Validation of Computational Methods for Triglyceride Composition of Fats and Oils by Liquid Chromatography and Mass Spectrometry

C. MERRITT, Jr., M. VAJDI[1], S.G. KAYSER, J.W. HALLIDAY and M.L. BAZINET,
Science and Advanced Technology Laboratory, U.S. Army Natick Research and Development Laboratories, Natick, MA 01760

ABSTRACT

A computer method for predicting triglyceride composition of fats and oils from fatty acid composition is described. The results of the method are compared with results of analyses performed by liquid chromatography (LC) and desorption chemical ionization mass spectrometry. An LC column technology is also described which provides a simple separation of triglycerides according to the equivalent carbon number of the triglyceride.

INTRODUCTION

A simple method for the total analysis of the triglyceride composition of fats and oils has long been sought by investigators of lipid chemistry, although many methods and procedures have been previously developed (1,2). Direct analysis of triglycerides based on chromatographic separation by gas chromatography (GC) or liquid chromatography (LC) has not yet been achieved, although partial separation and analysis by either method is readily accomplished (3,4). Analysis by mass spectrometric (MS) methods (1,2,5-11) likewise provides only partial analysis since the mass of several of the mixed triglycerides is isometric.

The fatty acid composition of lipids can now be determined easily by GC analysis of the methyl esters (or other derivatives) of the triglyceride hydrolysates (12). Several approaches to the computation of triglyceride composition from fatty acid analyses have been proposed (1,13), but a method to provide a quick estimate has not been previously devised.

This paper describes a simple procedure based on random probability for computing the triglyceride composition of a fat from its fatty acid composition. The validity of the computations is verified by using a combination of LC and MS methods to achieve actual triglyceride analysis of the corresponding fat. A new LC column technology is also described which provides a simple separation and analysis according to the equivalent carbon number of the triglyceride.

EXPERIMENTAL

The various fats and oils studied were obtained from commercial sources. The peanut oil was found to be a southwest variety, the olive oil was an imported, certified pure product, and the so-called fortified olive oil was a U.S. commercial product consisting of a mixture (90/10) of soybean and olive oils. The samples of meat fat were obtained by Soxhlet extraction with ethylether of the ground meat. The fatty acid analyses were performed according to the official AOAC method (12).

[1]Visiting Scientist, Department of Food Science and Nutrition, University of Massachusetts, Amherst, MA 01003.

Separation and analysis of the triglycerides was performed using reversed-phase liquid chromatography on a bonded silica-C_{18} column (Waters Associates, Inc.) and by direct liquid/solid chromatography with a Poragel PG, so-called triglyceride column (Waters Associates, Inc.). Details of column dimensions, eluents and operating conditions are given in the various figures. The chromatograph used was a Waters Associates, Inc., Model ALC-202 fitted with a solvent programmer and a refractive index detector. Integration of peak areas was performed with a Hewlett Packard Model 3390 recording integrator and checked by manual calculation from a simultaneous analog recording of the chromatogram using the triangulation (½ peak width x peak height) method.

Identification of triglycerides separated by LC was achieved by acquiring mass spectra of the eluted peaks. The mass spectra were obtained with a CEC Model 21-110 double focusing mass spectrometer in electron impact ionization mode using a solids insertion probe. The desorption chemical ionization mass spectra of the cooking oils were obtained with a MAT Model 312 mass spectrometer (Harvard University School of Public Health) using ammonia as reagent gas. The method was essentially that described by Schulte et al. (11). The MAT mass spectrometer was equipped with a MAT 200 data system.

The programs for computation of triglyceride composition were written in FORTRAN IV and were executed initially on a Digital Equipment Corporation Model No. PDP 15/76 computer. They were subsequently transcribed to be executed on a DEC PDP 11/34A computer. The plotting routines for the reconstructed chromatograms and the correlation graphs were written and executed on a Tektronix Model 5041 data terminal equipped with a Tektronix Model No. 4662 digital plotter.

