Research Trends in Optical Spectrum for Honey Analysis

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Abstract—The high demand for genuine honey leads to fraud practices in the market which have disadvantaged top graded genuine honey production. The conventional chemical analysis procedures are usually used to ensure the quality and authenticity of honey. Yet, some drawbacks, such as time-consuming, laborious, invasive and required complex sample preparation, in the chemical approaches make the optical spectrum based honey analysis an advantageous alternative method. This paper reports a comprehensive survey of peer-reviewed articles in honey analysis using spectroscopy techniques. The technologies, features, and preprocessing and prediction methods from the observed articles have been discussed to give an overview about optical spectrum approaches for honey analysis. This paper quickly introduces reseachers to modern honey analysis research.

I. INTRODUCTION

Optical spectrum based food analysis is a modern approach which provides contact-less, non-invasive, fast, and fully automatic methods with minimum sample preparation. Those characteristics give answers to the drawbacks of conventional chemical methods which are time-consuming, laborious and required complex sample preparations. Optical spectrum, which can be captured by spectrometers, is basically optical information showing the energy distribution in a particular range of wavelengths [1]. Different spectral responses from different materials introduce material fingerprints for prediction purposes. Chemistry analysis methods called chemometrics usually is used to do the prediction based on multivariate statistics, mathematical modeling and machine learning [2]. The utilization of chemometrics methods in spectral data makes superiority of optical spectrum based approaches compared with conventional methods.

Honey, which is an important commodity in market, has become a research focus in optical spectrum based analysis. The high demand of honey makes it a big business in food industry. Fig. 1 show upward trend of production and price of honey over years in New Zealand [3]. Indeed, this situation leads challenges for the honey industry to deliver good quality honey products.

This paper presents a comprehensive survey in honey analysis using the spectroscopy techniques and chemometric through an observation of peer-reviewed scientific journals. There was 61 papers in total recorded from 1998 to 2015 (Appendix A). The discussion about technology, features and methods in the honey analysis gives insight to researchers



Fig. 1: Honey production from 1961 to 2011 and producer prices from 1991 to 2003 in New Zealand.

about state of the art methodologies in optical spectrum based honey analysis.

II. RESEARCH AIMS IN OPTICAL SPECTRUM BASED HONEY ANALYSIS

In general, optical spectrum based honey analysis can be classified into two major groups, which are constituents prediction and types classification. Research aims were recorded from each research articles to investigate the trend. In case of more than one objective in an article, all objectives mentioned in the article would be recorded.

More than half studies were focused to differentiate many types of honey. Types of honey could be based on its botanical origin [4–20], geographical origins [15, 16, 21–27], authenticity (adulterated honey or not) [4, 7, 28–40] and brand identification [11]. The botanical origin and authenticity determination were the two most popular research focuses. A part from types classification, there were also studies which focused on visualization of the data, such as [5, 41–44].

Almost 40% of the studies investigated constituents prediction, such as Methylyoxal and antibacterial activity [45]; Melissopalynological characteristics and mineral composition [46], Glucose [43, 47–56], Fructose [47–56], Melezitose [47], Turanose [47, 52], Maltose [47–49, 51, 52, 55], Sucrose [48, 49, 51–53, 55–57] electrical conductivity [5, 52, 58], Pollen vectors [5], rice syrup adulterant [59], sugar syrups adulterant [60], jaggery syrup adulterant [61], Corn syrup adulterant [25, 53], High Fructose Corn Syrup (HFCS) adulterant [25, 32], invert sugar adulterant [25, 38], inverted beet syrup (IB) adulterant [32, 40], antioxidant compounds [62], Tetracycline (drug residues) [63], water content [58], pH [52, 58], HMF [55, 58], Ash [58], Colour [58], Trehalose [52], Isomaltose [52], Erlose [52], Moiseture [52, 54–56], free acidity [52, 55], Proline [52], Invertase [52], Polarimetric Parameters [57], cane invert adulterant [40], and Lactone [55]. It can be seen clearly that Fructose and Glucose, which are two

III. SPECTROSCOPY FOR HONEY ANALYSIS

major components of honey [64], were the two most popular

research focuses in the constituent prediction.

Spectroscopy which literally means *Ghost Watcher* from Latin and Greek words, gives foundation to the spectroscopic method and refers to a study related with interaction between matter and energy [65]. The responses from this interaction are used to determine a fingerprint of a particular object. The spectroscopy techniques used in honey analysis are listed below:

• Ultraviolet (UV), Visible-Near Infrared (VIS-NIR) and Infrared (IR) spectroscopy

UV, VIS and IR spectroscopies work with a same principle measuring the energy differentiation when molecules transit from one vibrational or rotational energy state to another state as interaction between matter and energy [65]. A difference among them is in wavelength regions. The UV spectroscopy works in the UV region which can be divided into far UV (10-200nm), and near UV region (200-350nm). The VIS-NIR spectroscopy works on the visible region (350-800nm) and near infrared region (800-2500nm). The IR spectroscopy works on the infrared region which can be divided into three subregions; Near-Infrared (NIR) covered $12,800-4000cm^{-1}$, mid-infrared (MIR) covered $4000 - 200 cm^{-1}$ and farinfrared covered $200 - 10cm^{-1}$ [65, 66]. Now days, Fourier transform (FT) spectrometer is more often used in Infrared (IR) spectroscopy (FT-IR, FT-NIR or FT-MIR) than the previous dispersive type spectrometer. The FT spectrometer has better signal-to-noise ratio, larger energy throughput, multiplex advantage, and wavelength precision than the dispersive spectrometer [65, 67]. Attenuated total reflectance (ATR) based on internal reflectance measurement is a sampling technique which is considered to have faster and simpler sample preparation than others and also can handle many form of objects including liquids, semi-solids, polymers, powders, and solids [67]. It is reasonable if a lot of researchers used the ATR-FT Spectrometer for honey analysis.

• Raman spectroscopy

Raman spectroscopy is a vibrational spectroscopy and working in a similar wavelength range as the IR spectroscopy. Raman and infrared spectroscopy complement each other. Raman spectroscopy uses symmetric vibration and infrared spectroscopy uses asymmetric vibrations [68]. Raman spectroscopy can uses Fourier transform spectrometer also, which is called FT-Raman, which has the similar advantages with FT-IR [65].

• Fluorescence spectroscopy

Fluorescence spectroscopy is quiet different with the two previous spectroscopy methods in terms of principles and also wavelength ranges. Fluorescence spectroscopy is related with phenomena of photon emission during transition of electrons from excited states to ground states which happens in the ultraviolet-blue-green region [69]. The fluorescence spectral data is recorded in twodimensional data according to the excitation and emission spectra [70]. The front-face technique is intended to

spectra [70]. The front-face technique is intended to examine original objects without prior sample preparation through measuring exiting and emitted light from the same cuvette face [71].

