Characterization of the TAG of Peanut Oil by Electrospray LC-MS-MS

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ABSTRACT: A study of processed peanut oil was undertaken to assess the utility of HPLC combined with tandem MS to obtain data easily regarding the number of TAG of fats and oils and their FA composition. Mass chromatograms and spectra corresponding to only TAG of a single M.W. were obtained for the full range of TAG in the sample. Analysis of the mass spectra allowed the identification of more than 160 TAG in the sample by their FA composition. In addition, it was possible to estimate relative abundances of the TAG and suggest the position of the FA on glycerol for a limited number of cases. This technique greatly simplifies the task of assigning FA to coeluting TAG and facilitates identification of TAG present in trace quantities in mixtures, with possible application in circumstances where such trace TAG could be significant markers. Results are quickly obtained without extensive sample preparation or prefractionation of the sample.

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Separation and identification of components of the complex mixtures of TAG that constitute fats and oils is a challenging analytical chemistry problem. Various approaches to separation by HPLC have been studied over the years (1). MS, and in particular combined HPLC and MS, has substantially improved the analysis of these mixtures (2).

Relatively little has been reported concerning the use of electrospray ionization (ESI) MS, ESI-LC-MS, and tandem MS (MS-MS) in the analysis of TAG mixtures. Duffin *et al.* (3) first reported ESI-MS-MS analysis of TAG (as ammonium or sodium ion adducts) by infusing a solution of the analytes in nonpolar solvents. Studies leading to complete structures of individual TAG by ESI or fast atom bombardment MS-MS on tandem magnetic sector instruments were undertaken by Cheng *et al.* (4). Hsu and Turk (5) described the use of ESI-MS-MS in a triple quadrupole instrument for the structural elucidation of lithium ion adducts of individual TAG. Marzilli and coworkers (6) studied the selectivity of FA loss from *sn*-1,3 vs. *sn*-2 positions in a small set of TAG under MS-MS and MS^3 conditions in an ion trap mass spectrometer. In a preliminary study for this paper, the FA composition of TAG components of cocoa butter was studied by ESI-MS-MS (7).

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Peanut oil was chosen as a test substance for the ability of LC-MS-MS to identify TAG components because it contains a wider range of FA (from at least C_{16} to C_{26}) than is typical for vegetable oils. Previous reports on the characterization of peanut oil have involved combinations of analytical methods. Myher *et al.* (8) analyzed natural and randomized peanut oils by HPLC coupled to direct inlet chemical ionization MS, identifying 35 TAG molecular species in a randomized sample and 16 TAG molecular species in natural samples. Sempore and Bezard (9) collected fractions from isocratic HPLC with refractive index detection, analyzed the FA of the fractions as methyl esters by GLC, and deduced the composition of the peanut oil TAG based on parameters derived from retention time data and mathematical treatment of the FA analysis data. They reported 75 TAG in their table of results. Singleton and Patee (10) also fractionated peanut oil by isocratic HPLC with UV detection at 210 nm, performed GLC on intact TAG and FAME, and obtained EI ionization mass spectra on the fractions using an insertion probe. The data thus obtained were used to characterize 23 TAG by their FA composition. Rezanka and Mares (11) fractionated several oils, including peanut oil, by gradient HPLC, GLC of intact TAG, and desorption CI-MS, the latter producing sets of pseudomolecular ions for the TAG fractions. These authors identified 42 TAG from peanut oil by these methods.

The present study was undertaken to explore the utility of LC-MS-MS for a similar characterization of refined peanut oil. The product ion scan mode of MS-MS allows the mass spectrometer to collect mass/intensity data only for fragment ions derived from precursor ions of a specified mass/charge ratio, thereby creating a "virtual fractionation" of the sample. The expectation is that these chromatograms and their associated mass spectra will be simpler to interpret than those obtained by ordinary LC-MS.