RESULTS AND DISCUSSION

Computer Predicted Composition

Several hypotheses have been proposed for the distribution of fatty acids among the various mixed triglycerides in fats. The several theories of mixed triglyceride structure and the triglyceride composition of various fats and oils have been extensively reviewed by Litchfield (1) and Coleman (13). Previously reported computer methods (14-17) for predicting triglyceride composition have been limited to calculating classes or have been concerned in detail with positional isomerism. Although a complete elucidation of triglyceride composition is possible invoking elaborate, time-consuming and tedious separations coupled with hydrolytic and/or enzymatic degradation, considerable uncertainty remains concerning the specific triglyceride composition of many common fats and oils. It is not the objective of this study to resolve these difficulties. Rather, it is intended to devise a utilitarian procedure to provide a rapid

means of obtaining the composition of the principal triglycerides in various natural fats. The methods described herein are an attempt to fulfill this need.

Newer methods of separation and analysis using chromatographic and mass spectrometric techniques can now be used to verify hypothetical predictions. In this study, a simple hypothesis for prediction of triglyceride composition based on random probability calculations from the fatty acid composition of the lipid hydrolysates is tested by comparing the results of computed composition with concomitant analyses by LC and desorption chemical ionization MS.

Since simple methods for determination of positional isomerism of the various fatty acid moieties in a triglyceride are unavailable and the chromatographic and mass spectrometric methods used here fail to distinguish such isomers, the computational procedure invoked likewise makes no attempt to assign positions to the fatty acid constituents. For many analytical applications, it is not necessary to know the precise isomeric configurations of the triglycerides. Therefore, an algorithm has been devised which follows the random theory of distribution. This theory assumes that the fatty acids are distributed both between the triglycerides and within each triglyceride molecule in a random manner and that the proportion of each triglyceride can be calculated from probability.

The algorithm used in the present computational prediction of triglyceride composition from fatty acid composition is:

$$\eta = n \times p,$$

where η is the probability of occurrence of a given triglyceride, n is a weighting factor for the number of times the same fatty acid occurs in the triglyceride and p is the percentage abundance of the fatty acid in the fat. Values of n are taken as shown in Table I.

TABLE I

Choice of Weighting Factors for Probability Calculations

No. of occurrences of a fatty acid	n
1	6
2	3
3	1

A flow diagram for the computational procedure is given in Figure 1. Included in the program output (not shown) is a listing of some of the MS data. The probability is expressed as a relative abundance in percentage normalized to the total possible number of triglycerides. Triglycerides having a probability of occurrence of less than 1.0% are disregarded in the considerations described below.

Since triglycerides are found to elute from liquid chromatographic columns according to equivalent carbon number (vide infra), a computer program (Fig. 2) was also written to plot the calculated triglyceride abundance data as a function of equivalent carbon number (1). Such a plot is seen in Figure 3. For comparison, a typical chromatogram obtained on the triglyceride column is also shown.

Liquid Chromatography

Partial separations of triglycerides have been achieved by both GC and reversed-phase LC (3,4). In this study, both methods were tried, but the use of a so-called triglyceride LC column (Waters Associates, Inc.) proved to be a more efficacious method for quantitative analysis. Prior applications of the triglyceride column have been described elsewhere (18-20). The chromatograms obtained for three typical oils and three meat fats are shown in Figure 4. The components of the mixture of triglycerides are separated into groups according to their equivalent carbon numbers. The composition of the individual peaks of the oils was ascertained by MS analysis of the collected fractions. Identification of the triglycerides was based on the appearance of the molecular ion and the M-RCOO peaks in the respective mass spectra. The data are given in Table II. The peak areas were acquired by means of a digital integrator. Data are given in Table III.

Chromatograms were also acquired by reversed-phase LC. These are shown in Figure 5. The separations obtained are essentially the same as those reported in the literature (21). As can be seen, there is partial separation of the so-called critical pairs found in each equivalent carbon number group. It was not possible to integrate the partly resolved peaks (reproducibility was very poor) on the digital integrator, but as shown below, integration by triangulation nevertheless gave good correlations with the computer predictions for the abundance of the individual triglycerides. Moreover, summation of the total peak areas by equivalent carbon number groupings gave correlations comparable to those obtained with the triglyceride (TG) column (vide