The survey of the spectroscopy methods is shown in Fig. 2. Fourier Transform Infrared Spectroscopy dominated with more than 34% articles and the Near Infrared spectroscopy was in the second place with more than 26% articles.



Fig. 2: The spectroscopic methods of the 61 studies listed in Appendix A.

The comparison among all spectroscopic techniques has not been done for honey analysis. However, Ruoff, Kaspar, et al. in 2006 wrote three different articles investigated NIR [17], MIR [16] and Fluorescence spectroscopy [15] to classify botanical origins of honey using relatively same samples and methodologies. It can be concluded from direct comparison of those three paper that the fluorescence spectroscopy was the best among the others.

IV. PREPROCESSING METHODS

Almost all researchers used preprocessing or pretreatment techniques prior learning processes. A preprocessing step is needed because multi or hyperspectral data generally contains noise. The common data pretreatment methods for optical spectrum data are baseline correction, scattering correction, smoothing and normalization.

Standard Normal Variate (SNV) and De-trending (DT) are the most common baseline correction methods. SNV tries to eliminate different slopes among samples with same constituents which may occur because of different particle size [72]. DT standardizes the spectra responses from offset and curvilinearity through an elimination using a general trend which can be calculated with a particular curve-fitting model [73]. DT can correct the baseline spectra and keeps the original pattern of particle size characteristic [72]. Other baseline correction methods are offset method using linear baseline subtraction and adaptive iteratively reweighted Penalized Least Square (airPLS) which a complex baseline will

be approximated using an iterative procedure and smoothness of the baseline will be determined using a penalty item [74]. airPLS is different from the other methods because it preserves small peaks.

Multiplicative Scatter Correction (MSC) is the only scattering correction method mentioned in the observed articles. MSC deals with phenomenon of light scattering which can lead to wrong spectral responses because of absorbance shift [75]. MSC uses intercept and slope properties of a linear regression between a spectrum and an average of an ideal spectrum form calibration set to correct an original spectrum [76].

Smoothing can efficiently remove random noise in the form of small fluctuations because of unknown low frequencies. Savitzky-Golay (S-G) smoothing fits original data points in a particular curve [77]. Another way to get a smoother spectral data is by lowering resolution which the total number of bands will be reduced by averaging several adjacent bands [43].

Several normalization techniques were mentioned in the observed articles to enhance original hyperspectral signals. Area normalization basically calculates a relative area under a spectra curve to correct spectral data where a path-length is unknown [78]. The different distances for light to travel through the object (path-length) will lead to different spectral responses according to Beer's law [79]. Autoscaling or unit variance scaling normalizes major and minor peaks in spectral data. Spectral data will be divided by a standard deviation from a training set after a mean-centering process [78]. Vector normalization is a normalization procedure based on an unit vector where the mean-centered original spectra is divided by a square of sum of each band in mean-centered original spectra squared [80]. Maximum normalization converts each spectral data in a range of 0 to 1 by dividing the spectral data by the maximum absolute value of the wavelength responses [81].

Almost half of the observed papers did performance comparison among preprocessing methods. However a firm conclusion could not be drawn because different papers used different set of preprocessing methods and concluded different best performance methods. It leads that the performance of preprocessing methods are vary for different samples, instruments and settings. It is highly recommended that each research work explores the best pretreatment methods based on their own configurations.

V. FEATURE SELECTION

Usually, spectral data needs to be transformed into different features to get better predictive power because the original spectral normally contains noise or overlapping information. The common feature extraction strategies in the observed articles are derivative spectral data, reduced spectral data and selective spectral data.

The derivative of the original spectral data produces more sensitive spectral to minor features [82]. The original spectra could be transformed to the first and second derivative spectral. Savitzky-Golay (S-G) algorithm is not only very common for smoothing but also the most common method to approximate derivative spectral data.

A transformation of spectral data into more compact features is also very common because spectral data is a high dimensional data which most of the recorded values are not informative or high correlated to each other. The feature reduction techniques are very important to visualize the data and also make more robust predictors. Feature reduction techniques used in the observed studies were Principal Component Analysis (PCA), Partial Least Square (PLS), PARAllel FACtor analysis (PARAFAC) modeling, and Wavelet coefficient. PCA has been used by around 80% of the observed articles utilizing feature reduction techniques. PCA uses the variance as a measurement for data separation. Actually, higher variance does not guarantee better discrimination power as depicted in Figure 3.



Fig. 3: The projection into PC 2 (36% of variance) has much better separation than projection into PC 1 (64% of variance).

Another strategy to prepare features is to select the most related bands to the targeted classes. Spectral selection techniques apparently were not quite popular to be explored. It may be because there was a firm research about relation between chemical constituents and related bands. For example, Glucose is observed at 1145, 1105, 1077, 1047, 1017 and 992 cm^{-1} [66]. Only four articles utilized feature selection techniques which are Fisher Ratios [22], PCA [7, 13] and Marten's Uncertainty Test [24].

More than 85% of the observed papers did not explore and compare the performances of features. A few papers which compared features also concluded the different best features and some of them had an opposite result. Features exploration is very important in classification problems which a good feature will perform very well even with a very basic classifier.

VI. PREDICTORS BASED ON HIDDEN FEATURES

As can be seen from CC (Classification) and R (Regression) section in Appendix A, predictors based on hidden features

were commonly used to build prediction models in honey analysis. These predictors use transformed independent variables instead of original independent variables, to determine discrete or continues targeted outputs. Projection of original spectral data from one to another space might be necessary to reduce noisy and to omit unnecessary information.

The predictors used in the observed studies were Soft-Independent Modeling by Class Analogy (SIMCA) which is based on Principal Components, Linear Discriminant Analysis (LDA), Partial Least Square (PLS), Canonical Variate Analysis (CVA), Artificial Neural Network (ANN) and Support Vector Machine (SVM). The comparison of the methods according to the number of usages is shown in Figure 4. Indeed, PLS based predictor has been the most widely successful method for both regression and classification problems.



Fig. 4: The predictors from the 61 recorded publications.

A same story with exploration of preprocessing method; there were almost 40% of papers which compared some predictors. Although most of them concluded that the PLS method was better than others, the performance of classifier is highly determined by the characteristics of data which is affected by samples, instruments and settings. The exploration of classifier methods for a specific configuration is highly recommended.

VII. PERFORMANCE EVALUATION

A proper choice of performance evaluation indicators will firmly convince readers and also be easier to be compared with other performances. In case of classification problems, one possible way to report a result is using overall correct classification accompanied by Cohen's kappa. Cohen's kappa (κ) is a coefficient of agreement between two predictors where 1 is the prefect agreement and below 0 is zero agreement [83]. Others possible measurements are sensitivity and specificity which measure the portion of positive and negative identified results in two classes (binary) classification problem. Sensitivity and specificity can be extended for a multi-class classification problem as discussed in [84].