EXPERIMENTAL PROCEDURES

Reagents. Refined, edible grade peanut oil was purchased at a local supermarket. HPLC grade chloroform was purchased from Aldrich Chemical Co. (Milwaukee, WI). Methanol (HPLC grade) and ammonium acetate (HPLC reagent) were purchased from J.T.Baker (Phillipsburg, NJ).

Columns. Two Waters Symmetry® C_{18} columns (2.1 mm i.d. × 150 mm; Milford, MA) connected in series were used for the separation of the peanut oil components.

MS and MS-MS. All MS measurements were performed on a triple quadrupole instrument (Quattro LC™; Micromass

Ltd., Manchester, United Kingdom) fitted with an electrospray ion source. Ion source parameters were adjusted to maximize the intensity of the $(M + NH_4)^+$ pseudomolecular ions. This was achieved with an electrospray capillary potential of 4.76 kV, cone voltage of 66 V, extractor voltage of 4 V, nebulizer gas flow of 80 L/min, desolvation gas flow of 530 L/min at 120°C, and a source block temperature of 100–120°C. Both mass analyzers were adjusted to give unit mass resolution. Single MS spectra were obtained using the first quadrupole as the mass analyzer. For MS-MS experiments, the collision cell contained argon at 3.5×10^{-4} mbarr, and the collision energy was 35 eV.

Infusion experiments. Peanut oil was dissolved in chloroform/methanol (7:3, vol/vol) containing ammonium acetate at 10 mM to a concentration of *ca.* 18 µL/mL. The solution was infused into the electrospray source at 10 µL/min using a syringe pump (Harvard Instruments, Holliston, MA).

HPLC. HPLC was performed with a Waters Alliance® 2690 chromatography module. Peanut oil samples were dissolved in chloroform (18 µL/mL). Injection volume was 10 µL. Elution was carried out using a linear gradient from 9:1 (vol/vol) to 55:45 (vol/vol) methanol/chloroform over 60 min at 250 µL/min, holding at the final composition for 10 min for a total run time of 70 min. The effluent from the columns was combined with a 100-mM solution of ammonium acetate in methanol delivered at 25 µL/min (syringe pump) by means of a T-connector a short distance from the inlet to the ion source. Detection was by means of MS or MS-MS in product ion mode.

FA analysis. A FA profile of the peanut oil by GLC was obtained from Krueger Food Laboratories, Inc. (Cambridge, MA).

RESULTS AND DISCUSSION

Examination of the TAG of peanut oil by product ion MS-MS requires acquisition of a chromatogram corresponding to each precursor species [$(M + NH_4)^+$ pseudomolecular ion] in the mixture. The mass range of these ions was obtained by simple infusion of a solution of the oil and ammonium acetate while operating the spectrometer in full-scan single MS mode. The spectrum thus obtained (Fig. 1) shows the $(M + NH_4)^+$ ions occurring in the *m/z* range of approximately 840 to 1020 Da. [The true monoisotopic M.W. of a TAG is some 0.8 Da greater than the number obtained by adding the integer atomic weights of the elements, owing to the mass defect of hydrogen (actual atomic weight 1.00794) and the large number of hydrogens in the molecule. For clarity, the masses of pseudomolecular ions and fragment ions have been rounded down to integers in each instance.] The monoisotopic precursor $(M + NH_4)^+$ ions are those whose integer mass (rounded down) is even. As expected for TAG containing even numbers of FA carbons, the ions are observed in clusters centered *ca.* 28 Da (= C_2H_4) apart in the spectrum. It is of interest that ions are also seen in the gaps between these clusters, most obviously in the 918 Da region, which may indicate the presence of an odd-carbon-number FA or an oxidation product (ketone or epoxide).

Because some collision-induced dissociation occurs in the ion source, some fragment ions are observed in the infusion spectrum. The fragments in the 550–700 Da region arise from the net loss of one FA and ammonia from the precursor ion, and have the general composition $[(M + NH_4) - (RCO_2H + NH_3)]^+$. These fragments are the most useful for determining the FA content of TAG and are referred to as "DG ions" for simplicity.