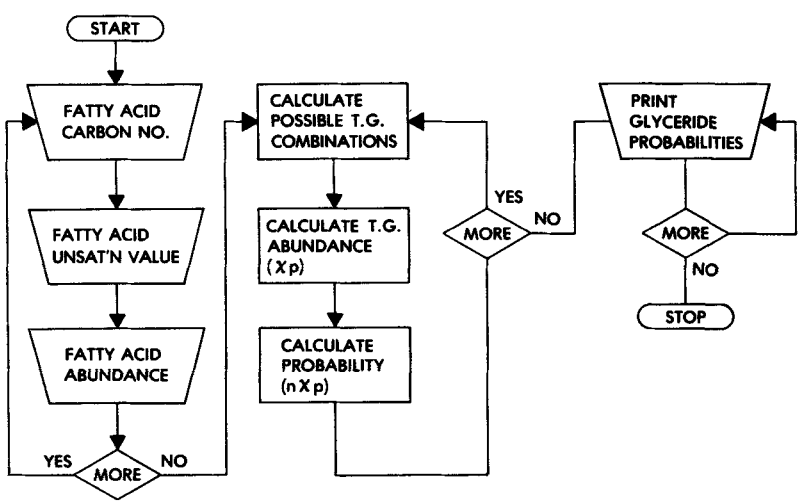

FIG. 1. Flow chart of computer program for calculation of triglyceride composition.

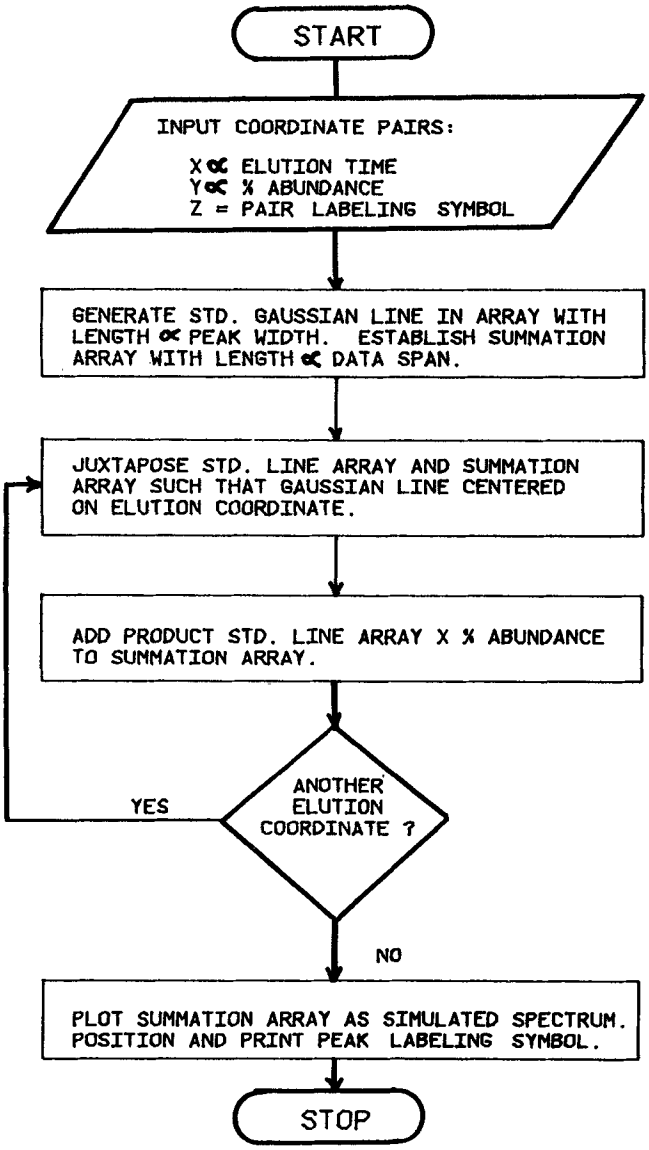

FIG. 2. Flow chart of computer program for generation of simulated liquid chromatograms based on computer predicted triglyceride composition as a function of equivalent carbon number.

infra). However, for purposes of quantitative analysis, the TG column is found to be preferable since integration of the smooth peaks provides reliable data in a simple manner. The peak area data from the RPLC column are given in Table IV.

In addition to the cooking oils studied, the validity of the correlation was also evaluated for various meat fats. Typical meat fat chromatograms are shown in Figure 4 and the peak area data are given in Table III.