In the case of regression problems, common performance evaluation indicators are correlation coefficient (r) or correlation of determination (r^2) . r can be explained as an association between a ground-truth and a predictor's output which is from -1 (strong negative correlation) to +1 (strong positive correlation); 0 means no correlation. r^2 can be interpreted as strength of a linear association or proportion of variable's variance that can be correctly predicted.

VIII. CONCLUSIONS

In this paper a survey of technologies, features and methods for honey analysis based on optical spectrum have been depicted. The aim of honey analysis can be classified into two groups. These are: types determination (majority in botanical origin and authenticity determination) and constituents prediction (majority in Fructose and Glucose prediction). Spectroscopy with chemometric has shown promising results for honey analysis with many advantages over the conventional methods. FT-IR Spectroscopy has been dominantly used as a spectral capturing technology. Baseline and scattering correction have become common pretreatment strategies to ensure correctness of spectral responses. PCA, as a dimensionality reduction technique, has been dominating to reduce an original spectral for data visualization and increasing predictors' performances. Performance of prediction methods could not be directly compared among different studies because it depends on experimental set ups which are normally different. However, PLS based predictors have been recorded as successful predictors in the majority of studies. Finally, the choice of performance evaluation indicators is very important for the development of honey analysis research.

References

- [1] Rüdiger Paschotta. *Encyclopedia of laser physics and technology*, volume 1. Wiley-vch Berlin, 2008.
- [2] Paul Gemperline. *Practical guide to chemometrics*. CRC press, 2006.
- [3] Food and Agriculture Organization of The United Nations Statistics Devision. Producer prices - annual and commodity balances - livestock and fish primary equivalent, 2015. URL http://faostat3.fao.org/.
- [4] Lea Lenhardt, Rasmus Bro, Ivana Zeković, Tatjana Dramićanin, and Miroslav D Dramićanin. Fluorescence spectroscopy coupled with parafac and pls da for characterization and classification of honey. *Food chemistry*, 175:284–291, 2015.
- [5] Lidija Svečnjak, Dragan Bubalo, Goran Baranović, and Hrvoje Novosel. Optimization of ftir-atr spectroscopy for botanical authentication of unifloral honey types and melissopalynological data prediction. *European Food Research and Technology*, pages 1–15, 2015.
- [6] L Lenhardt, I Zeković, T Dramićanin, Ž Tešić, D Milojković-Opsenica, and MD Dramićanin. Authentication of the botanical origin of unifloral honey by infrared spectroscopy coupled with support vector machine algorithm. *Physica Scripta*, 2014(T162):014042, 2014.
- [7] Lea Lenhardt, Ivana Zeković, Tatjana Dramićanin, Miroslav D Dramićanin, and Rasmus Bro. Determination of the botanical origin of honey by front-face synchronous fluorescence spectroscopy. *Applied spectroscopy*, 68(5):557–563, 2014.
- [8] Xiu Ying Liang, Xiao Yu Li, and Wen Jun Wu. Classification of floral origins of honey by nir and chemometrics. In *Advanced Materials Research*, volume 605, pages 905–909. Trans Tech Publ, 2013.

- [9] Abdul-Rahman A Roshan, Haidy A Gad, Sherweit H El-Ahmady, Mohamed S Khanbash, Mohamed I Abou-Shoer, and Mohamed M Al-Azizi. Authentication of monofloral yemeni sidr honey using ultraviolet spectroscopy and chemometric analysis. *Journal of agricultural and food chemistry*, 61(32):7722–7729, 2013.
- [10] Lanzhen Chen, Jiahua Wang, Zhihua Ye, Jing Zhao, Xiaofeng Xue, Yvan Vander Heyden, and Qian Sun. Classification of chinese honeys according to their floral origin by near infrared spectroscopy. *Food chemistry*, 135(2):338–342, 2012.
- [11] Xiangdong Zhao, Yong He, and Yidan Bao. Nondestructive identification of the botanical origin of chinese honey using visible/short wave-near infrared spectroscopy. *Sensor Letters*, 9(3):1055–1061, 2011.
- [12] Yan Yang, Peng-Cheng Nie, Wei Zhang, and Yong He. A novel method of pattern recognition for honey source based on visible/near infrared spectroscopy: Genetic algorithm combined with support vector machine. In Artificial Intelligence and Computational Intelligence (AICI), 2010 International Conference on, volume 1, pages 519– 523. IEEE, 2010.
- [13] D Bertelli, M Plessi, AG Sabatini, M Lolli, and F Grillenzoni. Classification of italian honeys by mid-infrared diffuse reflectance spectroscopy (drifts). *Food Chemistry*, 101(4):1565–1570, 2007.
- [14] Romdhane Karoui, E Dufour, J-O Bosset, and Josse De Baerdemaeker. The use of front face fluorescence spectroscopy to classify the botanical origin of honey samples produced in switzerland. *Food Chemistry*, 101 (1):314–323, 2007.
- [15] Kaspar Ruoff, Werner Luginbühl, Raphael Künzli, Stefan Bogdanov, Jacques Olivier Bosset, Katharina von der Ohe, Werner von der Ohe, and Renato Amadò. Authentication of the botanical and geographical origin of honey by front-face fluorescence spectroscopy. *Journal of agricultural and food chemistry*, 54(18):6858–6866, 2006.
- [16] Kaspar Ruoff, Werner Luginbühl, Raphael Künzli, María Teresa Iglesias, Stefan Bogdanov, Jacques Olivier Bosset, Katharina von der Ohe, Werner von der Ohe, and Renato Amadò. Authentication of the botanical and geographical origin of honey by mid-infrared spectroscopy. *Journal of agricultural and food chemistry*, 54(18):6873– 6880, 2006.
- [17] Kaspar Ruoff, Werner Luginbühl, Stefan Bogdanov, Jacques Olivier Bosset, Barbara Estermann, Thomas Ziolko, and Renato Amadò. Authentication of the botanical origin of honey by near-infrared spectroscopy. *Journal of agricultural and food chemistry*, 54(18):6867–6872, 2006.
- [18] Kaspar Ruoff, Romdhane Karoui, Eric Dufour, Werner Luginbühl, Jacques-Olivier Bosset, Stefan Bogdanov, and Renato Amadò. Authentication of the botanical origin of honey by front-face fluorescence spectroscopy. a preliminary study. *Journal of agricultural and food chemistry*,

53(5):1343–1347, 2005.

