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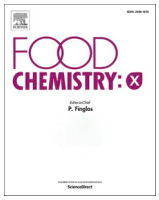

The application of emerging technologies for the quality and safety evaluation of oilseeds and edible oils

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ABSTRACT

Oilseeds and edible oils are an indispensable part for the human diet and provide nutritional support for the human health. It has been reported a total of above 170 million tons per annum of edible oils consumption were consumed worldwide. Safety and quality of oilseeds and edible oils cannot be ignored, which can pose risk to human health and cause agro-economic loss. Classical techniques widely used to detect the safety and quality attributes of oilseeds and edible oils often involve time-consuming and tedious operation; therefore, the development of low cost, rapid and non-destructive detection method is necessary. This review presents applications of four emerging spectroscopic techniques in recent ten years, such as Raman spectroscopy, fluorescence spectroscopy, fourier transform infrared spectroscopy and near-infrared spectroscopy for determining the quality and safety of oilseeds and edible oils. Meanwhile, the technical challenges and future prospects of these non-destructive spectroscopic technologies are also discussed.

1. Introduction

Oilseeds and edible oils are an indispensable part for the human diet and provide nutritional support for the human health, which contains essential nutrients and provides with energy. Examples of common consumed oilseeds include rapeseed, soybean, peanut, and sesame, being also the major sources of edible oils in China (Yang et al., 2018). Oilseeds and edible oils contain various natural nutrients including fat, protein, fatty acids, chlorophyll, tocopherol, squalene and carotenoids (Sundrasegaran & Mah, 2020; Xia et al., 2021), which have significant functions in anti-inflammatory, anti-cancer, anti-oxidation and preventing cardiovascular diseases (Trox et al., 2010). It has been reported a total of above 170 million tons per annum of edible oils consumption were consumed worldwide (Ng et al., 2015). However, oilseeds and edible oils are prone to be infected by fungi and mycotoxins during pre-harvest and post-harvest (Tao et al., 2018). Besides, pesticides are used to reduce diseases and insect pests of oilseeds, which can sometimes lead to the pesticide residues problem that need to be addressed (Jamshid et al., 2016). Moreover, the edible oils contain heavy metals with toxic properties such as arsenic with the range of 0.009–0.019μg/g (Zhu et al., 2011). Meanwhile, the polycyclic aromatic hydrocarbons (PAHs) are characteristics of carcinogenic and teratogenic, which can contaminate edible oil through various ways such as the oilseeds plants uptake PAHs by contaminated soil (Pandey et al., 2004). Mycotoxins, pesticide residue, heavy metals and PAHs are the common hazard factors in oilseeds and edible oils, which can pose risk to human health and cause agro-economic loss. It is therefore critical to evaluate the quality and safety of oilseeds and edible oils to ensure the high-quality development of oil industry.

Generally, chromatography and its hyphenation with mass spectrometry are the conventional and classical detection methods for quality and safety of oilseeds and oils, such as gas chromatography (GC), liquid chromatography (LC), gas chromatography mass spectrometry (GC–MS), liquid chromatography mass spectrometry (LC-MS) (Li, Wang,

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et al., 2020). Meanwhile, the enzyme linked immunosorbent assay and polymerase chain reaction are used to assess the contamination of aflatoxin and fungal (Wang et al., 2017). These technologies are widely used to detect safety and quality of oilseeds and oils. However, they are usually time-consuming, tedious operation and destructive, requiring some pretreatment or sample preparation. Therefore, evaluation trends of oilseeds and oils aim at developing advanced methods that are nondestructive, reliable, low cost, fast to measure. Emerging non-destructive spectroscopic technologies such as Raman spectroscopy, fluorescence spectroscopy, fourier transform infrared (FT-IR) spectroscopy and near infrared (NIR) spectroscopy are considered as promising tools for the quality and safety assessment of oilseeds and oils. The review of quality analysis in oilseeds and edible oils using NIR have been reported (Li, Zhang, et al., 2020). Raman spectroscopy has the narrow Raman band well resolved and the spatial resolutions, insensitive to water and temperature, lower sensitivity, high structural selectivity, provide qualitative, quantitative and structural analysis for food and agriculture nutritional components (Wang et al., 2021). Fluorescence spectroscopy has the ability to get 1 % accuracy and high sensitivity and selectivity for multiple potential analytes (Shaikh & O'Donnell, 2017). FT-IR is a high energy throughput, multiplexing capability, a good signal-to-noise ratio and highly reproducible technique (Duygu et al., 2009). It also can be used to determine the powdered, dehydrated, or aqueous samples (Delerisa & Petibois, 2003). NIR with probe flexibility and has the capability to detect the multiple components simultaneously (Fu & Ying, 2016).

Non-destructive technologies combined with chemometrics were applied to screen the safety and quality attributes in many kinds of agricultural products such as fish (Cheng et al., 2014), fruits (Arendse et al., 2018), staple foods (Su et al., 2017) and cereals (Hussain et al., 2019). This review is intended to have a comprehensive introduction of emerging non-destructive spectroscopic techniques, along with an overview of the application of these spectroscopic techniques in safety and quality evaluation of oilseeds and edible oils. Moreover, the future trends of application in non-destructive spectroscopic techniques are discussed.

In this review, the selection of references follows a set of strict criteria. The search engine of Web of Science was used and the keywords include "Raman/Fluorescence/FT-IR/NIR spectroscopy and oilseeds" and "Raman/Fluorescence/FT-IR/NIR spectroscopy and edible oils" to identify relevant literature. Only studies published in English between 2015 and 2024 were considered, ensuring the inclusion of the most recent advances in this research field. During the selection process, irrelevant studies, duplicates, and articles of low quality were excluded. In order to provide readers with a comprehensive, systematic, and reliable literature base that supports the arguments and conclusions presented.

2. Non-destructive spectroscopic techniques and applications

2.1. Raman spectroscopy

Raman spectroscopy was proposed by Raman and Krishnan, which is an inelastic scattering phenomenon that based on the exchange of light photon energy with molecules, and mainly causes the red shift of incident photon energy (Yin et al., 2018). The light source is monochromatic light with a certain frequency when analyzing the sample and monochromatic light incident into the medium leads to two different scattering processes. One is there is no energy exchange between the scattered photons and the sample molecules, the scattering frequency is the same as the excitation photons while the propagation direction of the scattered photons has changed. This elastic scattering is called Rayleigh scattering, which is the main part of scattering (Yaseen et al., 2017). The other is a minority of scattered photons exchange energy with the sample molecules. Not only has the direction of propagation changed, but also its frequency is different from the excitation photons. This inelastic scattering is called Raman scattering (Shoeman et al., 1993). Meanwhile, Raman scattering includes two types, one is Stokes scattering and the other is anti-Stokes scattering. With the rapid advancement of technology, Raman spectroscopy has various kinds of evaluation spectroscopy in order to meet different demands, including surface-enhanced Raman spectroscopy (SERS), fourier-transform Raman spectroscopy, micro-Raman spectroscopy, NIR Raman spectroscopy, and spatially offset Raman spectroscopy. Raman spectroscopy is a rapid and nondestructive vibration technique, it shows great potential to identify common and specific components in complex matrices combined with chemometrics. Furthermore, it has been applied to determine the quality and safety of the oilseeds and edible oils intensively. The overview of application of Raman spectroscopy in the detection of quality attributes of oilseeds and edible oils is shown in Table 1.

