Rapid Iodine Value Estimation Using a Handheld Raman Spectrometer for On-Site, Reagent-Free Authentication of Edible Oils

Sanoop Pulassery, Bini Abraham, Nandu Ajikumar, Arun Munnilath, and Karuvath Yoosaf

ABSTRACT: Edible oil adulteration is a common and serious issue faced by human societies across the world. Iodine value (IV), the total unsaturation measure, is an authentication tool used by food safety officers and industries for edible oils. Current wet titrimetric methods (e.g., Wijs method) employed for IV estimation use dangerous chemicals and elaborate procedures for analysis. Alternate approaches for oil analysis require sophisticated and costly equipment such as gas chromatography (GC), liquid chromatography, high-performance liquid chromatography, mass spectrometry (MS), UV-Visible, and nuclear magnetic resonance spectroscopies. Mass screening of the samples from the market and industrial environment requires a greener, fast, and more robust technique and is an unmet need. Herein, we present a handheld Raman spectrometer-based methodology for fast IV estimation. We conducted a detailed Raman spectroscopic investigation of coconut oil, sunflower oil, and intentionally adulterated mixtures with a handheld device having a 785 nm excitation source. The obtained data were analyzed in conjunction with the GC−MS results and the conventional wet Wijs titrimetric estimated IVs. Based on these studies, a specific equation for IV estimation is derived from the intensity of identified Raman spectral bands. Further, an algorithm is designed to automate the signal processing and IV estimation, and a stand-alone graphical user interface is created in user-friendly LabVIEW software. The data acquisition and analysis require < 2 minutes, and the estimated statistical parameters such as the $R^2$ value (0.9), root-mean-square error of calibration (1.3), and root-mean-square error of prediction (0.9) indicate that the demonstrated method has a high precision level. Also, the limit of detection and the limit of quantification for IV estimation through the current approach is $\sim$1 and $\sim$3 gI$_2$/100 g oil, respectively. The IVs of different oils, including hydrogenated vegetable oils, were evaluated, and the results show an excellent correlation between the estimated and reported ones.

INTRODUCTION

Food adulteration is a worldwide problem causing a threat to public health and the economy. Edible oil is one of the inevitable components of the human diet and is an excellent nutritional source for tissue development. Chemically, edible oils are triglyceride mixtures of various fatty acids. The chain length, the substitution pattern, and the unsaturation degree of fatty acids and their percentages vary from oil to oil. A meager fraction of sterols, phospholipids, carotenes, vitamins, and sugars are also present in edible oils. In general, the fatty acid composition of an edible oil determines its physiochemical properties. Adulteration changes the composition of edible oils and will disrupt lipid metabolism and signaling networks in human bodies. This can be a potential source of cancer, cardiovascular, neurodegenerative, and metabolic disorders. The rampant adulteration instances have necessitated an in-depth chemical analysis of foods and beverages. The essential analytical parameters used for edible oil quality estimation are the iodine value (IV), saponification value (SV), peroxide value (PV), acid value (AV), hydroxyl value, moisture content, and Polenske value. The SV and AV, respectively, provide information about the average molecular weight and the number of carboxylic acid groups of fatty acids present in the edible oil, while the IV measures the degree of unsaturation and the PV indicates its oxidative deterioration. The accurate estimation of IV is often used as an authentication tool by both the consumers and food industries and is a crucial parameter for lubricants and fuel industries.

Conventionally, a few wet chemical methods are available for the IV estimation. These include iodometry, Hübl, Wijs, Kaufmann, Rosenmund-Kuhnenn, and acid-base titrimetric methods. Among these, the Wijs method is the most widely practiced technique, and it is also accepted internationally by

