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アプリケーションノート

Rapid Identification of Adulteration in Edible Oils Using Direct Analysis Mass Detection Platform (RADIAN ASAP-LiveID)

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Abstract

In this application note learn how RADIAN ASAP is a compact, robust, and easy-to-use system that enables rapid screening of samples.

Benefits

- Ease of operation – Little to no sample preparation and the easiest instrument parameter optimization.
- Direct injection and analysis in real time – Based on direct analysis and LiveID real-time identification technology with easy data elucidation, analysis and results of identification can be done and generated in seconds, ideal for in-field and rapid monitoring and detection.
- Compact design with excellent performance – RADIAN ASAP System is designed with robust and reliable single quadrupole mass spectrometry technology in combination with Atmospheric Solids Analysis Probe (ASAP), featuring small footprint, ease of use, and the ability to provide high-quality data.

Introduction

Sesame oil is an edible vegetable oil derived from the seeds of Sesamum indicum, a plant in the genus Sesamum, through pressing or other processes. The main components in sesame oil include fatty acid glycerides of oleic acid, linoleic acid, palmitic acid, and stearic acid. In addition, it also contains vitamin E, sesamol, etc.[1] Because of its higher economic value compared with other vegetable oils, some unscrupulous producers adulterate the sesame oil with soybean oil, corn oil, or other vegetable oils and sell them as pure sesame oil. Therefore, ensuring the integrity and quality of raw materials is an important task within the food industry.

Adulterated oils are mainly detected by physical or chemical methods such as the widely used chromogenic methods (e.g. Villavecchia test,[2] Baudouin test,[3] and sulfuric acid chromogenic method),[4] chromatography methods,[5] NMR,[6] and so on. However, these methods are complicated and timeconsuming, and some of them require high costs, showing some limitation in rapid detection of adulterated oils.

Ambient Ionization Mass Spectrometry (AIMS) is the game changer in the field of mass spectrometry. Requiring little to no sample preparation and being able to analyze the sample directly at room temperature and under atmospheric pressure, AIMS is widely used in food authentication, drug quality control, material analysis, homeland security, and forensic applications. Featuring versatility, ease-of-use, speed and reliability, RADIAN ASAP with LiveID overcomes many barriers to entry associated with traditional mass spectrometry systems, empowering seamless deployment in existing lab environments and enabling those with minimal LC-MS training to obtain accurate results quickly.

Experimental

Sample Source

The edible oil samples were sesame oil, corn oil, and soybean oil purchased from supermarkets.

Sample Preparation

30 µL of sample and 970 µL of n-hexane were pipetted into a 2 mL centrifuge tube, which was then capped and shaken for 30 seconds. 2 µL of the sample extract was taken and applied onto the ASAP sampling capillary for analysis.

MS Conditions

MS system: RADIAN ASAP

Ionization parameters: See Table 1

Parameter	Setting
Ionization mode	ASAP+
Corona current	3 µA
Desolvation gas (N_2) temperature	600 °C
Desolvation gas (N_2) flow rate	3 L/min
Cone voltage	15 V
Acquisition mode	Full scan (Continuum)
Mass range	50–1200 Da
Scan speed	2 Hz

Table 1. RADIAN ASAP parameter settings.

LiveID chemometric model

In this experiment, MassLynx MS Software (v4.2) was used to acquire non-target full scan data, and multivariate statistical software LiveID (v2.0) was used for modeling and sample assignment and identification.

Results and Discussion

Establish the Experimental Model

The raw MS data of sesame oil, corn oil, soybean oil, and adulterated sesame oil (n=89, Figure 1) were acquired, and multivariate statistical analysis based on Principal Component Analysis-Linear Discriminant Analysis (PCA-LDA) was performed.