Correlations

To establish the validity of the computer prediction of triglyceride composition, the values obtained were compared with those ascertained by LC analysis. A statistical procedure was followed in which a plot of the computer data vis a vis the chromatographic data was constructed, and the correlation was established by linear least squares regression of the points to compute the slope and the correlation coefficient (22). In the figures shown, the points are distributed about a hypothetical line having a slope of 1.0 for perfect correlation, but the computed slope of the actual least squares regression line is given on the plot. Limit lines are shown corresponding to 95% confidence limits. The confidence limit is computed from the regression of x (LC data) on y (computer data) since y is invariant. The average deviation, d (taken in lieu of σ because of the small number of samples for each determination), is calculated for the entire population (N = 79) of LC measurements of abundance.

The chromatographic data used are given in Tables III and IV and the computer data are summarized in Table V. The correlation graph for the various oils is shown in Figure 6. In this figure, the analytical data are taken from the triglyceride column. The correlation was also established for data taken from the reversed-phase LC column. This is shown in Figure 7.

The partial separation of several of the critical pairs on reversed-phase LC also permitted a correlation of the predicted abundances of the individual triglycerides. The analytical data are given in Table IV and the data from the computer printouts are shown in Figure 8. The correlation graph is shown in Figure 9. It is seen that the computer predictions are verified not only for equivalent carbon number groups, but also for the individual triglycerides.

The hypothesis for a random distribution of the fatty acids among the triglycerides found in peanut, olive and soybean oils (the latter inferred from the results with the 90:10 soy/olive oil) has been verified by the correlation of the computer predictions with analytical data from LC. The results agree with earlier data by Dutton et al. (23-26) that such a random distribution is generally found for unsaturated vegetable oils. The present results are somewhat limited, being restricted to three oils, but further analyses are planned to test the hypothesis on a wider scope.

In connection with studies of the precursors involved in the formation of radiolysis products found in meat fats, it has become necessary to ascertain their triglyceride composition. A test of an analogous computer method for this purpose was also undertaken. In accordance with the generally accepted view (W.W. Nawar, private communication) that the abundance of simple triglycerides in such fats is quite small, the predictive algorithm was modified to exclude the simple triglycerides from the computation. A summary of the results for beef, ham and chicken fats is given in Table V. The correlation of these predictions with the LC analyses is shown in Figure 10.

The correlation coefficients obtained by linear least squares regression all demonstrate a high degree of correlation between the LC data and the computer predictions. The validity of excluding the simple triglycerides, however, is not readily established. If a computer algorithm for random distribution is used, the appearance of the equivalent carbon number distribution is essentially the same as that for one which excludes simple triglycerides. Moreover, the question of the absence of simple triglycerides cannot be easily resolved by MS since several pairs of triglycerides which coelute also have the same molecular weight and share some of the fatty acids. The fact that simple triglycerides are indeed absent is shown by the correspondence of the predictions to the actual chromatographic behavior.

A comparison of the computed individual triglyceride composition in ham fat based on a random and an exclusive hypothesis is given in Table VI. The relative proportions of the individual triglycerides is nearly the same for each equivalent carbon number group except for carbon number 48, in which triolein would appear if present. The reversed-

TABLE II

Mass Spectrometric* Identification of Triglyceride Components of HPLC Fractions

Equivalent carbon no.	Peanut oil M†	Peanut oil TG	Olive oil M	Olive oil TG	Soy/olive oil M	Soy/olive oil TG
38					874	LL_nL_n
40					850	PL_nL_n
					876	LLL_n[a]
					876	OL_nL_n[b]
42					852	PLL_n
	878	LLL			878	LLL
					878	OLL_n[c]
44	854	PLL	854	PLL	854	PLL
	880	OLL	880	OLL	880	OLL[d]
					880	OOL_n[e]
46	830	PPL				
	856	POL	856	POL	856	POL
	882	OOL	882	OOL	882	OOL
48			832	PPO	832	PPO
	858	POO	858	POO	858	POO
	884	OOO	884	OOO	884	OOO
	884	SOL[f,g]				
50			860	PSO	860	PSO
	886	SOO	886	SOO	886	SOO
	912	OLA			912	OLA
52	914	OOA				
	940	OLB				
54	942	OOB				

*Electron impact ionization
†M = Molecular ion.
[a]M - L = 597.
[b]M - O = 595.
[c]M - O = 597.
[d]M - L = 601.
[e]M - L_n = 603.
[f]M - S = 601.
[g]M - L = 605.