- [19] Anthony MC Davies, Branka Radovic, Tom Fearn, and Elke Anklam. A preliminary study on the characterisation of honey by near infrared spectroscopy. *Journal of near infrared spectroscopy*, 10(2):121–136, 2002.
- [20] Royston Goodacre, Branka S Radovic, and Elke Anklam. Progress toward the rapid nondestructive assessment of the floral origin of european honey using dispersive raman spectroscopy. *Applied spectroscopy*, 56(4):521– 527, 2002.
- [21] C Herrero Latorre, RM Peña Crecente, S García Martín, and J Barciela García. A fast chemometric procedure based on nir data for authentication of honey with protected geographical indication. *Food chemistry*, 141 (4):3559–3565, 2013.
- [22] Juan Antonio Fernández Pierna, Vincent Baeten, Ouissam Abbas, and Pierre Dardenne. Discrimination of corsican honey by ft-raman spectroscopy and chemometrics. *Base*, 2011.
- [23] Siobha'n Hennessy, Gerard Downey, and Colm P O'Donnell. Attempted confirmation of the provenance of corsican pdo honey using ft-ir spectroscopy and multivariate data analysis. *Journal of agricultural and food chemistry*, 58(17):9401–9406, 2010.
- [24] Tony Woodcock, Gerard Downey, and Colm P ODonnell. Near infrared spectral fingerprinting for confirmation of claimed pdo provenance of honey. *Food Chemistry*, 114 (2):742–746, 2009.
- [25] Tzayhri Gallardo-Velázquez, Guillermo Osorio-Revilla, Marlene Zuñiga-de Loa, and Yadira Rivera-Espinoza. Application of ftir-hatr spectroscopy and multivariate analysis to the quantification of adulterants in mexican honeys. *Food Research International*, 42(3):313–318, 2009.
- [26] Siobhán Hennessy, Gerard Downey, and Colm O'Donnell. Multivariate analysis of attenuated total reflection–fourier transform infrared spectroscopic data to confirm the origin of honeys. *Applied spectroscopy*, 62(10):1115–1123, 2008.
- [27] Tony Woodcock, Gerard Downey, J Daniel Kelly, and Colm O?Donnell. Geographical classification of honey samples by near-infrared spectroscopy: A feasibility study. *Journal of agricultural and food chemistry*, 55 (22):9128–9134, 2007.
- [28] Shuifang Li, Yang Shan, Xiangrong Zhu, Xin Zhang, and Guowei Ling. Detection of honey adulteration by high fructose corn syrup and maltose syrup using raman spectroscopy. *Journal of Food Composition and Analysis*, 28(1):69–74, 2012.
- [29] Lanzhen Chen, Xiaofeng Xue, Zhihua Ye, Jinghui Zhou, Fang Chen, and Jing Zhao. Determination of chinese honey adulterated with high fructose corn syrup by near infrared spectroscopy. *Food Chemistry*, 128(4):1110– 1114, 2011.
- [30] Xiangrong Zhu, Shuifang Li, Yang Shan, Zhuoyong Zhang, Gaoyang Li, Donglin Su, and Feng Liu. Detection

of adulterants such as sweeteners materials in honey using near-infrared spectroscopy and chemometrics. *Journal of Food Engineering*, 101(1):92–97, 2010.

- [31] Deirdre Toher, Gerard Downey, and Thomas Brendan Murphy. A comparison of model-based and regression classification techniques applied to near infrared spectroscopic data in food authentication studies. *Chemometrics and Intelligent Laboratory Systems*, 89(2):102–115, 2007.
- [32] J Daniel Kelly, Cristina Petisco, and Gerard Downey. Application of fourier transform midinfrared spectroscopy to the discrimination between irish artisanal honey and such honey adulterated with various sugar syrups. *Journal of agricultural and food chemistry*, 54(17):6166–6171, 2006.
- [33] J Daniel Kelly, Cristina Petisco, and Gerard Downey. Potential of near infrared transflectance spectroscopy to detect adulteration of irish honey by beet invert syrup and high fructose corn syrup. *Journal of Near infrared spectroscopy*, 14(2):139, 2006.
- [34] JF Daniel Kelly, Gerard Downey, and Vanessa Fouratier. Initial study of honey adulteration by sugar solutions using midinfrared (mir) spectroscopy and chemometrics. *Journal of agricultural and food chemistry*, 52(1):33–39, 2004.
- [35] Gerard Downey, Vanessa Fouratier, and J Daniel Kelly. Detection of honey adulteration by addition of fructose and glucose using near infrared transflectance spectroscopy. *Journal of Near Infrared Spectroscopy*, 11(6): 447–456, 2003.
- [36] J Irudayaraj, R Xu, and J Tewari. Rapid determination of invert cane sugar adulteration in honey using ftir spectroscopy and multivariate analysis. *Journal of food science*, 68(6):2040–2045, 2003.
- [37] Sakhamuri Sivakesava and Joseph Irudayaraj. Classification of simple and complex sugar adulterants in honey by mid-infrared spectroscopy. *International journal of food science & technology*, 37(4):351–360, 2002.
- [38] S Sivakesava and J Irudayaraj. Prediction of inverted cane sugar adulteration of honey by fourier transform infrared spectroscopy. *Journal of food science*, 66(7):972–978, 2001.
- [39] S Sivakesava and J Irudayaraj. Detection of inverted beet sugar adulteration of honey by ftir spectroscopy. *Journal of the Science of Food and Agriculture*, 81(8):683–690, 2001.
- [40] MM Paradkar and J Irudayaraj. Discrimination and classification of beet and cane inverts in honey by ftraman spectroscopy. *Food Chemistry*, 76(2):231–239, 2002.
- [41] Francesca Corvucci, Lara Nobili, Dora Melucci, and Francesca-Vittoria Grillenzoni. The discrimination of honey origin using melissopalynology and raman spectroscopy techniques coupled with multivariate analysis. *Food chemistry*, 169:297–304, 2015.
- [42] Seher Gok, Mete Severcan, Erik Goormaghtigh, Irfan

Kandemir, and Feride Severcan. Differentiation of anatolian honey samples from different botanical origins by atr-ftir spectroscopy using multivariate analysis. *Food chemistry*, 170:234–240, 2015.