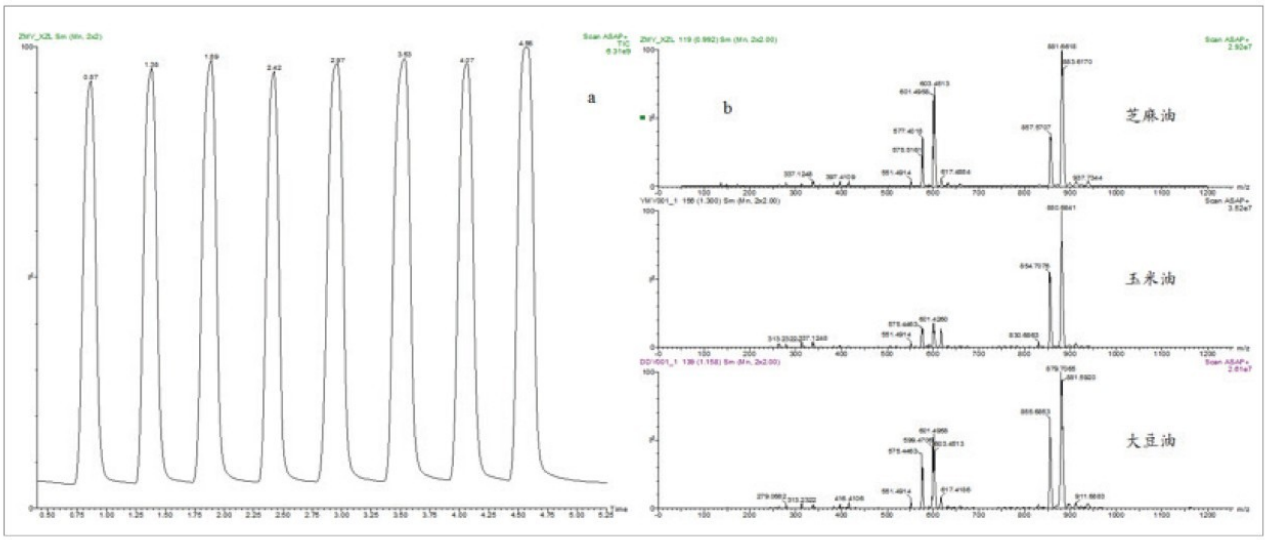

Figure 1. Total ion chromatogram of sesame oil sample acquired using RADIAN ASAP (a); mass spectra of three edible oils (sesame oil, corn oil, and soybean oil) acquired under positive ion mode (m/z 50–1200) (b).

The chemometric model was established based on 5 PCA components and 3 LDA components. As shown in the three-dimensional (3-D) PCA-LDA clustering scores plot in Figure 2, the three edible oils were clearly separated with the adulterated sesame oil.

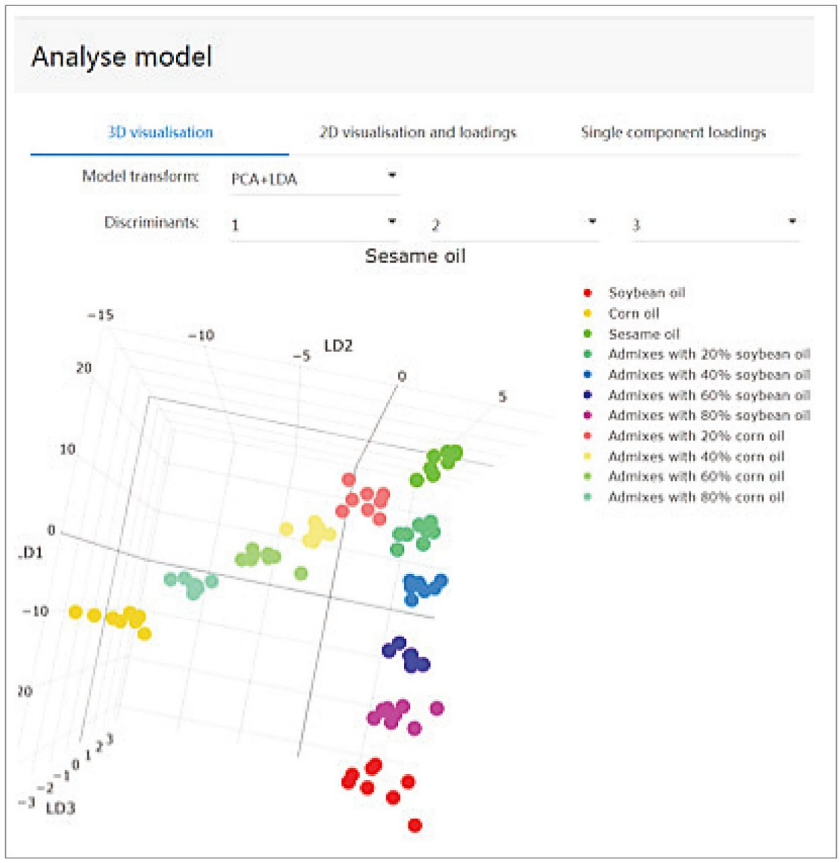

Figure 2. 3D model plot of PCA-LDA analysis for different edible oils and adulterated sesame oil.