Liquid chromatographic separations of TAG by nonaqueous RP-HPLC have been accomplished with several different mobile phases. One common approach has been to use a solvent gradient of acetonitrile and acetone on a C_{18} column (12). In preliminary experiments, mobile phases containing proton-accepting components such as acetone or THF completely suppressed ionization of TAG by ammonium ion under electrospray conditions. A methanol/chloroform mixture containing ammonium acetate was found by Duffin *et al.* (3) to be satisfactory for electrospray. A linear gradient of these solvents was found to give a satisfactory separation of peanut oil TAG on C_{18}, represented by the total ion current (TIC) chromatogram shown in Figure 2. A better separation was obtained using postcolumn addition of ammonium acetate rather than including the electrolyte in the mobile phase.

These chromatographic conditions were used to acquire a product ion chromatogram for each precursor ion mass $(M + NH_4)^+$ determined to be present. The mass spectrometer employed in this study allows up to eight such experiments to be programmed in a single run, but since only one experiment can be observed at any given moment, duty cycle data losses can be significant if many experiments are programmed simultaneously. Initially, four experiments were programmed

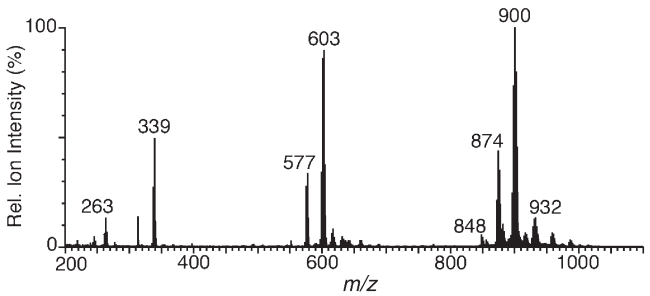

FIG. 1. Mass spectrum of peanut oil obtained by direct infusion into ion source.

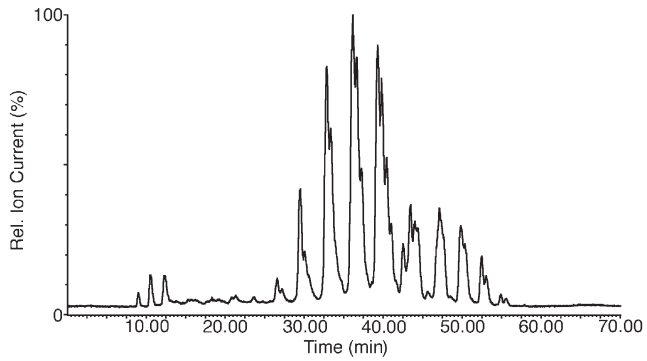

FIG. 2. Mass chromatogram (total ion current) of peanut oil (methanol/chloroform gradient on C_{18} column).

to run the entire length of the chromatogram. As retention time data were accumulated, it became possible to predict retention times with reasonable accuracy by interpolation, and the data acquisition strategy was revised. Under the new protocol, each chromatographic run was broken into four time segments. In each segment, two product ion experiments were programmed for TAG expected to elute in that segment. In this way, up to eight precursor ion masses could be studied per run while minimizing duty cycle losses. Still, given the wide range of M.W. of the TAG in the sample, more than 10 runs were required to cover all the TAG species, although further optimization may be possible.

The product ion TIC chromatograms typically consisted of one or two peaks sometimes with shoulders. Frequently, a peak(s) were seen at an earlier retention time. These were obtained from TAG whose M.W. is two less (i.e., one additional degree of unsaturation) than that under observation but which contain naturally occurring heavy isotopes (primarily ^{13}C). These species were easily identified by their mass spectra, which contained fragment ions whose integer M.W. was even. The loss (by fragmentation) of the elements of a FA (even M.W.) plus ammonia (odd M.W.) implies that only odd-weight fragments will be observed from monoisotopic precursors. The presence of such a heavy isotope species indicated the need to observe the lower M.W. precursor.