- [43] Abdul M Mouazen and Noura Al-Walaan. Glucose adulteration in saudi honey with visible and near infrared spectroscopy. *International Journal of Food Properties*, 17(10):2263–2274, 2014.
- [44] Lidija Svečnjak, Nikola Biliškov, Dragan Bubalo, and Domagoj Barišić. Application of infrared spectroscopy in honey analysis. *Agriculturae Conspectus Scientificus* (ACS), 76(3):191–195, 2011.
- [45] Yasmina Sultanbawa, Daniel Cozzolino, Steve Fuller, Andrew Cusack, Margaret Currie, and Heather Smyth. Infrared spectroscopy as a rapid tool to detect methylglyoxal and antibacterial activity in australian honeys. *Food chemistry*, 172:207–212, 2015.
- [46] Olga Escuredo, M Inmaculada González-Martín, M Shantal Rodríguez-Flores, and M Carmen Seijo. Near infrared spectroscopy applied to the rapid prediction of the floral origin and mineral content of honeys. *Food chemistry*, 170:47–54, 2015.
- [47] Ofélia Anjos, Maria Graça Campos, Pablo Contreras Ruiz, and Paulo Antunes. Application of ftir-atr spectroscopy to the quantification of sugar in honey. *Food chemistry*, 169:218–223, 2015.
- [48] Beril Özbalci, İsmail Hakkı Boyaci, Ali Topcu, Cem Kadılar, and Uğur Tamer. Rapid analysis of sugars in honey by processing raman spectrum using chemometric methods and artificial neural networks. *Food chemistry*, 136(3):1444–1452, 2013.
- [49] Jun Wang, Michael M Kliks, Soojin Jun, Mel Jackson, and Qing X Li. Rapid analysis of glucose, fructose, sucrose, and maltose in honeys from different geographic regions using fourier transform infrared spectroscopy and multivariate analysis. *Journal of food science*, 75(2): C208–C214, 2010.
- [50] Apostolos N Batsoulis, Nikolaos G Siatis, Athanasios C Kimbaris, Eleftherios K Alissandrakis, Christos S Pappas, Petros A Tarantilis, Paschalis C Harizanis, and Moschos G Polissiou. Ft-raman spectroscopic simultaneous determination of fructose and glucose in honey. *Journal of agricultural and food chemistry*, 53(2):207– 210, 2005.
- [51] Jagdish Tewari and Joseph Irudayaraj. Quantification of saccharides in multiple floral honeys using fourier transform infrared microattenuated total reflectance spectroscopy. *Journal of agricultural and food chemistry*, 52 (11):3237–3243, 2004.
- [52] Birgit Lichtenberg-Kraag, Christoph Hedtke, and Kaspar Bienefeld. Infrared spectroscopy in routine quality analysis of honey. *Apidologie*, 33(3):327–338, 2002.
- [53] S Sivakesava and J Irudayaraj. A rapid spectroscopic technique for determining honey adulteration with corn syrup. *Journal of Food Science*, 66(6):787–791, 2001.
- [54] M Garcia-Alvarez, JF Huidobro, M Hermida, and

JL Rodriguez-Otero. Major components of honey analysis by near-infrared transflectance spectroscopy. *Journal of agricultural and food chemistry*, 48(11):5154–5158, 2000.

- [55] PY Qiu, HB Ding, YK Tang, and RJ Xu. Determination of chemical composition of commercial honey by nearinfrared spectroscopy. *Journal of agricultural and food chemistry*, 47(7):2760–2765, 1999.
- [56] Jaeho Ha, Minseon Koo, and Hyunee Ok. Determination of the constituents of honey by near infrared spectroscopy. *J. Near Infrared Spectrosc*, 6:A367–A369, 1998.
- [57] M Garcia-Alvarez, S Ceresuela, JF Huidobro, M Hermida, and JL Rodriguez-Otero. Determination of polarimetric parameters of honey by near-infrared transflectance spectroscopy. *Journal of agricultural and food chemistry*, 50(3):419–425, 2002.
- [58] D Cozzolino and E Corbella. Determination of honey quality components by near infrared reflectance spectroscopy. *Journal of apicultural research*, 42(1-2):16–20, 2003.
- [59] Quansheng Chen, Shuai Qi, Huanhuan Li, Xiaoyan Han, Qin Ouyang, and Jiewen Zhao. Determination of rice syrup adulterant concentration in honey using threedimensional fluorescence spectra and multivariate calibrations. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 131:177–182, 2014.
- [60] MA Rios-Corripio, E Rios-Leal, M Rojas-López, and R Delgado-Macuil. Ftir characterization of mexican honey and its adulteration with sugar syrups by using chemometric methods. In *Journal of Physics: Conference Series*, volume 274, page 012098. IOP Publishing, 2011.
- [61] Sunita Mishra, Uma Kamboj, Harpreet Kaur, and Pawan Kapur. Detection of jaggery syrup in honey using nearinfrared spectroscopy. *International journal of food sciences and nutrition*, 61(3):306–315, 2010.
- [62] Olga Escuredo, M Carmen Seijo, Javier Salvador, and M Inmaculada González-Martín. Near infrared spectroscopy for prediction of antioxidant compounds in the honey. *Food chemistry*, 141(4):3409–3414, 2013.
- [63] Hongqian Chen, Zhenhua Tu, Zhaoshen Qing, Xiaobin Qiu, and Chaoying Meng. Feasibility study of veterinary drug residues in honey by nir detection. In *Computer and Computing Technologies in Agriculture VI*, pages 150– 156. Springer, 2013.
- [64] Landis W Doner. The sugars of honey?a review. *Journal* of the Science of Food and Agriculture, 28(5):443–456, 1977.
- [65] F James Holler, Douglas A Skoog, and Stanle R Crouch. Principles of instrumental analysis. *Belmont: Thomson*, 2007.
- [66] Da-Wen Sun. Infrared spectroscopy for food quality analysis and control. Academic Press, 2009.
- [67] Brian C Smith. Fundamentals of Fourier transform infrared spectroscopy. CRC press, 2011.
- [68] Peter Larkin. Infrared and Raman spectroscopy; princi-

ples and spectral interpretation. Elsevier, 2011.

- [69] Peter TC So and CHen Y Dong. Fluorecense spectrophotometry. In *Encyclopedia of Life Sciences*. Macmillan Publishers Ltd, Nature Publishing Group, 2002.
- [70] Joseph R Lakowicz. *Principles of fluorescence spectroscopy*. Springer Science & Business Media, 2007.
- [71] Josef Eisinger and Jorge Flores. Front-face fluorometry of liquid samples. *Analytical biochemistry*, 94(1):15–21, 1979.
- [72] RJ Barnes, MS Dhanoa, and Susan J Lister. Standard normal variate transformation and de-trending of near-infrared diffuse reflectance spectra. *Applied spectroscopy*, 43(5):772–777, 1989.
- [73] A Candolfi, R De Maesschalck, D Jouan-Rimbaud, PA Hailey, and DL Massart. The influence of data pre-processing in the pattern recognition of excipients near-infrared spectra. *Journal of Pharmaceutical and Biomedical Analysis*, 21(1):115–132, 1999.
- [74] Zhi-Min Zhang, Shan Chen, and Yi-Zeng Liang. Baseline correction using adaptive iteratively reweighted penalized least squares. *Analyst*, 135(5):1138–1146, 2010.
- [75] Tomas Isaksson and Tormod Næs. The effect of multiplicative scatter correction (msc) and linearity improvement in nir spectroscopy. *Applied Spectroscopy*, 42(7): 1273–1284, 1988.
- [76] P Geladi, D MacDougall, and H Martens. Linearization and scatter-correction for near-infrared reflectance spectra of meat. *Applied spectroscopy*, 39(3):491–500, 1985.
- [77] Abraham Savitzky and Marcel JE Golay. Smoothing and differentiation of data by simplified least squares procedures. *Analytical chemistry*, 36(8):1627–1639, 1964.
- [78] Jerry Workman Jr and Art Springsteen. *Applied spectroscopy: a compact reference for practitioners*. Academic Press, 1998.
- [79] Alan D McNaught and A Wilkinson. Compendium of chemical terminology, volume 1669. Blackwell Science Oxford, 1997.
- [80] Peter Kilz and J Cazes. Encyclopedia of chromatography, 2001.
- [81] Zoran Mandic. *Physico Chemical Methods in Drug Discovery and Development*. IAPC Publishing, 2012.
- [82] F Sanchez Rojas, C Bosch Ojeda, and JM Cano Pavon. Derivative ultraviolet?visible region absorption spectrophotometry and its analytical applications. *Talanta*, 35(10):753–761, 1988.
- [83] Jacob Cohen et al. A coefficient of agreement for nominal scales. *Educational and psychological measurement*, 20(1):37–46, 1960.
- [84] Vincent Labatut and Hocine Cherifi. Accuracy measures for the comparison of classifiers. *arXiv preprint arXiv:1207.3790*, 2012.
- [85] Einar Etzold and Birgit Lichtenberg-Kraag. Determination of the botanical origin of honey by fouriertransformed infrared spectroscopy: an approach for routine analysis. *European Food Research and Technology*, 227(2):579–586, 2008.