Protein, oil content, peroxide value (PV), iodine value, and fatty acids, are the important quality parameters for the oilseeds and edible oils, besides, carotenoids contributes to the oxidative stability for the edibles oil. These quality parameters have got progress with Raman spectroscopy. A model was established with different treatment of soybean, including ground bean, whole meal, and ground meal. Metric-based multiple linear regression (Metric-MLR) was the optimal method to measure bulk protein and oil content of whole meal soybean. As a result, coefficient of determination (R^2) were both 0.87 and root mean square error of prediction (RMSEP) were 1.15 ± 0.04 and 0.80 ± 0.02 (Singh et al., 2019). A surface-enhanced Raman spectroscopy analyzer based on plasmonic metal liquid-like platform was developed to detect the PV in edible oils, which showed the relative deviation was less than 10 % compared to the national standard method (Jiang, He, et al., 2021). Similarly, Raman spectroscopy was proved to outperform in assessment of PV and free acidity in extra virgin olive oil (EVOO). Partial least squares regression (PLSR) and principal component regression (PCR) were used to establish the model. The best result showed R^2 value of 0.989 and 0.994, low root mean square error (RMSE) value of 0.72 meq O^2/kg and 0.01 % for PV and free acidity (Gouvinhas et al., 2015). Edible oils were used to detect the PV, acid values and total polar compounds under frying conditions at real time by Raman spectroscopy (Castro et al., 2022). The model of acid value and peroxide value in flaxseed oil during frying was established coupled with peak-area-ratio method (Hua et al., 2024). Iodine value of unsaturated edible oils was determined and obtained the R^2 of 0.976 (Dyminska et al., 2017). Variable combination population analysis (VCPA) combined with support vector machine (SVM) were used to detect the acid value of edible oils during storage and obtained the determination coefficient of prediction (R_P^2) and RMSEP were 0.932 and 0.153 (Jiang, Su, et al., 2021). The least-squares support vector machine (LS-SVM) was used to build the model for predicting acid value in soybean oil, canola oil, and palm oil. The model obtained an RMSEP of 0.016 and a ratio of prediction to deviation (RPD) of 11.351 (Wang et al., 2023). PLSR was employed to build the model for saponification value of coconut-gingelly oil and coconut-sunflower oil systems, with the R^2 and RMSEP were 0.999 and 2.4, respectively (Ajikumar et al., 2025). Raman spectroscopy was a useful approach to monitor the fatty acid (FA) concentration of the vegetable oils. EVOO was used to detect the oleic acid, palmitic acid and linoleic acid, with R^2 between 0.80 and 0.92, the cross validation was nearly 0.68 (Portarena et al., 2019). A novel approach was proposed that the free fatty acid (FFA) of olive oil was detected by the relative intensity ratio of I_{1525}/I_{1655} (Qiu et al., 2019). In another study, a rapid method for determination of trans fatty acids (TFA) concentration in edible oils by stepwise multiple linear regression (SMLR) method and obtained residual predictive deviation was 4.639 (Gong et al., 2019). The saturated fatty acids (SAFA), monounsaturated fatty acids (MUFA) and polyunsaturated fatty acids (PUFA) in EVOO were determined by Raman spectroscopy. The result showed lower errors and all errors are close to 0 (Sánchez-López et al., 2016). A study was investigated to evaluate total MUFA and PUFA in vegetable oils, which had the great result that R^2 were 0.9555 and 0.9963, RMSEP were

Table 1
Overview of application of Raman spectroscopy in the detection of nutrient components of oilseeds.

Species	Spectral range (nm) (0()(()(s)11()()*()()(nm)	Model	Attribute(s)	Performance/Accuracy	Reference
Soybean	5128.2–25,000	Metric-MLR	Bulk protein, oil content	R^2–0.87-0.87, RMSEP-1.15 ± 0.04–0.80 ± 0.02.	Singh et al. (2019)
Edible oils	5000–20,000	–	PV	–	Jiang, He, et al. (2021)
Edible oils	2500–125,000	–	Iodine values	R^2–0.976	Dyminska et al. (2017)
EVOO	3278.7–40,000	PLSR, PCR	PV, free acidity	R^2–0.989-0.994 RMSE-0.72 meq O_2/kg −0.01 %	Gouvinhas et al. (2015)
Edible oils	3703.7–23,257.0	PLS	PV, acid values, Total polar compounds	RMSEP-0.03-0.95-1.89, R_P^2-0.91-0.86-0.96 RER-12.8-9.3-16.5, RPD-3.4-2.5-5.0	Castro et al. (2022)
Flaxseed oil	2777.8–100,000	–	PV, acid value	R^2–0.99179	Hua et al. (2024)
Edible oils	3030.3–100,000	SVM	Acid value	R_P^2. 0.932 RMSEP- 0.153	Jiang, Su, et al. (2021)
soybean oil, canola oil, palm oil	3125–100,000	LS-SVM	Acid value	RMSEP-0.016, RPD-11.351	Wang et al. (2023)
Edible oils	4347.8–25,000	PLSR	Saponification value	R^2–0.999, RMSEP-2.4	Ajikumar et al. (2025)
EVOO	3278.7–13,333.3	PLS	Oleic acid, palmitic acid, linoleic acid	R^2–0.80-0.92, cross validation-nearly 0.68.	Portarena et al. (2019)
Olive oil	–	–	FFA	–	Qiu et al. (2019)
Edible oils	2941.2–200,000	SMLR	TFA	residual predictive deviation-4.639	Gong et al. (2019)
EVOO	3225.8–100,000	PLS	SAFA, MUFA, PUFA	lower errors	Sánchez-López et al. (2016)
Vegetable oils	3846.2–57,142.9	PLS	Total MUFA, PUFA	R^2–0.9555-0.9963 RMSEP-0.0207- 0.0054	Bin et al. (2016)
Rapeseed and soybean oil	2857.1–50,000	SVR	MUFA, PUFA, SAFA	R^2–0.9670-0.9568-0.9553, RMSE-0.0273-0.0326-0.0340 R^2–0.9414-0.9562-0.9422, RMSE-0.0460-0.0378-0.0548	Pang et al. (2022)
Olive oil	3278.7–13,333.3	–	β-carotene	–	Anselmi et al. (2022)

Note: Metric-MLR: metric-based multiple linear regression, R^2: coefficient of determination, RMSEP: root mean square error of prediction, PV: peroxide value, PLSR: partial least squares regression, RMSE: root mean square error, PLS: partial least squares, R_P^2: determination coefficient of prediction, SVM: support vector machine, LS-SVM: least-squares support vector machine, FFA: free fatty acid, TFA: trans fatty acids, SAFA: saturated fatty acids, MUFA: monounsaturated fatty acids, PUFA: polyunsaturated fatty acids, SVR: support vector regression.

0.0207 and 0.0054, respectively (Bin et al., 2016). The MUFA, PUFA and SAFA of rapeseed and soybean oil were obtained a higher correlation coefficient and lower RMSE value (Pang et al., 2022). Only one drop olive oil was used to detect the β-carotene, which can be used to detect olive fly attack (Anselmi et al., 2022).