The product ion spectra were obtained by averaging across the peak (or portion of peak if shoulders were present) and subtracting a background spectrum. Interpretation of the spectra was generally straightforward. First, the identity of the FA lost to give each DG ion was determined: Subtraction of the mass of the DG fragment ion from the mass of the precursor ion (rounding the masses down to the nearest integer to remove the mass defect) and subtracting a further 15 for ammonia gave the M.W. of the FA lost in the fragmentation process. The M.W. of the FA indicates only the number of carbons and degree of unsaturation, but for FA identified in peanut oil by other methods, common names have been used (e.g., oleic for $C_{18:1}$). With the FA identities known, composition(s) were assigned to the DG ions, and the overall composition of the TAG was determined. In a straightforward case, the averaged product ion spectra from the chromatographic peak corresponding to precursors having an ion mass of 874.8 consisted only of fragment masses 575, 577, and 601. These DG ions resulted from loss of palmitic (P) (to 601), linoleic (L) (to 577), and oleic (O) (to 575) acids. The DG fragments thus have the composition LO (601), PO (577), and PL (575), and the overall composition of the single TAG of this mass observed at this retention time is PLO.

The situation can become more complex at higher precursor M.W. Figure 3 shows the DG fragments obtained from TAG of precursor ion mass 932. The mass losses indicated the presence of stearic (S), arachidic (A), $C_{20:1}$ "gadoleic" (G), and $C_{22:1}$ "erucic" (Er) acids, as well as O and P. From these FA, the fragment at *m/z* 577 resulting from loss of Er can be assigned only to the composition PO, thus establishing the presence of POEr. Similarly, the unique assignment of

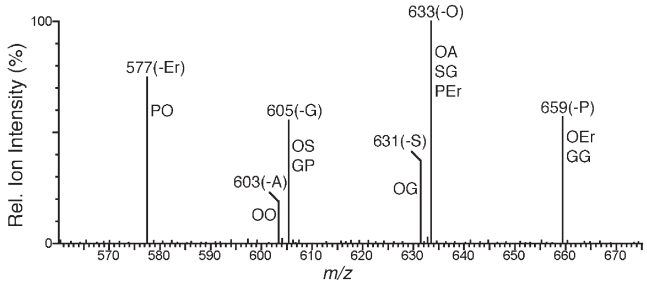

FIG. 3. Product ion spectrum of coeluting TAG POEr, AOO, GOS, and perhaps PGG. P, palmitic ($C_{16:0}$); O, oleic ($C_{18:1}$); Er, erucic ($C_{22:1}$); A, arachidic ($C_{20:0}$); G, gadoleic ($C_{20:1}$); S, stearic ($C_{18:0}$).

m/z 603 to OO established AOO, and the unique assignment of *m/z* 631 to OG established SOG. These assignments are supported by the fragments at 605 (OS), 633 (OA, SG, and PEr), and 659 (OEr). It is also possible to assign the structures GP to *m/z* 605 and GG to *m/z* 659 from this set of FA. This allows the possibility that a TAG of composition PGG could be included in the sample, but without a uniquely assigned DG fragment, the presence of PGG can be neither confirmed nor denied. This situation arises in a small number of instances in the analysis of peanut oil, particularly where a homogeneous TAG may appear in the presence of a mixed TAG, e.g., SSS in the presence of PSA where fragment mass 607 corresponds to SS and PA.

Altogether, over 160 TAG were identified by FA content. For each species, its relative abundance was estimated from the base peak intensities of the mass spectrum. The peak intensity is reported as a number in scientific notation, and the exponent was simply used to categorize abundance by order of magnitude. In some cases of redundant peak structure assignment, estimation of base peak intensity was required. Abundance exponent 5 represents the most abundant species, exponent 4 represents relative concentration on the order of 10% of the most abundant species, and so on. In addition, there are numbers representing a rough approximation of the relative abundance of each TAG and representing the degree of confidence in assigning the FA at the *sn*-2 position *(vide infra)*. Table 1 provides a partial listing of the TAG identified in this study, those with an abundance exponent of 4 or 5.