Model Verification and Sample Identification

Cross validation of the PCA-LDA classification model for multiple edible oils was performed with the method of “Leave 20% Out”. It can be seen from the validation results shown in Figure 3, the correctness score was as high as 96.63% and no false classification was noted.

Validation report

Description :

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Model details

Name : Sesame oil

Type : PCA-LDA

Outlier threshold : 7 (standard deviations)

PCA components : 5

LDA discriminants : 3

Mass range : 50 - 1200 (m/z)

Bin size : 1 (m/z)

Validation parameters

Validation type : 5 fold

Results summary

	Spectra	Passes	Failures	Outliers	Correctness score
Total	89	86	0	3	96.63%

Figure 3. Cross-validation results of the model of edible oils adulteration based on RADIAN ASAP data.

After the PCA-LDA model for edible oils was successfully constructed, it was verified and used for realtime identification of edible oil samples. The raw data files were acquired, and then processed in real time using the software to generate identification results in a near instantaneous way (Figure 4). There was a signal delay of approximately 2 seconds after sampling. The spectrum intensity limit was set to 4x10^8 to filter out background noise and ensure that the identification was based on the sample signal alone. The samples were correctly assigned and identified in all cases.

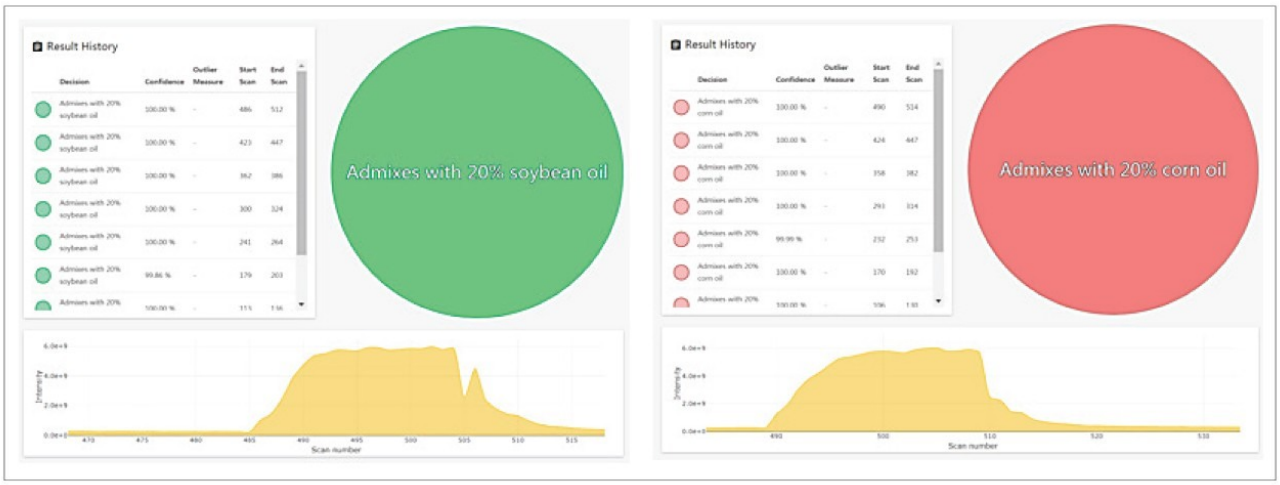

Figure 4. Real-time identification results of the samples using the PCA-LDA edible oil model.

Conclusion

RADIAN ASAP is a compact, robust, and easy-to-use system that enables rapid screening of samples. For non-MS users, the simplicity of direct analysis coupled with the LiveID software reduces the complexity of sample preparation and offers near-real time data processing with easy to interpret results typically obtained in a few minutes. RADIAN ASAP and LiveID offers a powerful combination of mass spectrometry and chemometric modelling, which allows users to easily and efficiently screen samples and make quicker decisions to assess food adulteration.

Using this platform to acquire the mass spectrum information of edible oils and in combination with the PCA-LDA method, it is possible to effectively differentiate sesame oil, corn oil, soybean oil, and even sesame oil adulterated with 20% corn oil or 20% soybean oil. The whole procedure takes only 2 minutes to accurately determine the adulteration of an edible oil, which can help the food industry and regulatory authorities to effectively address the threats and challenges arising from food adulteration, so as to protect brand reputation and the safety of food consumers.

References

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