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most regulatory authorities like the American Oil Chemical Society (AOCS), Food Safety and Standard Authority of India (FSSAI), and so forth. In general, these wet titration experiments use dangerous chemicals and involve time-consuming reagent preparation and chemical analysis procedures. For example, the Wijs reagent, iodine monochloride (ICl), is a corrosive chemical and can cause skin burn, eye damage, cough, or shortness of breath. Consequently, greener and simpler approaches have been sought. The titration method developed by Shimamoto et al. uses water and a less corrosive reagent, an ethanolic solution of iodine. Also, the procedure is faster (~15 min) and has comparable accuracy to the conventional Wijs method. Still, the titration experiments require a wet laboratory setup and are unsuitable for on-site analysis. Existing alternate approaches include modern spectroscopic and chromatographic techniques like gas chromatography (GC), liquid chromatography (LC), high-performance liquid chromatography (HPLC), mass spectrometry (MS), and ultraviolet-visible (UV-Vis), and nuclear magnetic resonance (NMR) spectroscopies. Most often, they are employed in combination and provide accurate and reliable results. Still, they rely on elaborate procedures and sophisticated instruments, demanding time and technical expertise. For an effective fight against adulterations, the methodologies need to be simpler, faster, and robust and must have adequate precision, aiding routine analysis in the market and industrial environment.

In this context, vibrational spectroscopies are of particular interest. They serve as fingerprint characterizing techniques and yield a wide range of information from single-shot measurements. Since the intensity of the vibrational band is directly proportional to the number of responsible molecules and functional groups, they are suitable for the composition examination of materials. Several researchers have illustrated the potential of infrared (IR) and Raman spectroscopies for the rapid characterization of edible oils and quantitative estimation of cis–trans composition and unsaturation of fatty acids present. At the same time, others have applied advanced spectroanalytical techniques such as multiple linear regression, genetic algorithm, principal component analysis, and partial least-squares regression for discriminating genuine samples from those adulterated and also for quantifying the extent of fraudulence. In particular, Raman spectroscopy is a noninvasive technique that allows rapid and nondestructive data acquisition from samples in their native state. The recent technological advancement has realized portable and handheld versions of Raman spectrometers, facilitating their on-site and industrial applications.

Herein, we present the possibility of a handheld Raman spectrometer for the rapid estimation of the IV of edible oils. The preference and type of edible oil consumption vary across the world and is largely influenced by availability, culture, different food processing traditions, and ethnicity. Table 1 lists some of the commonly used edible oils, their typical IVs, and major producers. Coconut oil (CO) is a vegetable oil having a global consumption of >3.59 million metric tons per annum. Though the health impact of CO was debated in the past decade, recent studies have unveiled the health benefits such as high nutritional and energy values, antiviral, antibacterial, antiprototzoal, and antioxidant properties. For example, lauric acid is a major component (~50%) in CO. Monolaurin produced from lauric acid can destroy lipid-coated viruses such as human immunodeficiency virus, herpes, and influenza in the human body. Trace amounts of a few identified phenolic acids in CO, such as vanillic, caffeic, ferulic, p-coumaric acids, and so forth, contribute to the antioxidant activity. Studies also show that consumption of CO reduces the risk of cardiovascular and Alzheimer’s diseases. Due to these established health benefits, recent years have witnessed an increased demand for CO. In addition to its use in cuisines, it is also being used to produce personal care cosmetics, detergents, and biodiesel. Presently, the incidence of CO adulteration is alarmingly increasing, and they are done mainly for economic benefits. From Table 1, it is clear that CO has one of the lowest IV. In comparison, sunflower oil (SO) is reported to have the highest IV. Therefore, it is expected that a combination of these two oils permits to have a broader range of IVs. Based on this assumption, Raman spectral studies of a model system, CO adulterated with SO, were conducted using a handheld Raman spectrometer with a 785 nm excitation laser. The obtained data were analyzed in conjunction with the GC–MS results and the conventional Wijs method-estimated IV. This helped to derive a specific relation between the intensity ratios of identified Raman spectral bands and the IV of CO. Further, an algorithm is designed to automate the signal processing and IV estimation, and a stand-alone graphical user interface (GUI) is created in LabVIEW software. The entire data acquisition and analysis process take < 2 minutes, and the demonstrated method has reasonably high accuracy and precision levels. The developed method is then used to predict the IV of different oils, including hydrogenated vegetable oils, and has proven to be a successful tool for IV estimation.

