

# Triacylglycerol Analysis of Potential Margarine Base Stocks by High-Performance Liquid Chromatography with Atmospheric Pressure Chemical Ionization Mass Spectrometry and Flame Ionization Detection

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Several margarine base stock candidates have previously been prepared for the purpose of finding better, more oxidatively stable food components: high-saturate vegetable oils, randomized vegetable oils, vegetable oil–hard stock blends, and interesterified vegetable oil–hard stock blends. Here are reported the triacylglycerol compositions of these products, determined using reverse-phase high-performance liquid chromatography (HPLC) coupled with a flame ionization detector or a quadrupole mass spectrometer with an atmospheric pressure chemical ionization source. Triacylglycerol percent composition results for samples of known composition (randomized and interesterified samples) exhibited less average error by HPLC coupled with a quadrupole mass spectrometer with an atmospheric pressure chemical ionization source, after application of response factors, than the results by HPLC coupled with a flame ionization detector. The fatty acid compositions calculated from the mass spectrometric data exhibited less average error than the fatty acid compositions resulting from the flame ionization detector data. The average error of the fatty acid compositions by the mass spectrometer was lowest for interesterified blend samples, next lowest for randomized samples, then followed by high-saturated fatty acid oils, normal oils, and blends. Analysis of the vegetable oil–hard stock blends by mass spectrometer required special treatment for calculation of response factors.

**Keywords:** *Atmospheric pressure chemical ionization mass spectrometry; flame ionization detector; margarine base stocks; triacylglycerol analysis; triglyceride; triacylglycerol*

## INTRODUCTION

The triacylglycerol (TAG) fraction of a margarine or shortening, called the base stock, is responsible for most of a product's physical properties, from texture to taste. Research has been directed toward improvement, through plant genetic manipulation, of the functional properties of vegetable oils (1–9), which may then be used as base stocks or components in base stocks (10, 11). Improvements have been accomplished by alteration of the fatty acid (FA) composition and TAG composition, resulting in oils with wide-ranging compositions. Alternatively, base stocks have been prepared from either the randomization of a single oil, the blending of a traditional vegetable oil with hard stocks (TAG mixtures containing mostly trisaturates), or the interesterification of the vegetable oil with hard stocks blend. Vegetable oil blends with hard stocks produce TAG mixtures that exhibit more solids at higher temperatures and are less susceptible to oxidative degradation (12, 13) than normal vegetable oil. Interesterification after blending, which may be chemically (14) or enzymatically (15) catalyzed, changes the TAG composition even further to provide improved food components (16, 17).

The ability to characterize the TAG composition of a potential fat or oil food product is integral to the formulation of a desirable end product. Reverse-phase high-performance liquid chromatography (RP-HPLC) with a detector such as a flame ionization detector (FID) (14, 18–20), refractive index (18), or evaporative light scattering detector (20) has become common for TAG analysis. These detectors have previously been shown to provide satisfactory qualitative and quantitative composition information for TAGs from a variety of sources. Quantification of TAG species using a FID has advantages over the other two-dimensional detectors in that it is linear over a broad range without the need for response factors (14, 18, 19), and it is not adversely affected by gradient runs. These various detectors have proven to be satisfactory for TAG analyses in which chromatographic standards were available for the TAG or in which structures could be identified by theoretical carbon number (14, 18) or equivalent carbon length. Unfortunately, however, these detectors do not allow characterization of unidentified TAGs for which no standards are available, and they cannot differentiate between TAG species that are completely chromatographically overlapped. Sometimes, the failure to resolve overlapped peaks can cause some TAG species to be overestimated while others go unidentified. As more is learned about how specific molecular species affect the lubricity (texture, mouthfeel) and other character-

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