Abbreviations: P = C_{16}; S = C_{18}; O = $C_{18:1}$; L = $C_{18.2}$; L_n = $C_{18:3}$; A = C_{20}; B = C_{22}.

TABLE III

Integrated Area Data for HPLC Peaks[a] from Various Oils and Meats

Equivalent carbon no. peak	Peanut oil Area %[b] $\bar{x} \pm d$[c]	Olive oil Area % $\bar{x} \pm d$	Soy/olive oil Area % $\bar{x}$[e] $\pm d$	Beef Area % $\bar{x} \pm d$	Ham Area % $\bar{x} \pm d$	Chicken Area % d, g
40			7.01 ± 0.38		1.90 ± 0.14	
42	2.04[d]		24.94 ± 0.95	0.66[d]		6.4
44	17.66 ± 0.14	8.10 ± 0.44	30.86 ± 0.16	5.48 ± 0.31	5.76 ± 0.33	23.9
46	33.93 ± 0.16	25.19 ± 0.19	22.12 ± 0.78	22.13 ± 0.87	22.91 ± 0.17	37.8
48	27.60 ± 0.77	61.28 ± 0.62	12.76 ± 0.56	48.36 ± 0.09	49.42 ± 0.47	25.9
50	7.03 ± 0.63	5.43 ± 0.86	2.13 ± 0.13	20.75 ± 0.11	20.03 ± 0.17	6.0
52	5.45 ± 0.26			3.26 ± 0.56	1.9[d,f]	
54	4.41 ± 0.22					
56	1.93 ± 0.66					

[a]See Fig. 4.
[b]Average from integrator printout.
[c]Average deviation.
[d]Single value.
[e]Three determinations.
[f]By triangulation.
[g]Rounded to nearest tenth.

phase chromatogram which shows partial separation of the components of the carbon number 48 peak is shown in Figure 11. The estimated resolution ($R = 2\Delta t/W_b + W_b'$) for the three major components is ~ 0.5. Using this value and the data of Table VI, a computer-constructed chromatographic peak for each hypothetical case also is plotted in Figure 11.

The shape of the peak for the situation predicted on the absence of triolein coincides nearly exactly with the actual reversed-phase chromatographic peak.

Desorption Chemical Ionization Mass Spectrometry

Electron impact ionization MS using a solids insertion

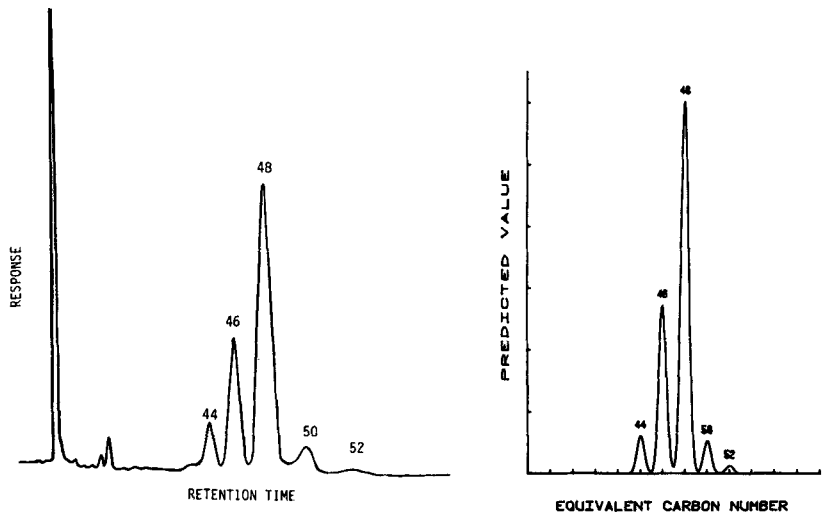

FIG. 3. Comparison of liquid chromatogram of olive oil on triglyceride column (left) with computer generated chromatogram from computer predicted composition (right). Unit separation factor, R = 1, is assumed.

