehyde content.
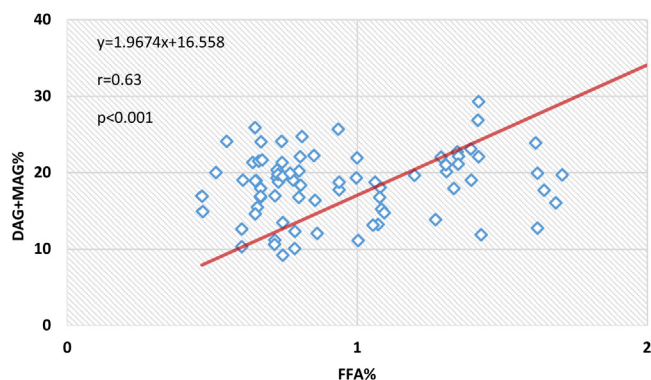

Fig. 1. Free fatty acid content (FFA%) versus monoacylglycerol and diacylglycerol content (MAG+DAG%) of samples during storage.

structured lipids interesterified with nut oil have lower FFA% compare to corn oil-butterfat samples throughout storage. The FFA content of interesterified lipids containing 50% and 30% of corn oil did not change during storage period. The samples structured with 40% corn oil had highest FFA content at the 20th day of storage. However, structured lipids interesterified with nut oil slightly increased throughout the storage at 7 °C. The increase in FFA content of interesterified lipids during storage was also observed in another studies [20,21].

The MAG, DAG and TAG contents of samples were determined in order to better understand the changes in the glycerol backbone associated with hydrolytic rancidity that occurred during storage process. The ranges of MAG, DAG and TAG contents of the samples are expressed in relative percentages of overall content (Table 1). The results are in accordance with the previous studies, which observed a decrease in TAG% and some increases in DAG-MAG% after interesterification reactions [22,23]. The decrease in TAG% contents of all samples after interesterification could be related to the production of partial mono- and diacylglycerols. The TAG% of interesterified lipids did not significantly change during storage period regardless of oil type. This result was also observed in a previous work examining storage stability of interesterified lipids [20]. The DAG and MAG contents of structured lipids with nut oil showed a slight increasing trend throughout storage. The MAG and DAG content of the sample with 40% corn oil reached highest ratio at the 20th day of storage as in the result of FFA content. In order to better analyze the changes in FFA, DAG and MAG content during storage process a correlation between FFA% and MAG+DAG content of samples was evaluated (Fig. 1). The correlation coefficient is calculated and found as 0.63. There was an increasing trend between FFA content and MAG+DAG% of the samples (Fig. 1). Generally, the samples having higher amounts of MAG+DAG content, also have higher FFA% as Fig. 1 indicated. Therefore, the increase in both FFA% and MAG+DAG% can be associated with increase in the hydrolytic rancidity of samples during storage.

The PV of samples was used as an index of the oxidative stability during storage. The PV of butterfat is 9.68 meq O_2/kg sample while blends without interesterification have a range of 2.64-11.38 meq O_2/kg sample (Table 1). In general, PV of interesterified samples decreased compared to starting blends. The PV of interesterified fats with nut oil less than structured lipids containing corn oil. This result could be associated with the high linoleic acid content of corn oil. There are some fluctuations in PV of samples interesterified with nut oil depending on storage period. However, the structured fat with 40% nut oil had lowest PV at the 20th day of storage time. There was an increase in PV of lipids that interesterified with corn oil at the 20th day of storage regardless of blend ratio. In general, interesterified lipids had PV less than 10 meq O_2/kg which is recommended as the limit value [24].

The MDA content is widely used as a measure parameter of lipid peroxidation. The initial MDA content of butterfat is 23.40 μg MDA/g. After both blending and chemical interesterification the MDA content of samples drastically decreased regardless of oil type. The MDA content of structured lipids ranged from 0.12 to 0.90 as shown in Table 1. The decrease in MDA content could be associated with the evaporation of MDA or the attachment to other compounds. The MDA content of structured lipids interesterified with nut oil slightly increased by advancing storage days. There were some ups and downs in MDA content of interesterified lipids containing corn oil during storage. However, the MDA content of sample with 40% corn oil reached maximum value at the 30th day of storage. Generally, the oxidative stability of samples is strongly affected by oil type chosen for interesterification reactions throughout storage.