Raman spectroscopy was not only used for quality analysis but also for detecting mycotoxins, PAHs and pesticide residues in oilseeds and edible oils. Raman spectroscopy combined with synergy interval partial least squares (siPLS) were used to screen zearalenone-contaminated maize (Guo et al., 2019). Meanwhile, aflatoxin B_1 (AFB1) in maize (Deng, Jiang, & Chen, 2022a) was detected with SERS. Detection of AFB1 in peanut oil was also investigated (Chen et al., 2020; Zhu et al., 2022). Recurrent neural network (RNN) was used to detect the AFB1 in edible oils with the accuracy of 100 %, R^2 and the ration of prediction to deviation were 0.95 and 4.86, respectively (Deng, Zhang, et al., 2022). Liquid-interfacial surface-enhanced Raman spectroscopy was employed to detect the PAHs in edible oils within 3 min (Su et al., 2021). Long short-term memory network (LSTM) combined with convolutional neural network (CNN) to detect the chlorpyrifos residues in corn oil, with the R_P^2 and RPD were 0.90 and 3.2, respectively (Xue & Jiang, 2023). Meanwhile, the use of a one-dimensional CNN (1D-CNN) to determine chlorpyrifos residues in corn oil obtained satisfactory results

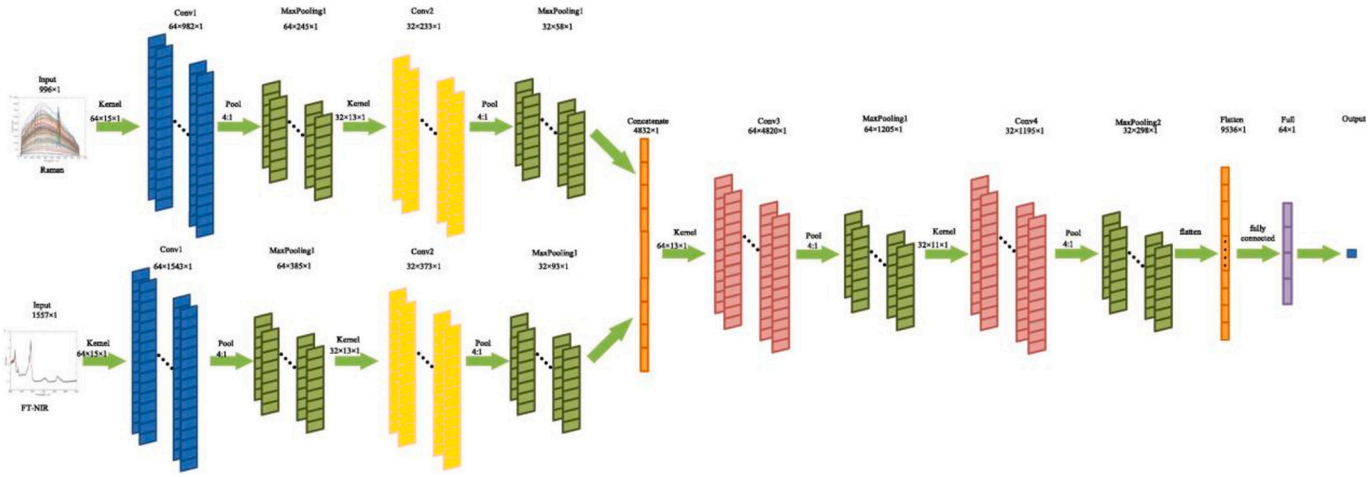

Fig. 1. Network structure of mid-level fusion technology (Mei et al., 2024).

when combined with data fusion from Raman and NIR spectrometers (Mei et al., 2024). The network structure of mid-level fusion technology was shown in Fig. 1. Raman spectroscopy has been applied to determine the oil content, protein, PV, iodine value and FA in oilseeds and edible oils, it has the unique advantage to differentiate the cis or trans double bonds in unsaturated fatty acids. Furthermore, the application of Raman spectroscopy for minor components like tocopherol, phenolic compounds and squalane in edible oils has been reviewed (Hu et al., 2019). Meanwhile, the hazards factors in oilseeds and edible oils are also introduced.

In summary, C═C, C═N, C–NO^2, C–X (X = F, Cl, Br or I), C—S and S—S have the strong Raman signals because the stronger change in polarization of these molecules, which showed satisfactory result for detection the quality parameters and the hazards factors of oilseeds and edible oils with these functional groups. Raman spectroscopy not only can obtain the information about the molecular fingerprinting but also acquire the bond structure changes compared to other spectroscopic technologies. However, fluorescence scattering light has much stronger intensity than Raman scattering light, some measures are required to restrict the fluorescence interference, such as fluorescence quenching method and the chemometrics. However, there are still some challenges for the removal methods, for example, the fluorescence removal effectiveness may change with the sample used, so exploring the reliable and efficient methods to eliminate the fluorescence is essential. Meanwhile, the food matrix is an important challenge, therefore, extraction, concentration and other basic preparation steps might be necessary prior to Raman spectroscopy used. Besides, the development of suitable signal enhancement substrates is essential for obtaining reliable results and improving the test sensitivity. Meanwhile, Raman spectroscopy coupled with mass spectroscopy or fluorescence spectroscopy has been used for bioanalytical applications recently (Das et al., 2017). Therefore, Raman spectroscopy connect with other analytical technique to evaluate the quality and safety in oilseeds and edible oils can be used. Furthermore, the future trends of the Raman spectrometer will be automatic and miniaturized portable instruments.

2.2. Fluorescence spectroscopy

Fluorescence is a high-energy light source excites molecules or moieties to emit light and release energy, which is a form of luminescence (Huang et al., 2022). Fluorophores are organic compounds that absorb (chromophore) and re-emit light, they have a core position in the fluorescence spectroscopy, and the components produce fluorescence in the molecules (Fellman et al., 2010). Fluorescence spectroscopy, also called fluorescence fingerprint, is used to measure the fluorescence characteristics of objects, and can detect organic components with fluorescence chromophores, offering information about the electronic structure of the objects (Li, Wang, et al., 2020). Generally, the fluorescence process includes the following steps: the molecules absorb light from the ground state to the excited state; then changing from the upper excited state to the lower electronic state without any radiation; and finally the electronic state returns to the ground state (Hussain et al., 2019). Single fluorescence spectroscopy and synchronous fluorescence spectroscopy are suitable for fluorescence spectrometer. Meanwhile, fluorescence spectroscopy, with its high sensitivity and selectivity, is well-suited for assessing the quality and safety of oilseeds and edible oils. The overview of application of fluorescence spectroscopy in the detection of quality attributes of oilseeds and edible oils is listed in Table 2.

The model of protein and oil contents in soybeans were built with the R^2 reached 0.86 and 0.74 (Saito et al., 2021). The model was based on the artificial neural network (ANN) method for the prediction of PV, acid value in peanut oil, which presented satisfactory results with MSE_{train} was 2.45, MSE_{test} was 4.10, correlation coefficient for training set (R_{train}) was 0.96 and correlation coefficient for test set (R_{test}) was 1.00 for PV, MSE_{train} was 0.03, MSE_{test} was 3.43, R_{train} was 1.00, and R_{test} was 1.00 for acid value in high temperatures (Gu et al., 2018). Four edible oils were stored at different days to measure the PV, multivariate curve resolution alternating least square (MCR-ALS) and ANN were used to build the model, the result showed the R_{train} and R_{test} were 1 and 0.96, respectively (Gu et al., 2019). The fuorescence intensity, reduced scattering coefficients and absorption of peanut oils were used to build the model for PV and acid value. ANN and support vector regression (SVR) revealed the optimal result of PV and acid value with the R_V^2 were 0.873 and 0.854, and root mean square errors for validation set (RMSEV) 2.896 meq·kg^{-1} and 0.154 mg/g, respectively (Wang et al., 2024). Unfolded partial least squares (U-PLS) was performed to build the oxidation index model of the EVOO with four different kinds of

Table 2
Overview of application of fluorescence spectroscopy in the detection of nutrient components of oilseeds.