| SI no. | oil     | IV (gI₂/100 g oil) | major producers       |
|-------|---------|--------------------|-----------------------|
| 1     | coconut | 6–11               | Asia, Africa, Latin America, Pacific regions |
| 2     | gingelly| 103–120            | Tanzania, Myanmar, India |
| 3     | olive   | 75–94              | Spain, Italy, Greece, Tunsia, Turkey, Morocco, Portugal, Syria and Algeria |
| 4     | palm    | 50–56              | Indonesia, Malaysia |
| 5     | rice bran| 90–115            | India, Japan, China, Korea, Taiwan, Thailand, and Indonesia |
| 6     | sunflower| 118–141           | Ukraine, Russia, North America, South America |
| 7     | butter  | 25–42              | India, European Union, USA |
| 8     | vanaspati| 37–47             | South Asia |

“Source: FDA Thailand and Codex Alimentarius. Food and Agriculture Organization Statistical Databases (FAOSTAT) and United States Department of Agriculture (USDA).”

### MATERIALS AND METHODS

**Materials.** Coconut oil, sunflower oil, butter, vanaspati, castor oil, gingelly oil, palm oil, paraffin oil, olive oil, and rice bran oil were purchased from local grocery stores. 1 M ICl in acetic acid, soluble starch, and methanol (HPLC grade) were purchased from Ms. SpectroChem Pvt. Ltd, India. Carbon tetrachloride, sulfuric acid, potassium iodide (KI) (>99%), potassium dichromate (>99.5%), glacial acetic acid (100%), and sodium thiosulfate (Na₂S₂O₃, >98.0%) were purchased from Ms. Sigma Aldrich Chemicals Pvt. Ltd. Hexane was purchased from SDFCL, India.
Sample Preparation. For calibration and validation, CO/SO mixtures of varying compositions (0–100 weight percentage) were prepared by mixing weighed amounts of oils and proper shaking. For Wijs titrations, two sets (15 mL each) of samples were analyzed using the standard procedure for IV estimation. For Raman analysis, not less than five spectra of each sample were taken for further analysis, and the average IV estimated was taken for the algorithm buildings.

IV Estimation through the Wijs Method. Herein, we adopted a literature-reported procedure for IV estimation. 19-20 ~2.8 g of oil in 15 mL of carbon tetrachloride was mixed with 25 mL of 0.25 N Wijs solution and kept in the dark for 1 h. It was then mixed with 10% KI solution (20 mL) and distilled water (100 mL) and titrated with 0.1 N sodium thiosulfate in the presence of starch until the blue color disappeared. The IV, grams of I₂ consumed per 100 g of oils, can be represented using eq 1

$$IV = \frac{(V_f - V_0) \times N \times 12.69}{W}$$

where $V_f$ and $V_0$ are the sodium thiosulfate volumes (in mL) required for decolorizing reference (blank) and oil samples, respectively. $N$ and $W$ are the normality of sodium thiosulfate solution and the gram weight of oil taken, and 12.69 is the conversion factor from mEq sodium thiosulfate to grams of iodine (the molecular weight of iodine is 126.9 g/mol).

GC–MS Analysis. In a typical experiment, the samples were first trans-esterified by treating with a mixture of 2% (v/v) methanol and sulfuric acid at 95 °C for 1 h. Then, 3 mL of hexane was added and vortexed for 1 min. The mixture was then centrifuged at 1000 rpm for 5 min. The upper layer was collected, diluted with hexane, and filtered. 47,48 The obtained fatty acid methyl esters were analyzed using GC–MS with a SHIMADZU GCMS-TQ8030 instrument. ~1 μL of the sample was injected (splitless) into the gas chromatograph equipped with a mass spectrometer and a medium polar capillary column Rxi-5Sil MS (30 m × 0.25 mm I. D. 0.25 μm). The detector and injection temperatures were 250 °C, and helium (99.999% pure) at a 1 mL/min flow rate was used as the carrier gas (Table S1). The total duration of the analysis was 51.67 min. The identity of chemical constituents was established by matching the mass spectra with the reference compounds in the NIST and WILEY library. The percentage composition of each component was estimated from their peak area.