All the TAG identified by Myher *et al.* (8), Singleton and Patee (10), and Rezanka and Mares (11) were also identified in the present study. Additionally, 72 of the TAG reported by Sempore and Bezard (9) were identified. Whether the few TAG in the Sempore and Bezard study not seen in the present study were the result of a different peanut oil sample or the methodology used by those authors to assign compositions by mathematical treatment of FA analysis data could not be determined.

The FA identified in the TAG species are listed in Table 2, with the results (as area percentage) of a FA profile of the oil sample performed by a contract laboratory. The FA not detected by GLC are, with few exceptions, found only in TAG species of low relative abundance (exponent 1 or 2, of the order of 0.01 to 0.1% of the most abundant species). Montanic acid ($C_{28:0}$), for instance, was identified in just two TAG of an abun-

TABLE 1
Partial Listing of TAG Species[a]

TAG species[b]	Retention time	M.W.[c]	Abundance exponent[d]	Substitution confidence[e]
LLL	28.52	896	5	1
LLO	31.63	898	5	1
PLL	32.13	872	4	1
LnOO	32.14	898	4	3
OLO	34.42	900	5	2
PLO	34.95	874	5	1
SLL	35.67	900	4	3
PLP	35.69	848	4	1
OOO	37.41	902	5	1
GLO	37.79	928	4	1
POO	38.22	876	5	2
SLO	38.66	902	4	2
POP	38.75	850	4	1
PLS	39.39	876	4	1
GOO	40.69	930	4	1
SOO	41.64	904	5	1
ALO	42.05	930	4	1
POS	42.29	878	4	1
BLL	42.51	956	4	1
AOO	44.89	932	4	2
BLO	45.24	958	4	1
PLB	45.81	932	4	1
BOO	47.75	960	4	1
LiLO	48.14	986	4	1
BLG	48.14	986	4	3
LiOO	50.41	988	4	2
BOG	50.41	988	4	3

[a]A total of 168 TAG species were identified in this study. Only the most abundant are listed here. A complete list may be obtained from the author.
[b]FA abbreviations: P, palmitic ($C_{16:0}$); Ln, linolenic ($C_{18:3}$; α, γ unspecified); L, linoleic ($C_{18:2}$), O, oleic ($C_{18:1}$), S, stearic ($C_{18:0}$), G, gadoleic ($C_{20:1}$), A, arachidic ($C_{20:0}$); B, behenic ($C_{22:0}$); Li, lignoceric ($C_{24:0}$).
[c]For convenience, M.W. are rounded down to the nearest integer value to eliminate hydrogen mass defect.
[d]Exponent of the observed base peak intensity (expressed in scientific notation) for the TAG, used to indicate relative abundance by order of magnitude.
[e]Assessment of confidence in assigning *sn*-positions of the FA: 1 = high confidence, substitution likely that expressed in column 1; 2 = moderate confidence, substitution may be that expressed in column 1; 3 = no substitution pattern implied.

TABLE 2
FA Identified in Refined Peanut Oil

FA[a]	Area % (GLC)[b]	FA	Area % (GLC)
14:0 (M)		19:2	
15:0		20:0 (A)	1.14
16:0 (P)	9.34	20:1 (G)	1.29
16:1 (Po)		20:2	
16:2		21:0	
17:0 (Ma)	0.09	22:0 (B)	2.78
17:1 (Mo)	0.11	22:1 (Er)	
17:2		22:2	
18:0 (S)	2.56	23:0	
18:1 (O)	52.07	24:0 (Li)	1.42
18:2 (L)	28.52	24:1	
18:3 (Ln)	0.69	25:0	
19:0		26:0 (Ce)	
19:1		28:0 (Mt)	

[a]FA abbreviations: M, myristic ($C_{14:0}$); Po, palmitoleic ($C_{16:1}$); Ma, margaric ($C_{17:0}$); Mo, margaroleic ($C_{17:1}$); Er, erucic ($C_{22:1}$); Ce, cerotic ($C_{26:0}$); Mt, montanic ($C_{28:0}$). For other abbreviations see Table 1.
[b]Area percentages are reported only for those FA found by GLC analysis of the oil.

dance exponent 1 level. The TAG uniquely identified in this study typically were also of low relative abundance (exponent 3 or less) and/or contained one or more of the FA not detected in the GLC analysis. It is possible, if not likely, that many of these TAG arise from randomization, cracking, and disproportionation resulting from processing. Without a raw sample of the same oil, however, it was impossible to verify this.