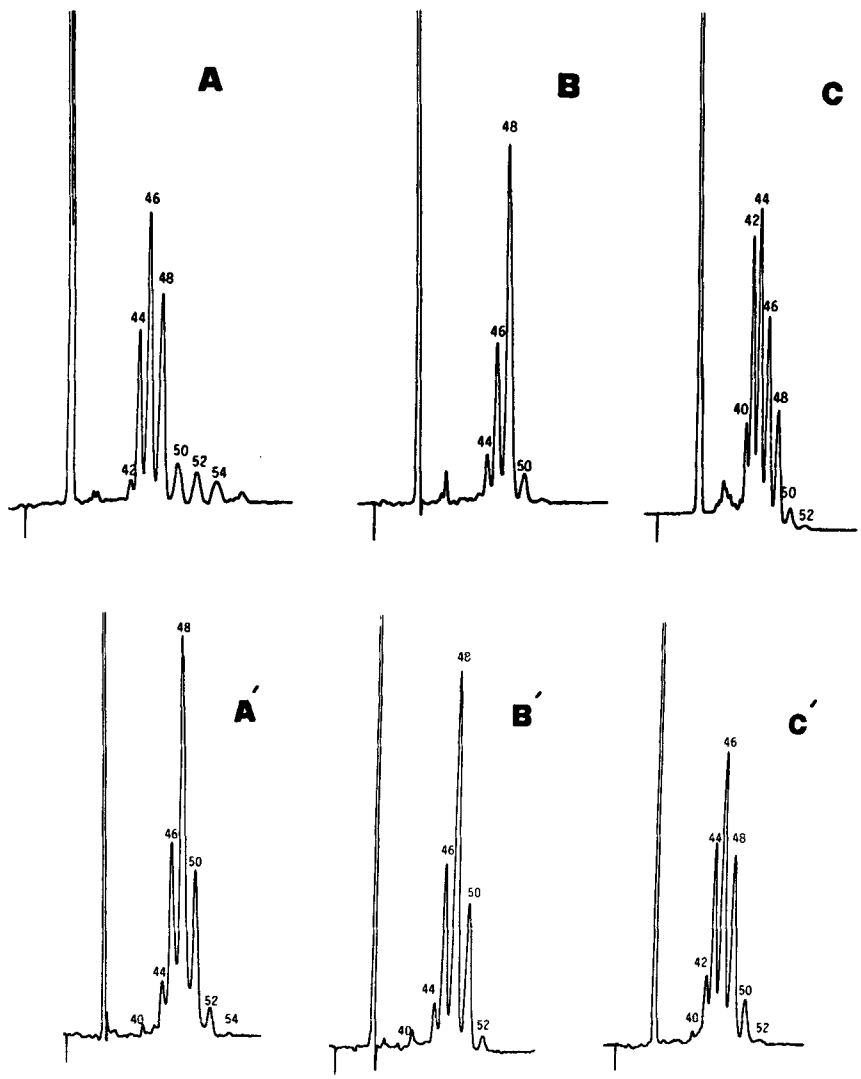

FIG. 4. Liquid chromatograms of various cooking oils and meat fats. A, peanut oil; B, olive oil; C, 90:10 soy/olive oil; A′, beef; B′, ham; C′, chicken. Column, triglyceride (30 cm x 7.8 mm); solvent, 20% THF/CH_3CN; flow rate, 2 mL/min; sample size, 10 μL.