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classifier, PLSR: Partial Least Square Regression, MPLSR: Modified PLSR algorithm, MLR: Multiple Linear Regression, HCA: Hierarchical Cluster Analysis, ÷ $10^7/a \ nm, \ 1D: \ 1^{st}$ derivative, 2D: 2nd derivative, AN: Area Normalization, BC: Baseline Correction, As: Autoscaling, Vn: Vector normalized, Mn: Maximum normalization, LDA: Linear Discriminant Analysis, PLS-DA: Partial Least Square Prediction - Discriminant Analysis, BP-ANN: Back-Propagation Artificial Neural Network, SVM: Support Vector Machine, LS-SVM: Least Square SVM, CVA: Canonical Variate Analysis, DUS: Discriminant based Univariate Split for Trees based P: to predict constituents, Avg: Averaging bands, Om: Offset method, S-G: Savitzky-Golay smoothing, MC: Mean Centering, SIMCA: Soft-Independent Modeling by Class Analogy, LV: Latent Variable, PC: Principal Component, RSQ:multiple correlation coefficient, RPD: Ratio of Performance to Deviation, AUC: Area Under Curve, ex: Excitation, em: Emission, a cm^{-1} = Note: PP: Preprocessing, FR/S: Feature Reduction/Selection, CC: Classification/Clustering, R: Regression D: to determine types, V: to visualize, Spec.: Spectroscopy, FS: Fluorescence, FF-FS: Front-face Fluorescence, unknown.

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|----|---|------|-----|-----------------|----------|------------------------------|------------------------------|--------------------|--------|--------|--|---|
| No | Citation | Year | Aim | # of Samples | Spec. | Range | PP | Method FR/S | cc | R | Features | Results |
| 1 | Sultanbawa, Yasmina, et al. [45] | 2015 | Ч | 144 | ATR-MIR | $4000-375 cm^{-1}$ | | PCA | | PLSR | ? PCs ? LVs | $r^2 = 0.63 - 0.75$ |
| 2 | Escuredo, Olga, et al. [46] | 2015 | Ь | 60 | NIR | 1100-2498nm | ID or 2D MSC DT SNV | PCA | | STAM | 5-14 PCs ? LVs | RSQ= 0.778 - 0.971 |
| 3 | Lenhardt, Lea, et al. [4] | 2015 | D | 95 | FF-FS | Em:270-640nm Ex:240-500nm | | PARAFAC | PLS-DA | | 6 factors | Fake vs authentic: sens. =1 spec. =1 Bothanical origins: sens. & spec. > 0.8 |
| 4 | Anjos, Oflia, et al. [47] | 2015 | Ч | 63 | ATR-FTIR | $4000-450 cm^{-1}$ | 1D MSC SNV | | | PLSR | 1500-750 <i>cm</i> ⁻¹ ? LVs | mostly $r^2 > 80\%$ |
| Ś | Corvucci, Francesca, et al. [41] | 2015 | > | 308 | Raman | $3500\text{-}200cm^{-1}$ | AN BC As | PCA | | | $200-3500cm^{-1}$ | Reasonable separation |
| 9 | Gok, Seher, et al. [42] | 2015 | > | 144 | ATR-FTIR | $4000-650 cm^{-1}$ | Vn 1D | PCA | HCA | | $1800-750cm^{-1}$ | Heterogenity value: up to 10 |
| | | | > | 506 | | | 20 | PCA | | | $3700-600cm^{-1}$ | For some types, a clear cut with some outliers was found. |
| ~ | Svecnjak, Lidija, et al. [5] | 2015 | ۵ | 000 | ATR-FTIR | $3700-600 cm^{-1}$ | USU MSC | | PLS-DA | | $1800-700 cm^{-1}$ | 100% correct classification |
| | | | Р | | | |) | | | PLSR | $1800-700cm^{-1}$ & 3700-600 cm^{-1} | Electrical conductivity: $r^2 = 0.987$ pH: $r^2 = 0.939$ |
| | | | P+D | 84 | | | | | LDA | PLSR | $\frac{1800-700cm^{-1}~\&}{3700-600cm^{-1}}$ | - 2 of 6 components; r^2 from 0.66-0.7. - 100% correct classification |
| ~ | Lenhardt, Lea, et al.[6] | 2014 | D | 130 | ATR-FTIR | $4000-500 cm^{-1}$ | S-G | PCA | SVM | | 22 PCs | 98.6% success classification |
| 6 | Lenhardt, Lea, et al. [7] | 2014 | D | 109 | FF-FS | Em:30-300nm Ex·240-500nm | | PCA for feature | PLS-DA | | 8 LVs; Em:160nm Ex:240-500nm; | Sens. and Spec. >0.9 |
| | | | | 72 | | LA:240-200000 | | selection | | | 7 LVs; Em: 215nm Ex: 240-500 nm | Sens. and Spec. >0.99 |
| 10 | Chen, Quansheng, et al. [59] | 2014 | Ч | 164 | FS | Em:250-750nm Ex:200-580nm | | PCA | | BP-ANN | 9 statistical parameters 5 PCs | r = 0.9787 |
| 11 | Mouazen, Abdul M., and | 2014 | > | 09 | VIS-NIR | 305-2200nm | Mn | PCA | | | PC1, PC2 | Good separation |
| | l c+j. wataan. [-c+j. | | Ч | 345 | | | Avg Om S-G | | | PLSR | 340-2148nm ? LVs | RPD=2.06 (good model predictioon) |
| 12 | Latorre, C. Herrero, et al. [21] | 2013 | D | 30 | NIR | $4000-9000cm^{-1}$ | SNV | PCA | ANN | | 10 PCs | Sens. = 1.0; Spec. = 0.933 |
| 13 | Liang, Xiu Ying, Xiao Yu Li, and Wen Jun Wu. [8] | 2013 | D | 147 | NIR | $4000 - 10000 cm^{-1}$ | D-S | STd | ANN | | 5 LVs (5303-6591 <i>cm</i> ⁻¹) | 100% correct classification |
| 14 | Ozbalci, Beril, et al. [48] | 2013 | Ч | 90 | Raman | $200-2000 cm^{-1}$ | BC | | | ANN | $2000-200cm^{-1}$ | r > 0.95 |
| 15 | Roshan, Abdul-Rahman A., et al. [9] | 2013 | D | 38 | UV | 200-400nm | | | SIMCA | | ć | interclass dist. = 380 discriminant power > 3 modeling power > 0.8 |
| | | | | | | | | | | | | |