Species	Spectral range (nm)	Model	Attribute(s)	Performance/Accuracy	Reference
Soybean	200–600	PLSR	Protein, oil content	R^2–0.86 - 0.74	Saito et al. (2021)
Peanut oil	200–800	ANN	PV, acid value	MSE_{train}-2.45-0.03, MSE_{test}-4.10-3.43, R_{train}-0.96-1.00, R_{test}-1.00-1.00	Gu et al. (2018)
Edible oils	200–800	MCR-ALS	PV	R_{train}-1, R_{test}-0.96	Gu et al. (2019)
Peanut oil	210–980	ANN, SVR	PV, acid value	R_v^2-0.873-0.854, RMSEV-2.896-0.154	Wang, Guo, et al. (2024)
EVOO	250–700	U-PLS	Peroxide index, K_{232}, K_{270}, Oxidative stability index	R_v^2-0.94-0.94-0.86-0.90, RMSEP-1.53-0.16-0.019-3.60mEqO_2·kg^{-1} REP(%)-14.98–9.22-12.25-8.12	Martín-Tornero et al. (2022)
EVOO	250–698.5	PLSR	Acidity, K_{232}, total tocopherol, peroxide index	R^2 close to 0.9, R^2 close to 0.7(peroxide index)	Baltazar et al., (2020)
Virgin olive oil	250–700	PLS	TPC	R^2–0.951, relative predictive deviation-4.0.	Squeo et al. (2018)
Rapeseed oil	250–500	MLR, PLSR	Pheophytin, carotenoids, total tocopherol content	R_{cal}^2-0.903-0.861-0.984, R_{cv}^2-0.825-0.735-0.972, RMSECV-27.2-0.25-6.65	Sikorska et al. (2019)
EVOO	250–730	PLS	Squalene	RMSEC-0.1500, RMSECV-0.1065, RMSEP-0.1310	Tarhan. (2020)

Note: PLSR: partial least squares regression, R^2: coefficient of determination, ANN: artificial neural network, PV: peroxide value, R_{train}: correlation coefficient for training set, R_{test}: correlation coefficient for training set, MCR-ALS: multivariate curve resolution alternating least square, U-PLS: unfolded partial least squares, SVR: support vector regression, R_V^2: determination coefficient of validation, RMSEV: root mean square error of validation, RMSEP: root mean square error of prediction, REP: relative error of prediction, TPC: total polar compounds, RMSECV: root mean square error of cross-validation, MLR: multiple linear regression, R_{cal}^2: determination coefficient of calibration, R_{cv}^2: determination coefficient of cross-validation.

containers (Martín-Tornero et al., 2022). Fluorescence emission spectra of EVOO was obtained to determine the characteristics including acidity, peroxide index, K_{270}, K_{232}, total tocopherols, α-tocopherol, β-tocopherol and γ-tocopherol, the model showed R^2 of acidity, K_{232} and total tocopherol content close to 0.9, while the peroxide index close to 0.7, and other characteristics had a bad performance (Baltazar et al., 2020). PLSR was employed to evaluate total tocopherol content of edible oils by fluorescence spectroscopy. The prediction accuracy presented regression coefficient (r) was 0.991 and root mean square error of cross-validation (RMSECV) was 36 mg/dm^3. As a result, the model can be used for prediction total tocopherol content of edible oils (Sikorska et al., 2005). A rapid analytical method based on fluorescence spectroscopy was developed for the determination of total phenolic content (TPC) in virgin olive oil. Partial least squares (PLS) with accuracy values for R^2 was 0.951, relative predictive deviation was 4.0 (Squeo et al., 2018). Cold-pressed rapeseed oil was used to determine the pheophytin, carotenoids and total tocopherol content. The result obtained determination coefficient of calibration (R^2_{cal}) were 0.903, 0.861 and 0.984, determination coefficient of validation (R^2_{cv}) were 0.825, 0.735 and 0.972, RMSECV were 27.2, 0.25 and 6.65 by using multiple linear regression (MLR) and PLSR. Therefore, fluorescence spectroscopy can be used to determine the pheophytin, carotenoids and total tocopherol content in cold-pressed rapeseed oil (Sikorska et al., 2019). The wavelength of 250–730 nm was chosen to detect the squalene content in extra virgin olive oils, which revealed the root mean square error of calibration (RMSEC), RMSEV and RMSEP were 0.1500, 0.1065 and 0.1310, respectively (Tarhan., 2020).

Fluorescence spectroscopy has developed rapidly and widely used in the detection of hazard factors of oilseeds and edible oils. The combination of multi-way method and fluorescence spectroscopy was employed to determine the aflatoxin B_1 and aflatoxin B_2 (AFB2) of peanuts (Sajjadi et al., 2016). The carbendazim and metiram pesticides residues of rapeseed and peanut oils was detected by collecting fluorescence spectrum. The R^2 between the fluorescence intensity and the pesticide concentration in the mixture was greater than 0.99. Limit of detection (LOD) were 7.07×10^{-4} mg/mL and 9.28×10^{-4} mg/mL for carbendazim and metiram pesticides residues. It was an efficient way to detect the pesticide residues in rapeseed and peanut oils (Chen et al., 2015). Fluorescence spectroscopy was used to determine the carbendazim and chlorothalonil pesticides residues of peanut oil. The carbendazim and chlorothalonil of peanut oil using excitation-emission matrix fluorescence coupled with alternating penalty trilinear decomposition (APTLD) can achieve high recoveries and sensitivity. It was verified that fluorescence spectroscopy can analysis the different pesticides residues of peanut oil (Yuan et al., 2019). A study was investigated that the extraction with the generation of hydride or cold vapor combined with atomic fluorescence spectrometry can determine the As, Se and Hg in crude palm oil. The concentrations of As and Se was limit of quantification (LQ) < -1.6 and 1.3–2.4 μg/L. However, the concentration of Hg was below the LQ. It was proved atomic fluorescence spectrometry is reliable to determine As and Se in crude palm oil (Valasques et al., 2020). Heavy PAHs in olive and sunflower oils were detected by fluorescence spectroscopy. The detection of PAHs obtained the satisfactory result though solid phase extraction with silica to remove the pigments and tocopherol (Alarcon et al., 2012). The PAHs of vegetable oils were successfully to detect using second-derivative nonlinear variable-angle-matrix isopotential synchronous fluorescence spectroscopy. The LOD of the chrysene (Chr), benzo(*a*)anthracene (BaA), benzo(*a*)pyren (BaP), and benzo(*b*)fluoranthene (BbF) were 13.0, 8.64, 0.16 and 7.68 μg/kg, respectively (Liu et al., 2016).

Generally, fluorescence spectroscopy was suitable for the determination of oil content, protein, PV, acid value, total tocopherol content, TPC and hazard factors in oilseeds. Fluorescence spectroscopy with rapidness and high sensitivity compared to other spectrophotometric techniques, it can be used to quantify fluorescent substances and monitor the molecular changes when it occurs during the food handling, processing and storage. However, fluorescence can be interfered by contaminants, which will lead to errors or no result. One photon induced fluorescence is the best option to detect the aflatoxin contaminants in solid foods, which can provide strong fluorescence signal to detect the low concentrations of contamination. Furthermore, on-line monitor quality of oilseeds is essential to use fiber optics connect with fluorescence spectrometer to make the real time detection of quality in oilseeds is possible.