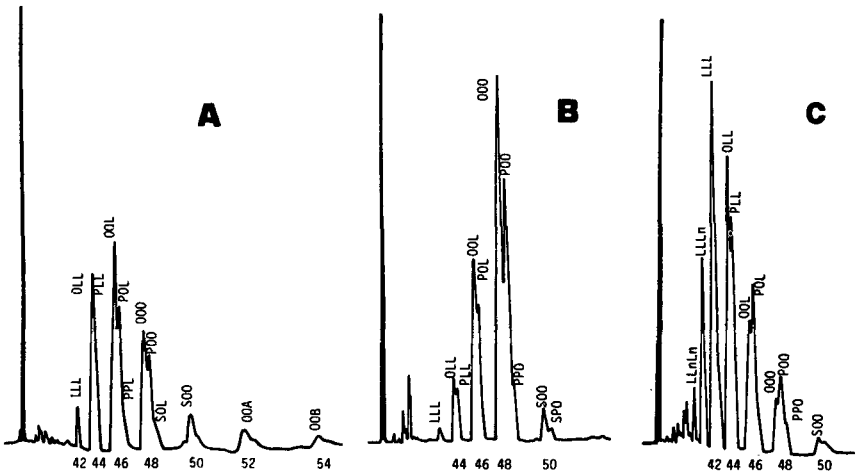

FIG. 5. Reversed-phase liquid chromatograms of various cooking oils. A, peanut oil; B, olive oil; C, 90:10 soy/olive oil. Column, Bondapak C_{18} (30 cm x 7.8 mm). Column conditions as in Fig. 4.

TABLE IV

Integrated Area Data for RPLC[a] Peaks

Equivalent carbon no.	Olive Oil TG[b]	Olive Oil Area %[c]	Olive Oil ΣA[d]	Peanut oil TG	Peanut oil Area %	Peanut oil ΣA
42	LLL	1.1		LLL	2.49	2.49
44	OOL_n	3.0		OLL	14.34	
			6.0			19.83
	OLL	3.0		PLL	5.49	
46	OOL	14.8		OOL	29.80	48.50
	POL	9.8	29.5	POL	18.70	
	P_OOO	4.9				
48	OOO	31.4		OOO	17.46	
						26.19
	POO	21.5	58.9	POO	8.73	
	PPO	6.0				
50	SOO	3.0		SOO	2.99	2.99
			4.5			
	PSO	1.5				

[a]See Fig. 5.
[b]In order of elution.
[c]By triangulation.
[d]Summation by equivalent carbon no.

TABLE V

Computer Predicted Triglyceride Composition of Various Oils and Meat Fats

Equivalent carbon no.	Abundance Peanut oil	Olive oil	Soy/olive oil	Beef	Ham	Chicken
40			5.1			1.5
42	4.6		19.6		3.8	22.2
44	19.1	6.1	31.7	20.0	29.3	42.4
46	36.0	27.2	27.6	44.9	41.5	25.6
48	26.9	60.1	13.4	29.8	23.0	8.4
50	5.1	5.3	2.5	5.3	2.4	
52	4.5	1.3				
54	3.8					

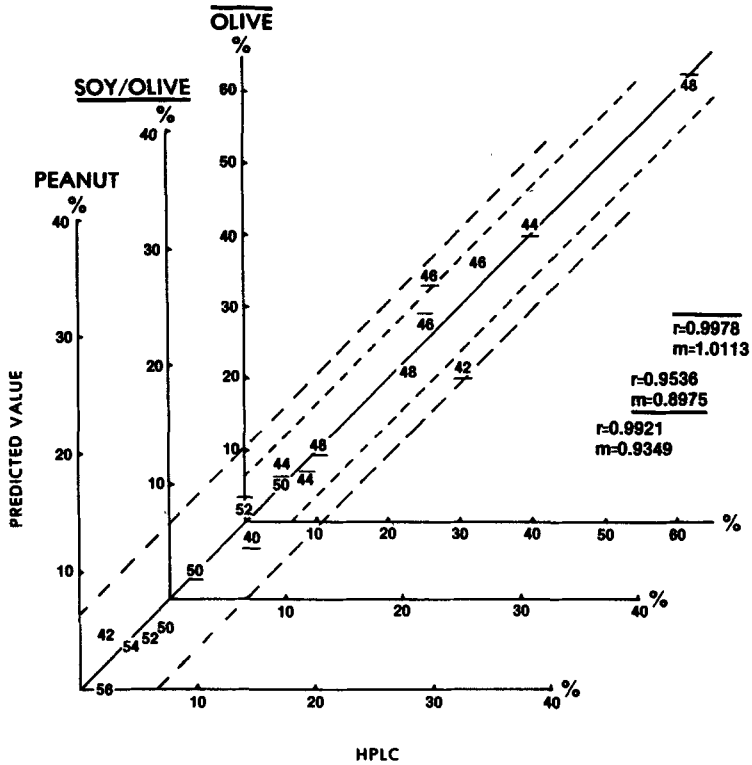

FIG. 6. Composite correlation graph of computer predicted triglyceride composition by equivalent carbon number with liquid chromatographic analyses of various oils. m = 1.0 for theoretical correlation line. Confidence limits, ± 0.95. Slope, m, and correlation coefficient, r, given for respective linear least squares regressions for each data set. Legends, data points and statistical values indicated by correspondence of no line, underline and overline designations.