Raman Spectral Studies. Raman spectra of CO, SO, and their laboratory prepared mixtures were acquired using a Mira DS handheld Raman spectrometer (Ms. Metrohm) having a 785 nm excitation source, 400–2300 cm⁻¹ spectral range, and 10 cm⁻¹ resolution. In a typical experiment, the samples were irradiated with laser power ~37 mW, and measurements were carried out in the single acquisition mode with 5 s integration time. The acquired Raman spectra were preprocessed for background removal through a Savitzky–Golay Coupled Advanced Rolling Circle Filter (SCARF), a method developed by T M James et al. 49 and implemented in LabVIEW software. For the validation of the developed method, similar experiments were conducted with different oils.

RESULTS AND DISCUSSION

Wijs Method of IV Estimation. Iodine value is defined as the weight of iodine in grams that reacts with 100 g of material. Iodine mainly adds to the unsaturated double bonds present in the fatty acids. Thus, the IV corresponds to the total unsaturation degree of fatty acids in oils. In the Wijs method, samples are treated with an excess of Wijs solution, that is, ICl solution in glacial acetic acid. The ICl reacts with unsaturated bonds resulting in halogenation. The excess unreacted ICl is then converted to molecular iodine by treating with KI. The amount of iodine formed is determined by titration with sodium thiosulfate as the titrant and starch as the indicator. Then, the IV is estimated from the difference of this value from that obtained for blank and using eq 1. The overall chemical reactions involved are represented in Scheme 1.

Scheme 1. Chemical Reactions Involved in the IV Estimation of Oils through the Wijs Method

![Scheme 1](image)

Table S3 (Supporting Information) present the estimated IV for CO/SO mixtures of varying compositions. It could be noticed that the CO exhibited the lowest IV (~9 gI₂/100 g oil), the sunflower has the highest (~129 gI₂/100 g oil), and the prepared laboratory mixtures have values in between.

Compositional Mapping through GC–MS. The compositional mapping of SO and CO obtained through GC–MS data is presented in Figure 1b and Figure S1 and Table S2 (Supporting Information). It is evident that the major components in SO are linoleic acid (~48%) and oleic acid (~32%); both are unsaturated fatty acids. They are present in meager amounts in CO (~4 and 11%, respectively). In contrast, saturated fatty acids such as lauric acid (~28%), myristic acid (18%), palmitic acid (12%), caprylic acid (12%), and capric acid (7%) are the major constituents in CO. Thus, the rich unsaturation present in SO is the primary reason for its highest IV, ~129 gI₂/100 g oil. Similarly, CO has a minor percentage of unsaturation and returned the lowest IV (9 gI₂/100 g oil). As the percentage of SO increases, the unsaturation present in mixtures also increases, which yields a linear trend in the measured IV (Figure 1a).

Raman Spectral Analysis. Figure 2a shows the raw Raman spectrum of edible oils. As expected, the spectrum is interfered with a band background causing a significant baseline shift. It may be caused by the fluorescence from other ingredients such as chlorophylls, pheophytins, vitamin E,
carotenes, and added coloring agents. This poses a significant challenge to quantitative analysis using Raman spectroscopy. Several spectral processing tools are described in the literature, and we found that SCARF is good enough for automated in-line background removal without losing much spectral information. The background-subtracted Raman spectra are presented in Figure 2a, and the significant peaks, their vibrational assignment, and relative intensities are tabulated in Table 2. The following observations can be derived from a close analysis of these data. The Raman spectra of CO and SO exhibited identical bands at the same frequencies. However, the notable difference was mainly in their relative intensities.