3.2. FT-MIR spectral profiles of interesterified lipids

The FT-MIR spectra of interesterified lipids, binary blends and butterfat during storage were shown in Fig. 2. The absorption of hydroxyl presents in the range of 2700-3000-cm^{-1} and was characterized by hydroperoxides and could be related to PV of interesterified fats (Fig. 2). The absorption of FFA occurs around 1700 cm^{-1}, which can be used to estimate the degree of hydrolysis of triglycerides throughout storage period (Fig. 2). Generally, the focus area of the MIR spectra is the fingerprint region which is provided in Fig. 3. In the fingerprint area, C-O-C vibration in esters, C−H bending and stretching vibrations, and the second overtone of C=O and −OH in fatty acid structure was observed. The carbon chain skeleton vibrations around 700 cm^{-1} is related to degree of oxidative reactions and could be associated with MDA content (Fig. 3). The out-of-plane bending vibrations and stretching of −C−O− and −CH_2 occurred between 1000−1500 cm^{-1} which are related to cis and trans form of fatty acids [25,26,27]. The FT-MIR spectra of samples interesterified with nut oil were given in Fig. 3. The spectra colored by blue presents the interesterified lipid stored for 20 days and the pink colored one belongs to 30 days stored sample. It is clearly understood that, 30 days of storage of structured lipids resulted in higher FFA content and increase in oxidation reactions as Fig. 3 indicated. As result, FT-MIR absorption
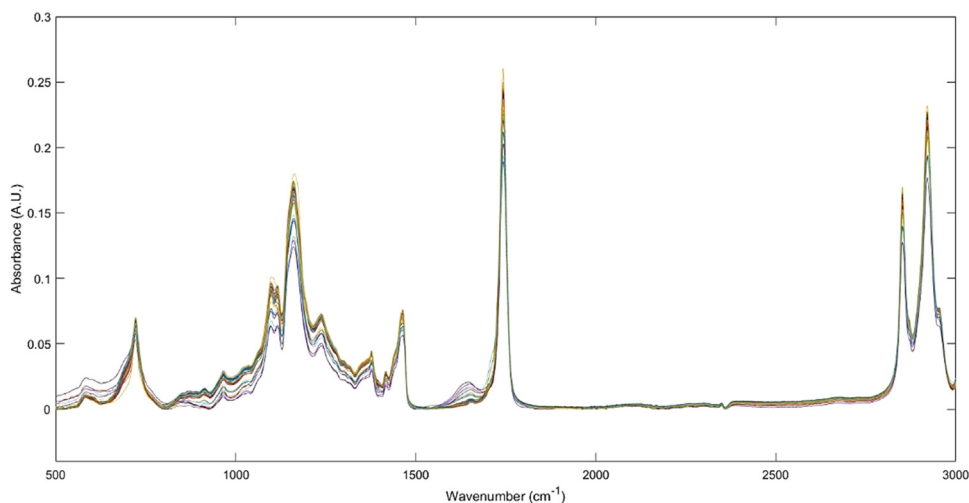
Fig. 2. The reduced FT-MIR spectra of chemically interesterified lipids and non-esterified blends and butterfat during storage at 7 °C.
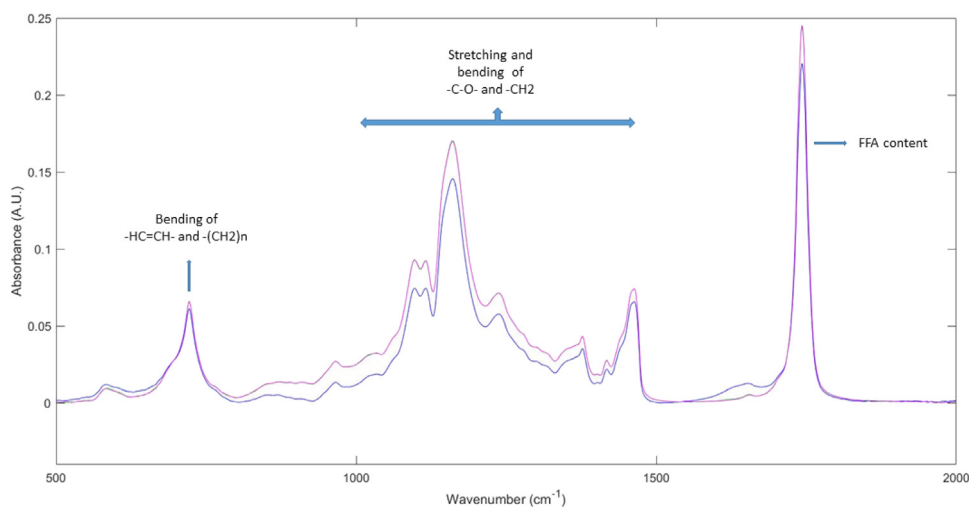