2.3. Fourier transform infrared spectroscopy

FT-IR spectroscopy is mainly the electromagnetic spectrum in the mid-infrared region with a wavenumber of 4000–400 cm^{-1}, which measures the basic vibration of substances and records frequency or intensity into the infrared spectrum (Rohman et al., 2020). It can be seen the wavelength of the light absorbed by the chemical bond in the spectrum (Fu et al., 2020; Jantasee et al., 2014). According to the characteristics of the sample and the required detection accuracy, precise and trustworthy data can be acquired by means of choosing appropriate accessories and sample preparation methods, thereby receiving chemical information about more samples (Li et al., 2019). Both wet and dry samples can be analyzed using FT-IR, which can obtain high-quality spectra from a small number of samples. Additionally, FT-IR is widely used in oilseeds quality detection due to its distinct advantages. The overview of application of FT-IR in the detection of quality attributes of oilseeds is listed in Table 3.

Multivariate regression analysis was applied to predict the iodine value of edible oils based on FT-IR data. Backward interval PLS (BiPLS) algorithms revealed great predictive results that R^2, RMSECV and RMSEP were 0.9885, 2.68 and 2.73, respectively (Meng et al., 2017). Disposable polyethylene films were selected to be the sample support to evaluate the iodine value and saponification number of edible oils. The method had a relative standard deviations (RSD) were 0.39 % and 0.32 % when compared to the standard methods, demonstrating its effectiveness in analyzing the iodine value and saponification number of edible oils (Xu et al., 2018). FT-IR was used to predict the PV in edible oils. It had the result of correlation coefficients (R) was 0.9972, prediction residual sums of squares (PRESS) and RMSEP were 66.46 and 0.579 (Shang et al., 2018). FT-IR data fusion were applied to determine the PV and acid value in edible oils, which showed the great performance that R^2_c and R^2_p were 0.964 and 0.939, RMSEC and RMSEP were 0.060 and 0.080 for PV, R^2_c and R^2_p were 0.955 and 0.919, RMSEC and RMSEP were 0.025 and 0.027 for acid value (Liu et al., 2020). FTIR-attenuated total reflection (FTIR-ATR) was applied to detect the PV, FFA and FA in edible oils, with correlation coefficients of calibration (R_c) higher than 0.99 and correlation coefficients of validation (R_v) higher than 0.86 using orthogonal signal correction-PLS (OSC-PLS) (Mahboubifar et al., 2016). Olive oil was studied to determine FFA with FT-IR. The accuracy obtained R, RMSEC and RMSECV were 0.9998, 0.0044 and 0.0107 (Tarhan et al., 2017). FFA, PV, thiobarbituric acid reactive substances (TBARS) and total oxidation (TOTOX) of the rapeseed oil in the process of storage were detected using FT-IR, the results showed that the R^2_p of the FFA, PV, TBARS were 0.99 while the R^2_p of TOTOX was 0.87 (Ghnimi et al., 2024). Quantitative model was developed for assessment TFA in edible oils by PLSR. The benchtop and portable attenuated total reflection-FTIR (ATR-FTIR) obtain the R^2 were 0.994 and 0.992. RMSECV were 0.23 and 0.14. The method provided a rapidly alternative method to detect TFA (Karunathilaka et al., 2018). Different quality parameters of olive oils were estimated by means of FT-IR, with R^2 more than 0.87 for oxidative stability, chlorophyll content, palmitic, oleic, linoleic acids, saturated, monounsaturated and polyunsaturated fatty acids, phenolic compound and TPC, which suggests FT-IR can be used to evaluate the quality of olive oil (Uncu & Ozen, 2015).

Meanwhile, FT-IR has made significant advances in detection of the specific nutrient components in oilseeds and oils. The study was

Table 3
Overview of application of FT-IR in the detection of nutrient components of oilseeds.

Species	Spectral range (nm)	Model	Attribute(s)	Performance/Accuracy	Reference
Edible oils	250–2500	BiPLS	Iodine value	R^2–0.9885, RMSECV-2.68, RMSEP-2.73	Meng et al. (2017)
Coconut, rapeseed, and linseed oil	200–2500	PLS	Iodine value, saponification number	RSD- 0.39 % -0.32 %	Xu et al. (2018)
Edible oils	167–400	PLS	PV	R-0.9972, PRESS-66.46, RMSEP-0.579	Shang et al. (2018)
Soybean, rapeseed, sunflower, peanut oils	526–1493	PLSR	PV, acid value	R_c^2-0.964-0.955, R_p^2-0.939-0.919, RMSEC-0.060-0.025 , RMSEP-0.080-0.027	Liu et al. (2020)
Canola, Corn, Sunflower, frying oil	250–1818	OSC-PLS	PV, FFA, FA	$R_c > 0.99$, $R_v > 0.86$	Mahboubifar et al. (2016)
Olive oil	250–1538	PLSR	FFA	R-0.99979, RMSEC-0.00441, RMSECV-0.0107	Tarhan et al. (2017)
Rapeseed oil	2500–15,384.6	PLSR	FFA, PV, TBARS, TOTOX	R_p^2-0.99-0.99-0.99-0.87	Ghnimi et al. (2024)
Edible oils	250–1429	PLSR	TFA	R^2–0.994-0.992, RMSECV-0.23-0.14.	Karunathilaka et al. (2018)
Olive oil	250–1538	PLS	Oxidative stability, chlorophyll, palmitic, oleic, linoleic acids saturated, monounsaturated, polyunsaturated fatty acids, phenolic compound, TPC	$R^2 > 0.87$	Uncu and Ozen (2015)
Corn, peanut, soybean, sunflower oil	250–1538	PLS	α-tocopherol	R-0.977, RMSEC-4.97	Silva et al. (2009)
Virgin olive oil	250–1538	PLS	Phenolic compounds	R^2–0.99, RMSEP-0.11	Hirri et al. (2016)
Amaranth seed oil	250–2500	PLS	Squalene	R^2–0.9989, RMSEC-0.0930, RMSECV-0.1301	Tarhan. (2021)
Soybean	250–1538	PLSR	Anthocyanin	R^2–0.86-0.88, SEP-9.7-21.8 %	Amanah et al. (2020)

Note: BiPLS: backward interval partial least squares, R: regression coefficient, RMSECV: root mean square error of cross-validation, PLS: partial least squares, PLSR: partial least squares regression, RSD: relative standard deviations, PV: peroxide value, PRESS: prediction residual sums of squares, RMSEP: root mean square error of prediction, R_c^2: Determination coefficient of calibration, R_p^2: determination coefficient of prediction, OSC-PLS: orthogonal signal correction-partial least squares, FFA: free fatty acid, FA: fatty acid, TBARS: thiobarbituric acid reactive substances, TOTOX: total oxidation, R_c: correlation coefficients of calibration, R_v: correlation coefficients of validation, RMSEC: root mean square error of calibration, TFA: trans fatty acids, R^2: coefficient of determination, SEP: standard error of prediction.

analyzed to examine α-tocopherol of vegetable oils by PLS method, the result showed FT-IR have the potential to be utilized for the determination of α-tocopherol in vegetable oils (Silva et al., 2009). The wavenumber range 4000-600 cm^{-1} of FT-IR was used to measure the phenolic compounds of virgin olive oil. With R^2 and RMSEP were 0.99 and 0.11, respectively (Hirri et al., 2016). The findings revealed potential in detection sesamol in sesame seed oil. The determination of squalene in amaranth seed oil with the FT-IR, UV–visible and fluorescence techniques, which showed FT-IR obtained the great result with the RMSEC, RMSECV and R^2 were 0.0930, 0.1301 and 0.9989, respectively (Tarhan., 2021). Besides, FT-IR detected the anthocyanin of single soybean seed successfully (Amanah et al., 2020).