For example, the peak at 1658 cm$^{-1}$, due to C=C stretching vibrations, is the strongest for SO and is at least one order of magnitude less intense for CO. This could be understood from the fact that SO is highly unsaturated, and hence the peak corresponding to C=C stretching vibrations gets the highest intensity. The highest intensity peaks for CO appeared at 1442 and 1300 cm$^{-1}$, corresponding to CH$_2$ bending modes. Also, the band at 1262 cm$^{-1}$ assigned to cis RCH=C=CHR, that is, C=H bending (scissoring), is negligible in the case of CO when compared with SO. Figures 2b and S2 (Supporting Information) represent the observed Raman spectra of CO/SO mixtures of varying compositions. As expected, a steady rise in the peak intensities at 971, 1265, and 1658 cm$^{-1}$ is evident as the percentage of SO in the mixture increases. This is because the main components of SO are unsaturated linoleic acid and oleic acid, and the mentioned Raman spectral bands are contributed by C=C stretching and bending modes.

**Figure 2.** Raman spectra of (a) CO and SO and (b) mixtures of varying compositions. Measurement parameters: $\lambda_{\text{exc}} = 785$ nm, laser power = 37 mW, integration time = 5 s, and no. of averages = 1. The red arrow indicates the direction of peak intensity variation at 1658 cm$^{-1}$ with the percentage composition of SO in the mixture.

Table 2. Observed Raman Spectral Peaks for CO and SO and Their Vibrational Assignments

| Raman peak (cm$^{-1}$) | intensity (counts) | vibrational assignment |
|------------------------|-------------------|------------------------|
| 1750                   | 2413              | 2017  | C=O symmetric stretching |
| 1658                   | 699               | 11478 |  |
| 1442                   | 7181              | 7842  | CH$_2$ bending (scissoring) |
| 1300                   | 3933              | 4330  | CH$_2$ bending (twisting) |
| 1265                   | 728               | 4195  | cis RCH=C=CHR bending (scissoring) |
| 1125                   | 1914              | 987   | C=C aliphatic in-phase bending |
| 1080                   | 2263              | 2537  | -CH$_3$ bending |
| 968                    | 1554              | 2617  | trans RCH=C=CHR bending |
| 860                    | 2123              | 2617  | C=C stretching |

**Figure 3.** Plot showing the (a) variation of the peak ratio against the weight percentage of SO in the mixture, (b) comparison of IVs estimated through the Wijs method and software at different known compositions of SO in CO, and (c) comparison of the values estimated through Wijs method and software for blind samples.

The iodine value, IV, is a measure of the number of double bonds in a hydrocarbon. It is calculated as the weight of iodine that is engaged in a given weight of the hydrocarbon. The relation between the Wijs method-measured IV and w/w % composition of SO in the mixture can be represented by eq 2.

$$\text{IV} = m_1 \left( \frac{W_{\text{SO}}}{W} \right) + C_1$$

where the slope, $m_1$, is the rate of change of IV with the percentage variation of SO in the mixture. The y-intercept, $C_1$, is the IV of pure CO. The linear fitting of the plot returned an $R^2$ value of 0.999 (Figure 1a), and the extracted values of $m_1$ and $C_1$ are, respectively, 1.208 and 7.672.
A few previous studies have illustrated that the intensity ratio of peaks corresponding to C≡C and CH₂ can be used to measure the unsaturation degree in oils and lipids in biological samples.²⁵,⁵¹ In the current work, these peaks appeared at 1658 and 1442 cm⁻¹. Hence, we studied the variation of peak ratio of these bands as a function of the percentage composition of SO in the mixture (Figure 3a). The obtained linear plot is best fitted with eq 3

\[ \text{peak ratio} = \frac{I_{1658}}{I_{1442}} = m_2 \left( \frac{W_{\%}}{W_{SO}} \right) + C_2 \]  

(3)

Slope, \( m_2 \), corresponds to the rate of change of peak ratio against the percentage composition of SO in the mixture. The y-intercept, \( C_2 \), is the peak ratio of pure CO. The linear fit of Figure 3a yielded an \( R^2 \) value of 0.999, and the estimated values of \( m_2 \) and \( C_2 \), respectively, are 0.01363 and 0.0864. From eqs 2 and 3, the equation for calculating the IV from the peak ratio can be deduced as

\[ \text{iodine value} = m_1 \frac{I_{1658}}{I_{1442}} + C_3 \]  

(4)

where

\[ m_3 = \frac{m_1}{m_2} \]  

(5)

and

\[ C_3 = C_1 - \frac{m_1}{m_2} C_2 \]  

(6)

From eqs 5 and 6, slope \( m_3 \) and intercept \( C_3 \) are calculated as 88.644 and 0.012, respectively.

