Discrimination of soybean oil and olive oil by benchtop linear MALDI-TOF

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1. Overview

Soybean oil and olive oil were discriminated successfully using benchtop linear MALDI-TOF.

2. Introduction

The safety of edible oil has always been a concerned issue by the public. Various methods have been developed for analysis of edible oil, such as PCR, low field nuclear magnetic resonance, ion mobility spectrometry, chromatography, MALDI-TOF-MS. Among these methods, MALDI-TOF-MS has prominent advantages for its convenient operation, high throughput and high sensitivity. As reported by Ng et al (Food chemistry, 2018), a comprehensive spectral database for analysis of edible oils was established using MALDI-MS. Edible oils were analyzed using large MALDI-TOF Mass Spectrometer with high specifications in reflection mode, which is difficult to popularize due to their size and initial/running costs. In this study, we attempt to analyze edible oil using a novel benchtop linear MALDI-TOF. The result showed that soybean oil and olive oil were distinguished successfully, which indicates that benchtop linear MALDI-TOF can be used for edible oil analysis.

3. Methods and Materials

1 µL of 20 mg/mL DHB (2,5-dihydroxybenzoic acid) in Tetrahydrofuran was spotted on MALDI plate and oil sample was then transferred by a medical cotton tip onto the spot after matrix layer formed. The plate was then introduced into a benchtop linear MALDI-TOF mass spectrometer (MALDI-8020, Shimadzu Corporation, Japan) for MALDI-MS analysis. Mass spectrometer was operated in positive mode. Umetrics Simca 13.0 was used for principal component analysis (PCA) and partial least square-discriminant analysis (PLS-DA) of monoisotopic peaks' normalized intensities.

Figure 1. MALDI-8020 Benchtop Linear MALDI-TOF Mass Spectrometer

4. Result

MALDI-TOF-MS conditions

Tuning: linear
Polarity: positive
Mass range: 500-2000 Da
Laser rep. rate: 200 Hz
Power: 85
Ion gate blanking: 500
Accumulation rate (shots/profile): 10
Profiles: 200

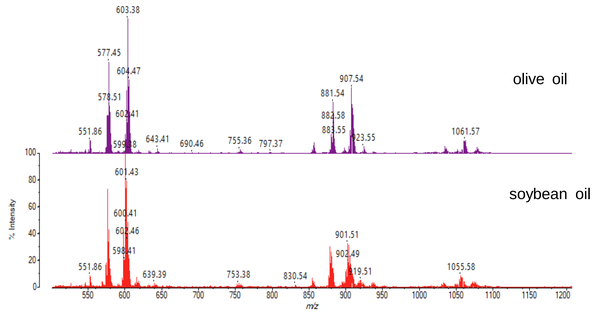

Figure 2. MALDI mass spectrum of olive oil and soybean oil (m/z range 500–1200 Da)

Soybean oil and olive oil were collected from five different brands respectively. Soybean oil includes two types, genetically modified and non-genetically modified. Each sample was spotted three spots, and each spot was analyzed three times. The mass region was set as m/z 500-2000. From the result of mass spectra, the distribution pattern of peaks of different samples of the same edible oil are similar (Figure 2), mainly concentrated in the diacylglycerols (DAGs)-like region (Figure 3) and sodium adducts of triacylglycerols (TAGs) region (Figures), typically at the region of m/z 573-579,595-606,853-855,875-883,899-909 for soybean oil while at the region of m/z 575-579, 601-606, 879-883, 905-910 for olive oil (Figured 3 and Figure 4). Soybean oil showed higher abundance of peaks at m/z 599, 601, 603, 877, 879, 901, 903, 905, while olive oil showed higher abundance of peaks at m/z 577, 603, 604, 881, 907, 908. The signal intensities of characteristic peaks of soybean oil and olive oil were quite different, which may be related to the different types and proportions of fatty acids in soybean oil and olive oil.

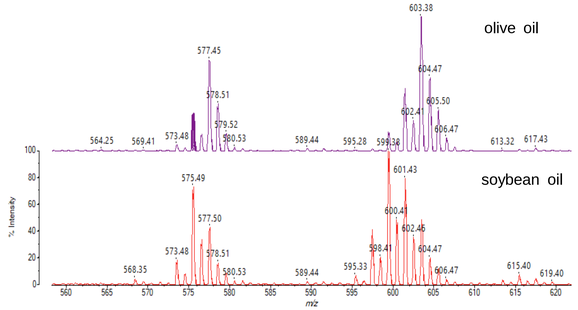

Figure 3. DAGs-like regions of MALDI mass spectra of oil and soybean oil

The DAGs-like fragments were observed in the spectrum, which could be due to fragmentation of TAGs ions and the higher laser energy used in the current study.

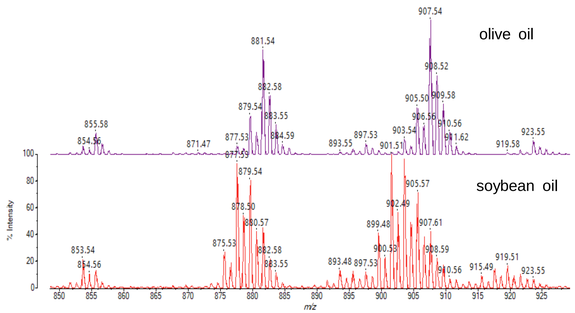

Figure 4. The TAGs regions of MALDI mass spectra of olive oil and soybean oil

TAGs were clearly observed in the spectrum, which are composed of major fatty acids, such as palmitic acid, oleic acid and linoleic acid.

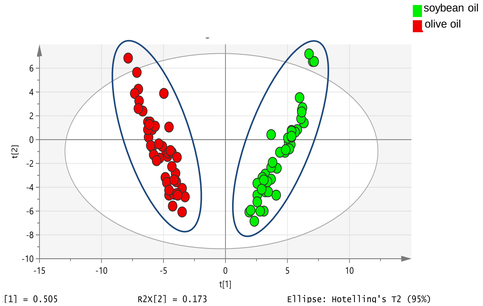

Figure 5. PCA score plot for olive oil and soybean oil based on their MALDI-MS results. The first principal accounted for 51% of variance and second principal accounted for 17% of variance.

For signals with intensity higher than 2%, the relative intensities of monoisotopic peaks (the ratio of absolute intensity of the peak observed to absolute intensity of the highest peak observed in the mass spectra) were input into the statistics software for PCA and PLS-DA analysis. The PCA result showed that samples from the same species were clustered individually and different edible oil could be clearly differentiated from each other (Figure 5). All of the tested samples were classified correctly using PLS-DA even though they are from different manufacturers. Genetically modified and non-genetically modified soybean oils showed no significant difference in PCA analysis and were clustered together.

5. Conclusions

In this study, with DHB (2,5-dihydroxy benzoic acid) as matrix, we analyzed a variety of olive oil and soybean oil samples using bentop linear matrix assisted laser desorption/ionization time of flight mass spectrometry (MALDI-8020). Spectral patterns were obtained and ninety spectra were analyzed with multivariate statistical analysis software Simca for PCA and PLS-DA. The result showed that soybean oil and olive oil were discriminated successfully. This indicates that benchtop linear MALDI-TOF can be used for edible oil analysis, which is conducive to the popularization of this method.