These studies have revealed the applicability of FT-IR for the quality evaluation in oilseeds due to its rapidness, better signal to noise ratio and quantitative and qualitative analysis. However, it is critical to improve spectral acquisition way and obtain the representative background to collect FT-IR spectra effectively. Usually, diffuse reflection accessory, ATR-FTIR and transmission mode are used to acquire the spectra. Meanwhile, selecting suitable chemometric methods to solve the spectral signal problems is an important way to realize effective calibrations.

2.4. Near infrared spectroscopy

NIR is a kind of high-energy vibrational spectroscopy covers the wavelength of 780-2500 nm, reflected or transmitted radiation is recorded when radiation the sample with NIR light, which provides low cost, rapid and greater penetrative power potential (Li et al., 2022; Zhou et al., 2020). NIR is the overtones and combinations of fundamental bands vibrations involves the functional groups of C—H, N—H and O—H and conforms to Lambert-Beer's law (Johnson, 2020). In our previous work, the quality analysis of oilseeds and edible oils using NIR spectroscopy has been reviewed (Li, Zhang, et al., 2020). Therefore, the process of quality and safety assessment in oilseeds and edible oils were introduced recently. Different wavelength selection methods were used to build the model of oil content, protein, moisture and starch in corn, as a result, eXtreme Gradient Boosting (XGBoost) was used to extract the feature wavelengths and one-dimensional shallow CNN was applied to build the model of oil content, protein, moisture and starch in corn, the result revealed that the R^2 of the main four parameters were higher than 0.99 (Zou et al., 2025). The prediction results with different wavelength selection methods were revealed in Fig. 2. The moisture and protein in corn were detected using PLSR method (Zheng et al., 2024). Single-kernel NIR was used to detect the oil content and protein in single flax seed, with the R^2 were 0.82 and 0.62, standard error of prediction (SEP) were 1.72 and 0.96, respectively (Armstrong & Hacisalihoglu, 2025). Oil content in single kernel of maize was measured based on SVM pretreatment, which showed the R^2 and RPD were 0.845 and 2.55, respectively (Gürbüz et al., 2023). Also, the amylose content of single maize was measured (Dong et al., 2023). Portable NIR instrument was employed to detect the acidity index of peanut, the result showed great performance that RMSEP, R_p^2 and RPD were 0.61 g/kg, 0.95 and 4.31, respectively (Liu et al., 2022). Protein, ether extract, crude fiber, ash, starch and moisture of maize and sorghum were determined successfully (Simeone et al., 2024). Moreover, NIR applied as a fast method to detect the total flavonoids and phenolic content in peanut, the R_p^2 were 0.9137 and 0.9042, and the external validation set showed satisfactory result with scores of 0.88 and 0.86 of total flavonoids and phenolic content (Haruna et al., 2023).

NIR showed great potential to detect AFB1 in peanuts and maize. Gramian angular summation field image coding combined with two-dimensional convolutional neural network (2D-CNN) to detect AFB1 in peanuts, RMSEP, R_p^2 and RPD were 2.0 μg/kg, 0.99 and 8.3, respectively (Jiang et al., 2023). Another study was that the PLS model was

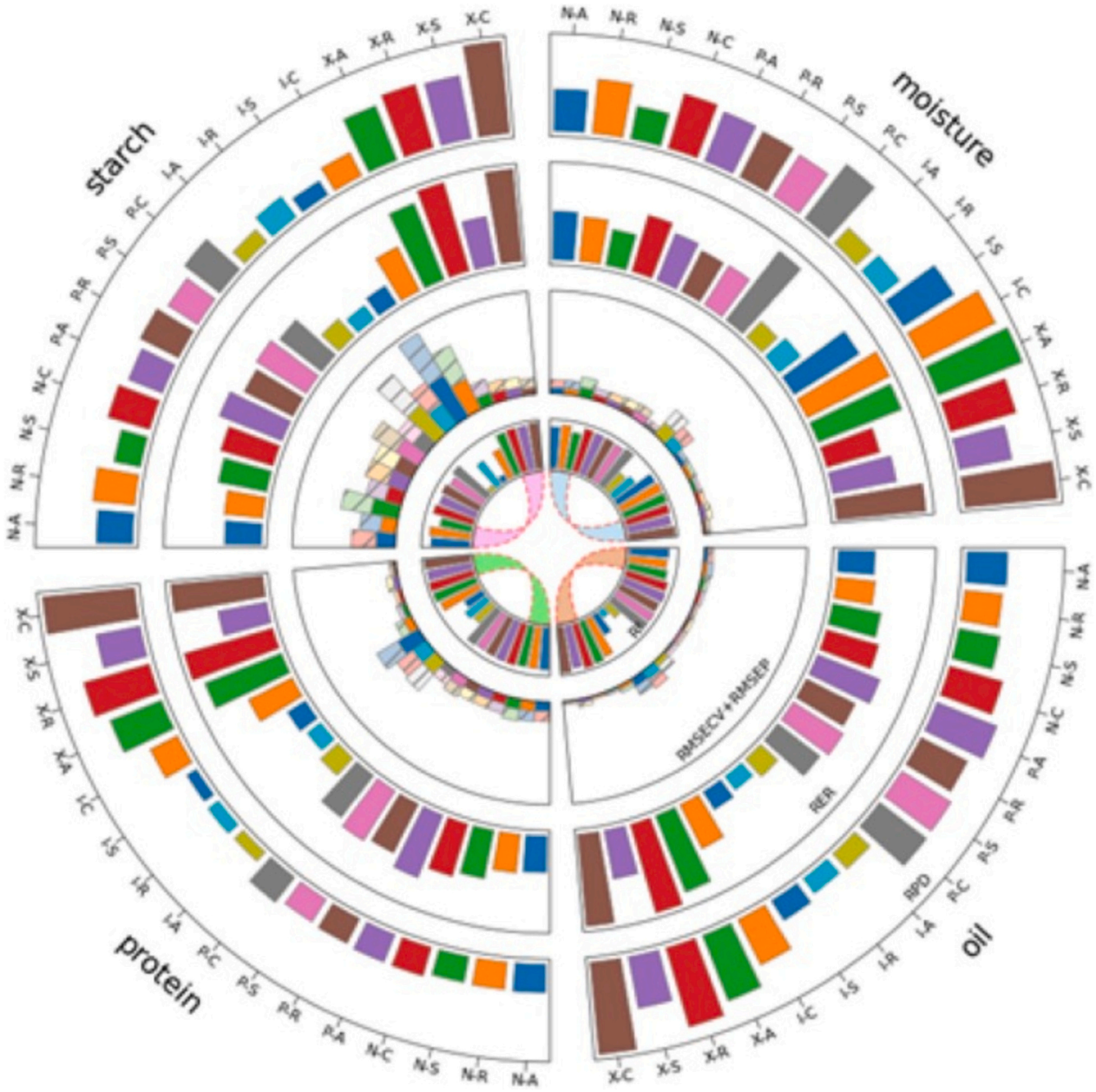

Fig. 2. The prediction results of four quality parameters in corn with different wavelength selection methods (Zou et al., 2025).

used to measure AFB1 in peanuts (Yao, Liu, Xu, et al., 2022). Particle swarm optimization combined moving window were used to select the important variables to detect the AFB1 in maize, the SVM model showed RMSEP, R_p^2 and RPD were 3.5967 μg /kg, 0.9707 and 5.7538, respectively (Deng, Jiang, & Chen, 2022b). A PLS model for AFB1 in peanut oil was established (Yao, Liu, Zhang, et al., 2022). Moreover, chlorpyrifos residues in corn oil was detected with the 1D-CNN method (Xue et al., 2023). SVR was used to build the model for procymidone residues in rapeseed oil, the result showed the R_p^2 was 0.9939 and RMSEP was 2.3435 mg/kg, respectively (Zhao et al., 2023). Cadmium (Cd) in the peanut was detected and the R_p^2 and RMSEP were 0.9539 and 0.0341, respectively (Gao et al., 2023). Meanwhile, NIR was used to detect Cd in peanut oil (Wang, Deng, et al., 2024a; Wang, Deng, et al., 2024b). In summary, the overview of application of spectroscopic techniques in the detection of hazard factors of oilseeds and edible oils was shown in Table 4.