Fig. 3. The reduced FT-MIR spectra interesterified lipids with 40% of nut oil throughout storage
*(blue spectra presents 20 days of storage; pink spectra presents 30 days of storage).

peaks are influenced by functional groups of interesterified fats and provide the foundation for establishing accurate and efficient models by choosing the relevant spectral regions.

3.3. Prediction of chemical parameters from middle infrared spectra with partial least square analysis

The capability of predicting chemical properties of interesterified fats by PLS regression from FT-MIR spectra was investigated. The various transformations of spectral data including; SNV, MSC, d1 and d2 derivatives were also applied. PLS models was constructed by each pre-treated data matrices in order to predict the chemical properties of the interesterified lipids. The PLS results were summarized in Table 2 and significant components (PCs), coefficients of determination in calibration (R^2_{cal}), cross-validation (R^2_{cv}), root mean square errors of calibration (RMSEC), validation (RMSECV) were listed. The best models were chosen according to lower number of PCs, higher R^2, and lower errors for each response variable.

The chemical properties including PV, MAG, DAG, TAG, MDA and FFA content were provided as separate responses (Y matrices) and models were developed for each of these responses. The models constructed by d2 transformation data were chosen as the best due to higher determination coefficients with lower RMSEC and RMSECV values.

The PLS regression of FFA contains 3 significant components (PCs). The regression coefficient of the model determined with calibration set was found as 0.71 (Table 2). Since the RMSEC and RMSECV values are low enough (RMSEC=5.02 and RMSECV =4.28), the model could be regarded as satisfactory according to the comparison criteria. The PLS model for TAG content showed a good predictive ability with higher R^2_{cal}=0.98, R^2_{cv}=0.96 and lower RMSE values. The PLS model for DAG also had good capability of prediction due to higher R^2 =0.98 and lower RMSE values. For the prediction of MAG content of interesterified lipids, regression coefficient of calibration set was found as 0.88 (Table 2). The model has lower error values (RMSEC=0.67 and RMSECV=0.68). The constructed model was useful for MDA prediction of the interesterified lipids. The limited errors and the high determination coefficients (R^2_{cal}=0.84, R^2_{cv}=0.82) indicated the reliability of the PLS model (Table 2). The PLS regression of PV with 6 PCs has moderate regression coefficient of calibration and cross validation (R^2_{cal}=0.57 and R^2_{cv} =0.75) meaning that PV of structured lipids could be estimated from MIR spectra (Table 2). Generally, all the models constructed for the prediction of chemical properties based on FT-MIR spectra were satisfactory. The results of this research are in agreement with the studies about prediction of chemical properties of

Table 2

Statistical parameters of developed PLS models for the prediction of chemical properties of structured lipids by FT-MIR data. The best models are reported in bold.

Response	Pretreatment	PCs	RMSEC	R^2_{cal}	RMSECV	R^2_{CV}
FFA	d1	5	4.93	0.73	3.95	0.78
	d2	**3**	**5.02**	**0.71**	**4.28**	**0.73**
	SNV	7	6.29	0.57	5.48	0.59
	MSC	10	5.86	0.64	5.26	0.64
PV	d1	8	1.52	0.57	1.15	0.76
	d2	**6**	**1.50**	**0.57**	**1.13**	**0.75**
	SNV	10	1.65	0.51	1.47	0.62
	MSC	10	1.79	0.42	1.72	0.47
MDA	d1	8	2.20	0.83	2.19	0.82
	d2	**7**	**2.18**	**0.84**	**2.18**	**0.82**
	SNV	10	2.60	0.78	2.61	0.75
	MSC	10	3.14	0.67	2.98	0.68
TAG	d1	6	0.91	0.98	0.81	0.99
	d2	**4**	**1.05**	**0.98**	**1.43**	**0.96**
	SNV	10	1.97	0.92	2.14	0.92
	MSC	10	3.12	0.81	3.31	0.78
DAG	d1	6	0.75	0.98	0.63	0.99
	d2	**5**	**0.75**	**0.98**	**0.69**	**0.98**
	SNV	10	1.80	0.88	1.76	0.91
	MSC	10	2.38	0.80	2.70	0.78
MAG	d1	4	0.75	0.86	0.75	0.88
	d2	**3**	**0.67**	**0.88**	**0.68**	**0.90**
	SNV	8	1.01	0.76	0.94	0.83
	MSC	8	1.13	0.70	1.08	0.77