**Algorithm for the Estimation of IV.** Knowing the relationship between the IV and the peak intensity ratio and the values of \( m_1 \) and \( C_3 \), we designed a stand-alone GUI to automate the signal processing and IV estimation. The data flow involved in the algorithm is presented in Figure 4 and is described as follows. In the first step, the raw spectrum (csv format) recorded using a handheld Raman spectrometer is loaded into the IV estimator. Subsequently, the data undergo automated background subtraction through the SCARF method with a set of fixed values such as third-order polynomial, rolling circle filter radius (rcf) as 60, zero baseline, and Savitzky–Golay filtering side points as 60. In the consecutive steps, the software measures the intensities at 1658 and 1442 cm⁻¹. The estimated ratio of these intensity values is fed to the equation of the form (4), and finally, the calculated IV is displayed. The whole process takes place within a few seconds.

To test the accuracy and reliability of the method, we analyzed the statistical error parameters such as the \( R^2 \) value, mean percentage error (MPE), and root-mean-square error of calibration and prediction (RMSEC and RMSEP) for both known and blind samples (Figure 5 and Table S4, Supporting Information). Figure 3b and 3c represent the comparison of predicted versus Wijs method estimated IVs. The IV versus composition returned a linear plot with \( R^2 \) values (0.9) for known samples, indicating higher linearity and correlation between software predicted IVs and those from the Wijs titrimetric method.

The relative error calculated for calibration and blind samples varied from −0.07 to 0.04 (Tables S3, S5 and Figure S3, Supporting Information). MPE is the measure of the precision of the experimental value to the predicted one. The obtained values are 0.6% and 1.4% for known and blind samples, respectively, suggesting good agreement between IVs obtained from the developed GUI and the Wijs method of titration. RMSEC and RMSEP are the square roots of the average of squared differences between IVs predicted by software and the Wijs method for calibration and blind samples, respectively. Generally, a lower value of RMSE infers a classic match between the predicted and observed values of

![Figure 4. Algorithm for the estimation of IV.](https://doi.org/10.1021/acsomega.1c05123)
measurement. In the present case, RMSEC and RMSEP are 1.3 and 0.9, respectively, indicating the excellent performance of the developed method.

Listed in Tables S6–S11 of the Supporting Information are the results of some of the matrix effects investigated. In general, it is observed that experimental parameters, such as the type of sample container, the environment of measurements, and the presence of other chemicals, and instrumental parameters such as laser power, integration time, and the number of accumulations have a negligible effect on the determined IV. For the quantitative evaluation of the intra/interday precisions and accuracies, IVs of five different compositions (0, 25, 50, 75, and 100% w/w SO in CO) were estimated through both Wijs and developed methods at four different time intervals (Table S12, Supporting Information). For a particular composition and method, the IVs estimated at different time intervals varied by a maximum of ±0.5. However, the relative standard deviation percentage showed a value of 6.4% for the samples with low IVs (pure SO). As such, the relative cumulative deviation shows a negligible effect on the measured IV.52 For the quantitative evaluation of the intra/interday precisions and accuracies, IVs were determined using the formula 3σ/m, where σ is the standard deviation and m is the slope of the residual linear regression plot (Figure S4, Supporting Information). The RMSEC and RMSEP of the developed method, LoD, and LoQ are estimated to be ~1 gI2/100 g oil and ~3 gI2/100 g oil, respectively.53,54

To evaluate the wider applicability of the developed method further, 10 different oils were analyzed, including hydrogenated vegetable oils. Reported in Figure S5 (Supporting Information) are the Raman spectra of these oils, and Table S13 (Supporting Information) shows the comparison of the estimated IVs along with literature reported values. It is found that for the samples investigated, the IVs calculated from Raman spectra fall well within the range of literature-reported values. Table S14 (Supporting Information) lists the comparison of the cost and easiness of the current method against some of the presently available techniques. As stated before, techniques like NMR and GC–MS provide accurate results, but the instruments are highly sophisticated and require trained technicians to operate. The titrimetric methods involve the use of wet chemical laboratory, corrosive chemicals, and sample preparation procedures. UV–vis spectroscopy requires reaction with certain chemicals. The IR and NIR instruments require specific sample containers and a closed chamber. On the contrary, as illustrated in Table S15 (Supporting Information), Raman spectroscopy allows direct measurements using simple glass containers and works even in an open environment (Figure S6, Supporting Information).