NIR is a promising tool to detect the quality and safety in oilseeds and edible oils. However, it has weaker absorption overtones than mid-infrared spectra range. It is critical to develop NIR methods to measure more specific compounds in oilseeds and edible oils due to the weaker sensitivity. Moreover, decreasing the cost of instrument and improving the software and hardware are also important. On-line analysis is another direction in the future. The quality and safety assessment with emerging spectroscopic were shown in Fig. 3.

3. Limitations and future prospects

Spectroscopic techniques, including Raman spectroscopy, fluorescence spectroscopy, FT-IR spectroscopy and NIR spectroscopy are superior to be fast, sensitive, preprocessing-free and high efficiency, have been used to analyze the quality and safety of oilseeds and edible oils, which provide reliable quality and safety assessment for oilseeds and edible oils. However, it has some limitations of these technologies in oilseeds and edible oils. Concerning Raman spectroscopy, the interference with biological fluorescence is strong, it may influence the detection efficiency. Besides, the low Raman scattering cross-section, weak

Table 4
Overview of applications of spectroscopic techniques in the detection of hazard factors of oilseeds and edible oils.

Species	spectroscopy techniques	Spectral range (nm)	Model	Attribute(s)	Performance/Accuracy	Reference
Maize	RS	5555.6–200,000	SiPLS	Zearalenone	R_p^2-0.9260, RMSEP-87.9132 μg/kg	Guo et al. (2019)
Maize	SERS	3225.8–50,000	SVM	AFB1	R_p^2-0.9715, RMSEP-3.5377 μg/kg, RPD-5.8258 5 ng/mL-100 ng/mL: R_P-0.9283, RMSEP-10.1 100 ng/mL-1000 ng/mL: R_P-0.9332, RMSEP-90.4	Deng, Jiang, and Chen (2022a)
Peanut oil	SERS	190–1100	BP-AdaBoost	AFB1	from 5 ngmL−1 to 100 ngmL−1	Chen et al. (2020)
Peanut oil	RS	3030.3–100,000	PLS	AFB1	R_p^2-0.99, RMSEP-22.6 μg/kg	Zhu et al. (2022)
Edible oil	RS	2941.2–200,000	RNN	AFB1	R_p^2-0.95, ration of prediction to deviation −4.86	Deng, Zhang, et al. (2022)
Edible oil	SERS	–	–	PAHs	R^2–0.9959	Su et al. (2021)
Corn oil	RS	2202.7–119,047.6	LSTM-CNN	Chlorpyrifos	R_p^2-0.90, RPD-3.2	Xue and Jiang (2023)
Corn oil	RS	2202.7–119,047.7	1D-CNN	Chlorpyrifos	RPD-11.6517, R_p^2- 0.9874.	Mei et al. (2024)
Peanut	FS	300–550	PARAFAC	AFB1, AFB2	AFB1: R^2–0.9856, RMSEC-0.06 ppb AFB2: R^2–0.9822, RMSEC-0.06 ppb	Sajjadi et al. (2016)
Repeseed and peanut oils	FS	220–700	–	Carbendazim, metiram	R^2>0.99, LOD: 7.07 × 10–4 mg/mL-9.28 × 10–4 mg/mL	Chen et al. (2015)
Peanut oil	FS	200–900	APTLD	Carbendazim, chlorothalonil	R>0.96, LOD: 11 ng/mL-4.3 ng/mL	Yuan et al. (2019)
Palm oil	FS	–	–	As, Se and Hg	LQ < −1.6 and 1.3–2.4 μg/L Hg: below LQ	Valasques et al. (2020)
Edible oil	FS	–	PLS, U-PLS	PAHs	R-0.9940-0.9946, LOD-2.6-0.8	Alarcon et al. (2012)
Vegetable Oil	FS	350–600	–	Chr, BaA, BaP, and BbF	LOD: 13.0–8.64-0.16-7.68 μg/ kg	Liu et al. (2016)
Peanuts	NIR	1000–2500	2D-CNN	AFB1	R_p^2-0.99, RMSEP-2.0 μg/kg, RPD-8.3	Jiang et al. (2023)
Peanuts	NIR	1111.1–2500	PLS	AFB1	R_C^2-0.984, RMSECV-2.2 %, RPD-7.91	Yao, Liu, Xu et al. (2022)
Maize	NIR	901.8–1661.2	SVM	AFB1	R_p^2-0.9707, RMSEP-3.5967 μg/kg, RPD-5.7538	Deng, Jiang, and Chen (2022b)
Peanut oil	NIR	833.3–2500	PLS	AFB1	R^2–0.951, RMSEC-3.87 %, RPD-4.52	Yao, Liu, Zhang, et al. (2022)
Corn oil	NIR	970–1700	1D-CNN	Chlorpyrifos	R_p^2-0.9492, RPD-4.4569	Xue et al. (2023)
Rapeseed oil	NIR	950–1700	SVR	Procymidone	R_p^2-0.9939, RPD-2.3435	Zhao et al. (2023)
Peanut	NIR	800.1–2777.8	PLS	Cd	R_p^2-0.9539, RPD-0.0341	Gao et al. (2023)
Peanut oil	NIR	1000–2500	PLSR	Cd	R_p^2-0.9675, RMSEP- 3.7753 mg/kg RPD-5.5485	Wang, Deng, et al. (2024a)
Peanut oil	NIR	955.8–1702.6	PLSR	Cd	R_p^2-0.9666, RMSEP- 2.8207 mg/kg RPD-5.5705	Wang, Deng, et al. (2024b)

Note: RS: raman spectroscopy, SiPLS: synergy interval partial least squares, R_p^2: determination coefficient of prediction, RMSEP: root mean square error of prediction, SERS: surface-enhanced raman spectroscopy, SVM: support vector machine, AFB1: aflatoxins B_1, R_P: correlation coefficients of prediction, PLS: partial least squares, RNN: recurrent neural network, R^2: coefficient of determination, LSTM-CNN: long short-term memory network-convolutional neural network, RPD: ratio of prediction to deviation, 1D-CNN: one-dimensional convolutional neural network, AFB2: aflatoxins B_2, RMSEC: root mean square error of calibration, R: regression coefficient, LOD: limit of detection, APTLD: excitation-emission matrix fluorescence coupled with alternating penalty trilinear decomposition, LQ: limit of quantification, U-PLS: unfolded partial least squares, PAHs: polycyclic aromatic hydrocarbons, Chr: chrysene, BaA: benzo(*a*)anthracene, BaP: benzo(*a*)pyren, BbF:benzo(*b*)fluoranthene, 2D-CNN: two-dimensional convolutional neural network, R_c^2: determination coefficient of calibration, RMSECV: root mean square error of cross-validation, SVR: support vector regression, PLSR: partial least squares regression.