*FFA, Free Fatty Acid Content; TAG, Triacyglycerol content; DAG, Diacylglycerol content; MAG, monoacylglycerol content; PV, Peroxide Value; MDA, Malondialdehyde content; SNV,Standard Normal Variate; MSC, Multiplicative Scatter Correction; d1, first derivative; d2, second derivative; PCs, Significant Components; RMSEC, root mean square error of calibration; R^2_{cal}, determination coefficient of calibration; RMSECV, root mean square error of cross-validation; R^2_{cv}, determination coefficient of cross-validation.

interesterified fats. The authors demonstrated that FT-MIR analysis of the interesterified products combined by conventional and instrumental methods exhibited higher correlations associated with fatty acid profile, free fatty acid and peroxide contents, solid fat content and melting points [28,29,30].

4. Conclusion

The structured lipids were produced by chemical interesterification of butterfat blended by vegetable oils and some chemical properties of produced samples were investigated throughout storage. The storage time over 20 days resulted in negative effects on the chemical properties of the structured lipids regardless of oil type. Generally, the oil type highly affects the chemical properties of the products during storage. The samples produced with corn oil have higher contents of free fatty acid content compared to the others. Oxidative stability parameters (MDA and PV) of the samples containing nut oil is lower than other structured lipids. Interesterified lipids produced from nut oil have more desirable properties (lower oxidative stability, lower free fatty acid content) compared to corn oil. Therefore, chemically interesterification of butterfat with %40 nut oil could be suggested as an alternative lipid source due to its good chemical properties and the storage period of this interesterified lipid should be limited by 20 days at 7 °C.

Mid-infrared spectra of all samples were collected and used in the prediction of chemical properties. FT-MIR estimated malondialdehyde, mono-di-triacylglycerol contents very well and prediction ability of free fatty acid and peroxide value are also good. Therefore, IR spectroscopic techniques can be used for analyzing the changes of interesterified fats during storage and provide rapid and non-destructive techniques as good alternatives to the traditional analytical methods.

Conflict of Interest and Authorship Conformation

- All authors have participated in (a) conception and design, or analysis and interpretation of the data; (b) drafting the article or revising it critically for important intellectual content; and (c) approval of the final version.
- This manuscript has not been submitted to another journal, while it is under review.
- The authors have no affiliation with any organization with a direct or indirect financial interest in the subject matter discussed in the manuscript.
- The following authors have affiliations with organizations with direct or indirect financial interest in the subject matter discussed in the manuscript.

Ethical Statement for Solid State Ionics

Hereby, I Ayse Burcu Aktas, consciously assure that for the manuscript 'Application of Fourier Transform Infrared Spectroscopy with Chemometrics for Chemical Property Prediction of Interesterified Lipids during Storage' the following is fulfilled:

1) This material is the authors' own original work, which has not been previously published elsewhere.
2) The paper is not currently being considered for publication elsewhere.
3) The paper reflects the authors' own research and analysis in a truthful and complete manner.
4) The paper properly credits the meaningful contributions of co-authors and co-researchers.
5) The results are appropriately placed in the context of prior and existing research.
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7) All authors have been personally and actively involved in substantial work leading to the paper, and will take public responsibility for its content.

I agree with the above statements and declare that this submission follows the policies of Solid State Ionics as outlined in the Guide for Authors and in the Ethical Statement.

Declaration of Competing Interest

The authors do not have any conflict of interest.

Data availability

Data will be made available on request.

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