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| mostly RPD >2.5 | r = 0.6618 | 89.3% overall correct classification | Sens. = 0.7188; Spec. = 0.8462 | 100% correct classification | good separation | Sens. = 0.9373; Spec. = 0.8419 | $r^2 > 0.9$ | 78.57% overall correct classification 100% overall correct classification | $r^2 = 0.948 - 0.988$ | AUC = 0.952 | 90.62% correct classification | 87% overall correct classification | $r^2 = 0.81$ | Correct classification Coarcian = 90.4% Non-Coarcian = 86.3% | $r^2 = 0.97 - 0.99$ | 100% correct classification | 96% overall correct classification | vary | 100% correct classification | 90% correct classification | 75%-100% correct classification | >90% correct classfication | 91% overall correct classification Unifloral: > 90% correct classification Polyfloral: 55% correct classification | 90.9% correct classification | BI: $r=0.79$ HFCS: $r=0.72$ | 45% overall correct classification Unifloral: 29-100% correct classification Polyfloral: 19% correct classification |
|-----------------------------|-----------------------------|--------------------------------------|--------------------------------|-----------------------------|------------------------------|---|-----------------------------------|--|------------------------|-----------------------------|-----------------------------------|--|-----------------------------|--|--------------------------------|-----------------------------|---|---|--|---------------------------------------|---------------------------------|--|---|------------------------------|--------------------------------|---|
| ? LVs | $12500-3600cm^{-1}$ | $10000-4200 cm^{-1}$ | $1300-300cm^{-1}$ | $10000-6000 cm^{-1}$ | $1200-700 cm^{-1}$ | 15 bands | i | 10 PCs | 4-11 LVs | 102 Wavelet Coefficients | 10 PCs | 7 LVs | ż | Selected bands | 4-8 LVs | 3 PCs | 9 LVs | Distants between a sample and the mean of calibrated honey types | $3649-2401cm^{-1}+$ $1501-751cm^{-1}$ | 10 PCs Ex: 290nm; Em: 305-500nm | 5 LVs | 10-40 LVs | Ex: 220-440nm; Em: 420nm | 5 PCs | BI: 7 LVs HFCS: 8 LVs | 20 PCs 9947-4112 <i>cm</i> ⁻¹ |
| MPLS | LS-SVM | | | | | | PLSR | | PLSR | LS-SVM | SVM | | PLSR | | PLSR | | | | | | | | | | PLSR | |
| | | BP-ANN | PLS-DA | PLS-DA | | MVS | | BP-ANN | | | | PLS-DA | | PLS-DA | | SIMCA | PLS-DA | LDA | DUS | FDA | PLS-DA | PLS-DA | LDA | SIMCA | | LDA |
| | | | | | PCA | Fisher Ratio | | PCA | | МТ | PCA | | | Martens' Uncer- tanty Test | | | | PCA | PCA for feature selection | PCA | | | PCA | | | PCA |
| MSC | | ID | airPLS As | 1D MC | S-G | MSC | | S-G | 2D MC | 2D SNV | BC Smoothing Standarization | 2D | | 2D | | 1D | SNV | | | AN | SNV | | | | | |
| 1100-2798nm | $12500-3600cm^{-1}$ | $12000-4000 cm^{-1}$ | $2600-175 cm^{-1}$ | $10000-4000cm^{-1}$ | $1200-700 cm^{-1}$ | $3500\text{-}200cm^{-1}$ | $4000-650 cm^{-1}$ | 325-1075nm | $4000-400 cm^{-1}$ | $10000-4000cm^{-1}$ | 346-1038nm | 2500-12500nm | 1380-1960nm | 1100-2498nm | $4000-650 cm^{-1}$ | $1500-700 cm^{-1}$ | 2500-12500nm | $5012-926cm^{-1}$ | $4000-600 cm^{-1}$ | Em:280-480nm Ex:250,290,373nm | 1100-2498nm | 400-2498nm | Em:420 & 490nm & Ex:220-440nm Em:220-600nm & Ex:210,270,310,350, 390,440nm | 1100-2498nm | | $10000-4000 cm^{-1}$ |
| NIR | FT-NIR | FT-NIR | Raman | FT-NIR | FT-IR | Raman | FT-IR | VIS-NIR | ATR-FTIR | NIR | VIS-NIR | ATR-FTIR | NIR | NIR | ATP_FTTP | | ATR-FTIR | FTIR | FT | FS | NIR | NIR | FS | NIR | | FT-NIR |
| 09 | 153 | 250 | 149 | 144 | 144 | 374 | i | 230 109 | 37 | 135 | 232 | 373 | 56 | 373 | 235 | 78 | 150 | 1,075 | 82 | 62 | 292 | 478 | 371 | 179 | 96 | 364 |
| Ь | Ч | Ω | D | D | > | D | Ч | DD | Р | D | D | D | Ч | D | Ч | D | D | D | D | D | Ω | D | D | D | Ь | Q |
| 2013 | 2013 | 2012 | 2012 | 2011 | 2011 | 2011 | 2011 | 2011 | 2010 | 2010 | 2010 | 2010 | 2010 | 2009 | 0000 | 6007 | 2008 | 2008 | 2007 | 2007 | 2007 | 2007 | 2006 | 2006 | | 2006 |
| Escuredo, Olga, et al. [62] | Chen, Hongqian, et al. [63] | Chen, Lanzhen, et al. [10] | Li, Shuifang, et al. [28] | Chen, Lanzhen, et al. [29] | Svenjak, Lidija, et al. [44] | Pierna, Juan Antonio Fernndez, et al. [22] | Rios-Corripio, M. A., et al. [60] | Zhao, Xiangdong, Yong He, and Yidan Bao. [11] | Wang, Jun, et al. [49] | Zhu, Xiangrong, et al. [30] | Yang, Yan, et al. [12] | Hennessy, Siobhan, Gerard Downey, and Colm P. ODonnell. [23] | Mishra, Sunita, et al. [61] | Woodcock, Tony, Gerard Downey, and Colm P. ODonnell. [24] | Gallardo-Velzquez, Tzayhri, et | al. [25] | Hennessy, Siobhn, Gerard Downey, and Colm O'Donnell. [26] | Einar Etzold and Birgit Lichtenberg-Kraag [85] | Bertelli, D., et al. [13] | Karoui, Romdhane, et al. [14] | Woodcock, Tony, et al. [27] | Toher, Deirdre, Gerard Downey, and Thomas Brendan Murphy. [31] | Ruoff, Kaspar, et al. [15] | Kelly, J. Daniel, Cristina | Petisco, and Gerard Downey[33] | Ruoff, Kaspar, et al. [17] |
| 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 10 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 30 | 5 | 40 |