Mottram *et al.* (13) have used the relative abundances of the DG ions derived from $(M + H)^+$ precursors in atmospheric pressure chemical ionization LC-MS to assign the *sn* position of FA, based on the observation that fragmentation loss of the *sn*-1(3) FA is generally preferred to FA fragmentation at *sn*-2. Thus, the intensities of the –A and –B ions will be more nearly equal from a TAG of substitution type AAB than will be the case from a substitution type ABA. The intensity of the AC ion will be the lowest of the three arising from a TAG of substitution type ABC. The situation with ESI is less clear. Duffin *et al.* (3) declined to draw any conclusions based on intensity of fragments derived from $(M + NH_4)^+$ using a triple quadrupole instrument, where the selectivity of the FA fragmentation did not seem as pronounced. In contrast, using an ion trap mass spectrometer to fragment $(M + NH_4)^+$ ions, Marzilli *et al.* (6) observed a much larger ratio of 605(SO)/607(SS) for SOS than for SSO and suggested the intensities may indicate FA position on glycerol. Pittenauer *et al.* (14), however, claimed that when using sector instruments, it is possible to determine positional information only from $(M + Na)^+$ ions but not from $(M + NH_4)^+$ ions. In the present work, the peak intensity ratio for 605:607 was 3.2 for SOS and 1.5 for SSO, suggesting at least limited applicability of these ratios for positional assignments. Accordingly, an assignment has been suggested for 64 of the peanut oil TAG. Assignments deemed to be highly likely were given a confidence level of 1 in Table 1 (35 cases). Where an assignment seemed likely but less certain (i.e., narrower ratios), a confidence level of 2 was given (29 cases). In the majority of cases, it was not possible to assign an *sn*-position (confidence level 3) owing to coelution and redundant FA assignments of peaks. A more thorough study of FA fragmentation susceptibility considering such factors as associated cations and FA chain length and degree and sites of unsaturation as well as substitution position on glycerol would be required to increase the confidence of these positional assignments.

Finally, the data permit study of chromatographic behavior of TAG in the methanol/chloroform/C_{18} separation system. Examination of the retention times of the TAG indicates that the "peaks" observed in the TIC chromatogram (Fig. 2) are actually envelopes of overlapping peaks. A clearer picture is obtained by determining the equivalent carbon number (ECN) for each species [ECN = FA chain length – 2 × (no. olefinic double bonds)]. Retention time is then seen to be essentially linear with respect to ECN, although there is a spread in retention times for each ECN value. The retention

times of TAG that appear to have an odd number of FA carbons fall neatly between adjacent sets of even-numbered TAG, thus supporting the conclusion that the odd-numbered TAG are indeed that, and not ketones or epoxides of even-numbered TAG. In that case, shorter retention times would be expected. This observation is further supported by the identification of $C_{17:0}$ and $C_{17:1}$ FA in the GLC analysis. Examination of subsets of the retention time data sorted by the total number of olefinic double bonds in the FA shows that retention time is related to the distribution of double bonds among the FA. Longer retention times are associated with saturation. For example, TAG containing two saturated and one diunsaturated FA have consistently longer retention times than TAG containing one saturated and two monounsaturated FA. This phenomenon accounts for the typical appearance of two peaks in the product ion chromatograms. In one anomalous case, the retention times of the TAG having 62 FA carbons were reproducibly shorter than expected, suggesting that one or more of the very long chain FA was folding back on itself and reducing interaction with the stationary phase.

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