CHARACTERIZATION OF VEGETABLE OILS: DETAILED COMPOSITIONAL FINGERPRINTS DERIVED FROM ELECTROSPRAY IONIZATION FOURIER TRANSFORM ION CYCLOTRON RESONANCE MASS SPECTROMETRY

Zhigang Wu (NHMFL/FSU, Chemistry and Biochemistry), Ryan P. Rodgers (NHMFL/FSU, Chemistry and Biochemistry) and Alan G. Marshall (NHMFL/FSU, Chemistry and Biochemistry)

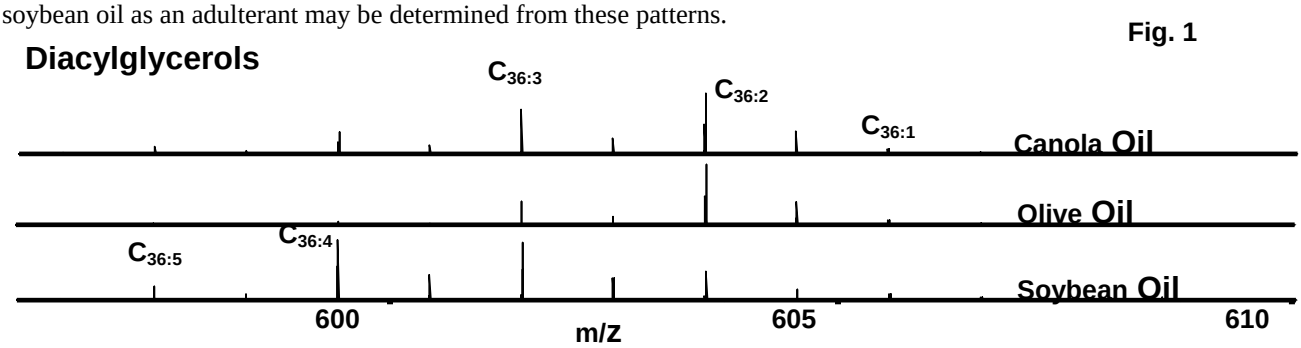
Introduction

Adulteration of vegetable oil is of concern for both commercial and health reasons. Compositional based fingerprints can potentially reveal both the oil source and its possible adulteration. Here, electrospray ionization (ESI) Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) resolves and identifies literally thousands of distinct chemical components of commercial canola, olive, and soybean oils, without extraction or other wet chemical separation pretreatment. In negative-ion ESI FT-ICR MS, the acidic components of soybean oil are easily distinguished from those of canola and olive oil based on relative abundances of C_{18} fatty acids, whereas olive oil differs from canola and soybean oil based on relative abundances of tocopherols. In positive-ion ESI FT-ICR MS, the three oils are readily distinguished according to the relative abundances of di- and triacylglycerols with various numbers of double bonds in the fatty acid chains.
We demonstrate the detection of soybean oil as an adulterant of olive oil, based on relative abundances of members of each of several chemical families. We suggest that the detailed chemical compositions of vegetable oils can be used to characterize them and to detect and identify adulterants.[1]

Results and Discussion

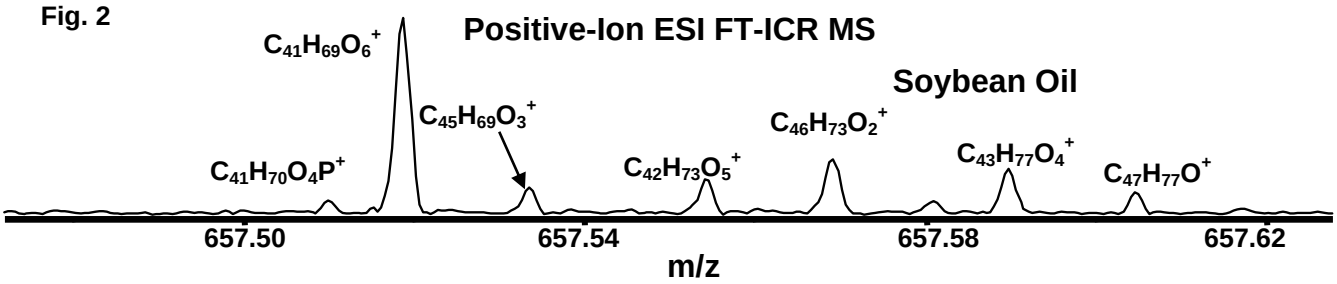
For example, Figure 1 shows the fatty acid distributions for mixtures of olive oil and soybean oil. The presence and extent of soybean oil as an adulterant may be determined from these patterns.

Fig. 1



It is important to understand that low-resolution mass analysis is not adequate to determine these distributions, because (see Figure 2) there are species of many different chemical compositions at every nominal (nearest-integer) mass. Thus, ultrahigh mass resolution is required to distinguish the desired species from all of the rest.

Fig. 2



Acknowledgements

We thank Daniel McIntosh for machining all of the custom parts required for the 9.4 T instrument, John P. Quinn for maintenance of the instrument, and Christopher L. Hendrickson for help in optimizing instrument-operating parameters.

References

[1] Wu, Z., *et al*., J. Agric. Food Chem., **52**, 5322-5328 (2004).