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| assification | t classification ct classification classification | with HPLC | assification | classification | | - Adulterated: 99 | îcation | | | ation adulteration | | tion | tion | | classification | assification | | classification | | nponents | |
|---|---|---|--|---|---|--|---|---|---|---|---------------------------------|---------------------------------|--|--|---|------------------------|--|------------------------|--|-------------------------|--|
| 54.5% total correct cli | 82.65% overall correc Uniflora: >90% corre Plyfloral: 26% correct | Statistically equivalent | 94% overall correct cl | 93.7% overall correct | $r^2 > 0.95$ | Correct classification: - Unadulterated: 96% | 93.75% correct classif | $r^2 = 0.61 - 0.97$ | $r^2 = 0.84 - 0.98$ | 100% correct classific for simple & complex | mostly r^2 >98% | 68% correct classifica | 93% correct classifica | $r^2 = 0.818$ | 78.4% overall correct $r^2 > 0.9$ | 91% overall correct cl | $r^2 = 0.824$ | 78.4% overall correct | $r^{2} = 0.700$ $r^{2} > 0.95$ | Reliable for major con | r = 0.68-0.98 |
| 6 PCs 2500-12500nm | 20 PCs | 6 | 19 PCs Ex:250mm; Em:20480nm Ex: 290; Em:305-500nm Ex:373nm; Em:305-600nm Ex:320400nm; Em:450nm | 6 LVs | 6 LVs | 9 LVs | - 5 PCs - 1500-800 <i>cm</i> ⁻¹ | 5-12 LVs | 2971-926 <i>cm</i> ⁻¹ 5-17 LVs | 2PCs 1500-800 cm^{-1} | 8-10 LVs | 10 PCs | 10 PCs | 1500-950 <i>cm</i> ⁻¹ 14 LVs | 10 factors $1600-200 \text{ cm}^{-1}$ | 3-4 LVs 10 factors | 15 LVs | 10 Factors | 7-9 LVs | 400-2500nm 2-8 LV s | 1100-2500nm |
| | | PLSR | | | PLSR | | | MPLS | PLSR | | WPLS | | | PLSR | PI_SR | | PLSR | DI CD | MPLS | MPLS | MLR |
| SIMCA | LDA | | LDA | PLS-DA | | PLS-DA | -LDA -BPNN | | | LDA | | CVA | BP-ANN | 1110 | CVA | CVA | | CVA | | | |
| | PCA | | PCA | | | | -PCA - none | | | PCA or PLS | | PCA | PCA | | PCA | PLS | | | | | |
| | Spectral cutting $3718-631 cm^{-1}$ | | Vn | AN 1D | | Ð | AN | SNV DT ID | | | SNV DT ID | 2D | | ID | 6 | | MC | AN | DT DT DT | SNV DT | |
| 2500-12500nm | $4000-550 cm^{-1}$ | $1700-700 cm^{-1}$ | Ex:250nm and Em:280-480nm Em:280-480nm Em:205-500nm Em:373nm and Em:373nm and Em:370-600nm Em:250-440nm and Em:450nm | $4000-800 cm^{-1}$ | $1500-750cm^{-1}$ | 400-2498nm | $1500-800 cm^{-1}$ | 400-2500nm | $5012-926cm^{-1}$ | i | 400-2500nm | 1100-2498nm | $3000 - 100 cm^{-1}$ | $4000-800 cm^{-1}$ | | $4000-200 cm^{-1}$ | $4000-400 cm^{-1}$ | $1500-800 cm^{-1}$ | 400-2500nm | 400-2500nm | 1100-2500nm |
| ATR-FTIR | FT-MIR | FT-Raman | FF_FS | ATR-FTIR | ATR-FTIR | NIR | ATR-FTIR | NIR | FTIR | FTIR | NIR | NIR | Raman | ATR-FTIR | | FT-Raman | ATR-FTIR | ATR-FTIR | NIR | VIS-NIR | NIR |
| 1380 | 411 | 21 | 57 | 320 | 112 | 300 | 48 | 110 | 1707 | ć | 156 | 51 | 43 | 50 | | 47 | 153 | 53 | 161 | 74 | 126 |
| D | D | Р | Q | D | Р | D | D | Р | Р | D | Р | D | D | Р | | , D | Р | D | Ъ | Р | Р |
| 2006 | 2006 | 2005 | 2005 | 2004 | 2004 | 2003 | 2003 | 2003 | 2002 | 2002 | 2002 | 2002 | 2002 | 2001 | | 2001 | 2001 | 2001 | 2000 | 1999 | 1998 |
| Kelly, J. Daniel, Cristina Petisco, and Gerard Downey. [32] | Ruoff, Kaspar, et al. [16] | Batsoulis, Apostolos N., et al. [50] | Ruoff, Kaspar, et al. [18] | Kelly, JF Daniel, Gerard Downey, and Vanessa Fouratier [34] | Tewari, Jagdish, and Joseph Iru- dayaraj. [51] | Downey, Gerard, Vanessa Fouratier, and J. Daniel Kelly. [35] | Irudayaraj, J., R. Xu, and J. Tewari. [36] | Cozzolino, D., and E. Corbella. [58] | Lichtenberg-Kraag, Birgit, Christoph Hedtke, and Kaspar Bienefeld. [52] | Sivakesava, Sakhamuri, and Joseph Irudayaraj. [37] | Garcia-Alvarez, M., et al. [57] | Davies, Anthony MC, et al. [19] | Goodacre, Royston, Branka S. Radovic, and Elke Anklam. [20] | Sivakesava, S., and J. Irudayarai. [39] | Paradkar M M and I | Irudayaraj. [40] | Sivakesava, S., and J. Iruda- varai. [53] | Sivakesava, S., and J. | nuuayaraj. [30] Garcia-Alvarez, M., et al. [54] | Qiu, P. Y., et al. [55] | Ha, Jacho, Minseon Koo, and Hyunee Ok. [56] |
| 41 | 42 | 43 | 4 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 | 55 | | 26 | 57 | 58 | 59 | 09 | 61 |