CONCLUSIONS

Herein, we demonstrated a simple, reagent-free, and rapid method to determine the IV of edible oil. The judicious analysis of Raman spectra with GC–MS and the Wijs method–estimated IV helped us correlate unsaturation with spectral information. A specific relation is derived to estimate the IV of the oils using the peak ratio of contributions from unsaturation (1658 cm−1) to saturation (1442 cm−1). The incorporation of SCARF helped us automate the process of background subtraction and IV estimation. The estimated statistical error parameters for blind samples such as the R2 value (0.9), MPE (∼0.6 known 1−α) blind), RMSEC (1.3), and RMSEP (0.9) indicate the high precision of the developed technique. The paired-t test estimated for sample compositions located in the low, medium, and high concentration levels of the calibration graph indicated more than 95% of confidence level. Also, the current method has got reasonably good LoD (∼1 gI2/100 g oil) and LoQ (∼3 gI2/100 g oil) for the estimation IVs. Compared to other presently available techniques, the present method is completely reagent-free, and the measurements can be performed using simple glass vials or in their native state. Yet, another attraction of the method is that the analysis is performed using a handheld Raman spectrometer, and the developed software module enables even a layperson to perform the analysis. Similar approaches can be developed to estimate other quality parameters such as peroxide and acid values of edible oils. We believe that the work described herein can elevate the use of Raman spectroscopy for fast quality analysis and authentication of edible oils from the market and industrial environment.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.1c05123.

GC–MS measurement conditions, chromatogram, estimated chemical composition, Raman spectra of different oils and CO/SO mixtures, comparison of IV estimated through Wijs and Raman spectral method, equations and results of statistical error parameters, matrix effects, calibration graph used for LoD and LoQ estimation, validation results with various oils, cost and convenience comparison with other presently available methods, and pictorial representation of data acquisition using a handheld Raman spectrometer (PDF)

AUTHOR INFORMATION

Corresponding Author

Karuvath Yoosaf – Photosciences and Photonics Section, Chemical Sciences and Technology Division, CSIR-National Institute for Interdisciplinary Science and Technology, Thiruvananthapuram 695019, Kerala, India; Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India; Research Centre, University of Kerala, Thiruvananthapuram 695034, Kerala, India; orcid.org/0000-0002-8837-4490; Phone: 0091-471-2515477; Email: yoosafk@niist.res.in

Authors

Sanoop Pulassery – Photosciences and Photonics Section, Chemical Sciences and Technology Division, CSIR-National Institute for Interdisciplinary Science and Technology, Thiruvananthapuram 695019, Kerala, India; Research Centre, University of Kerala, Thiruvananthapuram 695034, Kerala, India; orcid.org/0000-0003-1836-9618

Bini Abraham – Photosciences and Photonics Section, Chemical Sciences and Technology Division, CSIR-National Institute for Interdisciplinary Science and Technology, Thiruvananthapuram 695019, Kerala, India; Academy of
Nandu Ajikumar — Photosciences and Photonics Section, Chemical Sciences and Technology Division, CSIR-National Institute for Interdisciplinary Science and Technology, Thiruvananthapuram 695019 Kerala, India; Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India; orcid.org/0000-0002-1694-4204

Arun Munnilath — Photosciences and Photonics Section, Chemical Sciences and Technology Division, CSIR-National Institute for Interdisciplinary Science and Technology, Thiruvananthapuram 695019 Kerala, India; orcid.org/0000-0002-5832-9920

Complete contact information is available at: https://pubs.acs.org/10.1021/acsomega.1c05123

**Notes**

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