scattering signals of some materials, and the large degree of optical sampling variance for solid samples will affect the result (Hussain et al., 2018). The drawback of fluorescence spectroscopy is not all elements and compounds show fluorescence, so the application range will be limited (Bose et al., 2018). FT-IR is a single beam and has the trouble to obtain representative background. Meanwhile, the instrument with high cost (Tahir et al., 2019). In addition, Raman spectroscopy and FT-IR spectroscopy hardly offer the information about spatial distribution in the sample in terms of detection mycotoxins and toxigenic fungi of oilseeds (Xing et al., 2019). NIR as the classical spectral sensor, it has some limitations to detect the inhomogeneous contaminations due to its nature of "point" detection (Tao et al., 2018). NIR has requirements for sample thickness, homogeneity and dilution to avoid saturation (Lohumi et al., 2015). The application of non-destructive technologies in oilseeds and edible oils still have some challenges. We can avoid some limitations by means of choosing the available techniques according to different characteristics of quality parameters. Furthermore, the spectroscopic techniques combined with chemometrics in the agricultural product industry have a bright future. It is reported that Raman spectroscopy has been applied to determine the vitamins B2 and B12 in cereals (Radu et al., 2016), the determination of n-6 and n-3 fatty acid ratios in cereal grains by ^{1}H NMR spectroscopy (Prema et al., 2016). The next direction is to explore the direction of vitamins B2 and B12, as well as the ratios of n-6 to n-3 fatty acids, in oilseeds using spectroscopic techniques. Meanwhile, it is hopeful that resolving issues related to instrumental and software limitations, along with effective data fusion, will improve the accuracy and precision of the detection results. Hyperspectral imaging, particularly multispectral imaging combined with deep learning and using a few important bands instead of full wavelengths to assess the food quality and safety. Additionally, developing new chemometric algorithms and the exploration of data are essential. There is also a need for portable, high-performance, and cost-effective instruments for real-

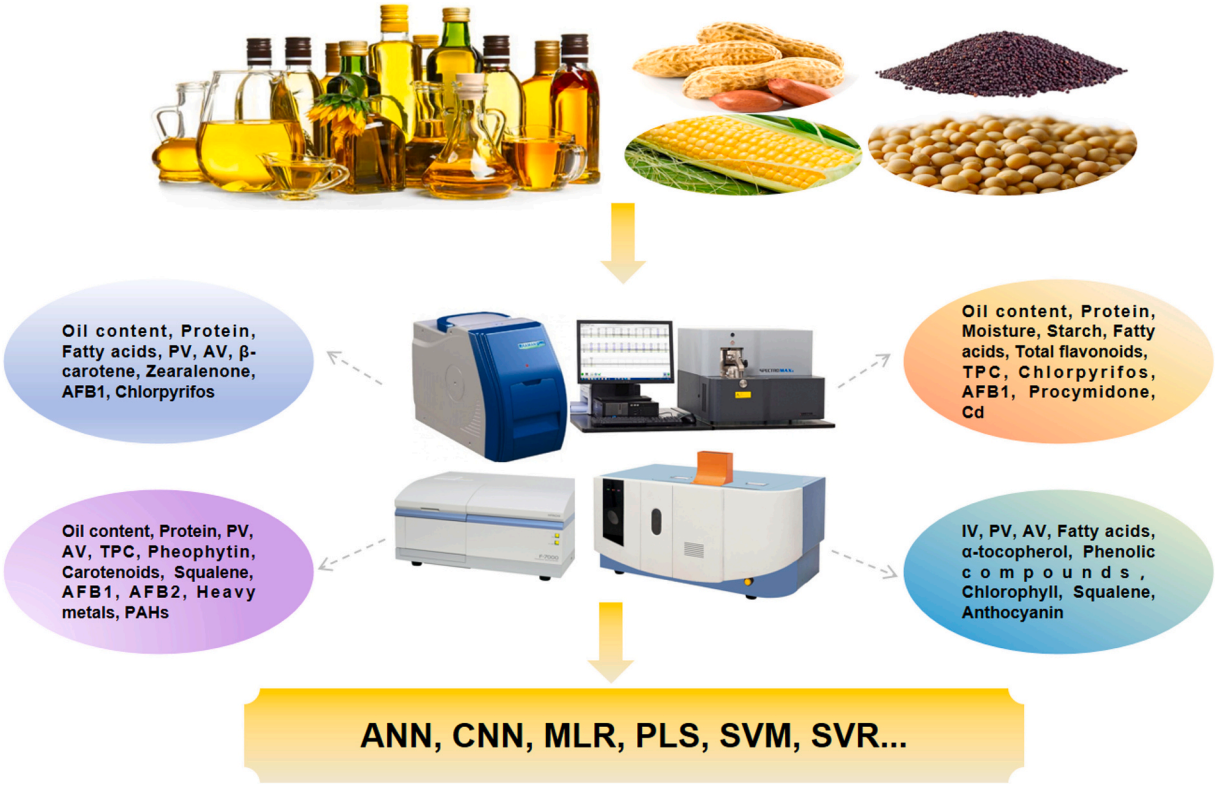

Fig. 3. The quality and safety assessment with emerging spectroscopic.

time applications.

4. Conclusions

Spectroscopic techniques have been developed rapidly over the past few decades, which widely used in different fields of research due to its rapidness, short analysis time, noninvasive and simultaneous determination. This review summarized non-destructive technologies, including Raman spectroscopy, fluorescence spectroscopy, FT-IR and NIR spectroscopy along with their major applications in the quality and safety assessment of oilseeds and edible oils. Raman spectroscopy has the potential to detect physicochemical and specific nutrient components, as well as mycotoxins, pesticide residue, and PAHs in oilseeds and edibles oils, such as protein, oil content, fatty acids, tocopherol phenolic compounds, squalene, zearalenone, AFB1, chlorpyrifos and PAHs. Fluorescence spectroscopy provides information of quality and safety in oilseeds and edible oils, especially total tocopherol content and pesticide residue in edible oils. FT-IR spectroscopy revealed great performance in determining the anthocyanin of soybean. NIR spectroscopy is considered a classical and widely used technique for analyzing the quality and safety of oilseeds and edible oils. Recently, NIR has been used to detect quality parameters in single seed, such as oil content in single maize. Besides, it has been applied to detect contaminants like AFB1, chlorpyrifos, procymidone and Cd, providing new insights into its potential for safety assessments in oilseeds and edible oils. The applications of spectroscopic techniques in oilseeds and edible oils jointly guarantee the quality control of oilseeds and edible oils and promote the development of agricultural products.

CRediT authorship contribution statement

Xue Li: Writing – review & editing, Writing – original draft, Investigation, Formal analysis. **Wenwen Liu:** Investigation, Formal analysis. **Lu Xiao:** Investigation, Formal analysis. **Jie Zhao:** Investigation, Formal analysis. **Yan Chen:** Investigation, Formal analysis. **Liangxiao Zhang:** Investigation, Conceptualization. **Peiwu Li:** Supervision, Conceptualization. **Dolores Pérez-Marín:** Writing – review & editing, Investigation, Conceptualization. **Xu Wang:** Supervision, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

No data was used for the research described in the article.

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