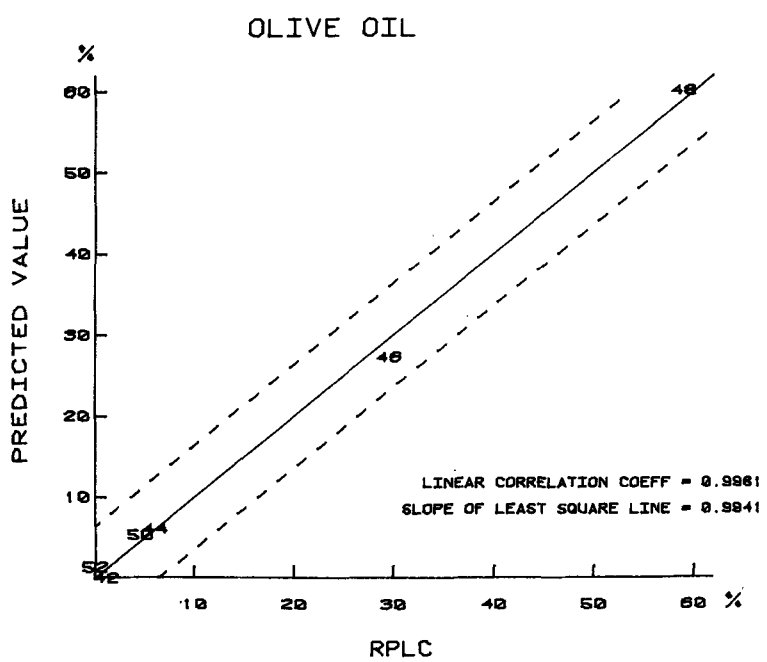

FIG. 7. Correlation graph of computer predicted triglyceride composition of olive oil by equivalent carbon number with an analysis by reversed-phase liquid chromatography. Format as in Fig. 6.

NAME= OLIVE OIL
INPUT COMPOSITION

FATTY ACID	ABUNDANCE(%)
1. 1610	15.3
2. 1611	1.6
3. 1810	2.5
4. 1811	65.8
5. 1812	11.8
6. 1813	1.3
7. 2010	0.9
8. 2014	0.8

TRIGLYCERIDES BELOW 1.0% ARE EXCLUDED
TRIGLYCERIDES ARE ORDERED BY PROBABILITY

TRIGLYCERIDES	EQUIV. CARBON #	PROBABL
1811 1811 1811	48	28.5
1610 1811 1811	48	19.9
1811 1811 1812	46	15.3
1610 1811 1812	46	7.1
1610 1610 1811	48	4.6
1810 1811 1811	50	3.3
1811 1812 1812	44	2.7
1611 1811 1811	46	2.1
1811 1811 1813	44	1.7
1610 1810 1811	50	1.5
1811 1811 2010	52	1.2
1810 1811 1812	48	1.2

NAME= PEANUT OIL (SOUTHWEST)
INPUT COMPOSITION

FATTY ACID	ABUNDANCE(%)
1. 1610	12.2
2. 1810	2.9
3. 1811	47.5
4. 1812	29.5
5. 1813	1.8
6. 2010	1.8
7. 2210	3.2
8. 2410	1.0

TRIGLYCERIDES BELOW 1.0% ARE EXCLUDED
TRIGLYCERIDES ARE ORDERED BY PROBABILITY

TRIGLYCERIDES	EQUIV. CARBON #	PROBABL
1811 1811 1812	46	20.0
1811 1812 1812	44	12.4
1811 1811 1811	48	10.7
1610 1811 1812	46	10.3
1610 1811 1811	48	8.3
1610 1812 1812	44	3.2
1811 1812 2210	52	2.7
1812 1812 1812	42	2.6
1810 1811 1812	48	2.4
1811 1811 2210	54	2.2
1610 1610 1811	48	2.1
1810 1811 1811	50	2.0

FIG. 8. Computer printouts of predicted triglyceride composition of olive and peanut oils.

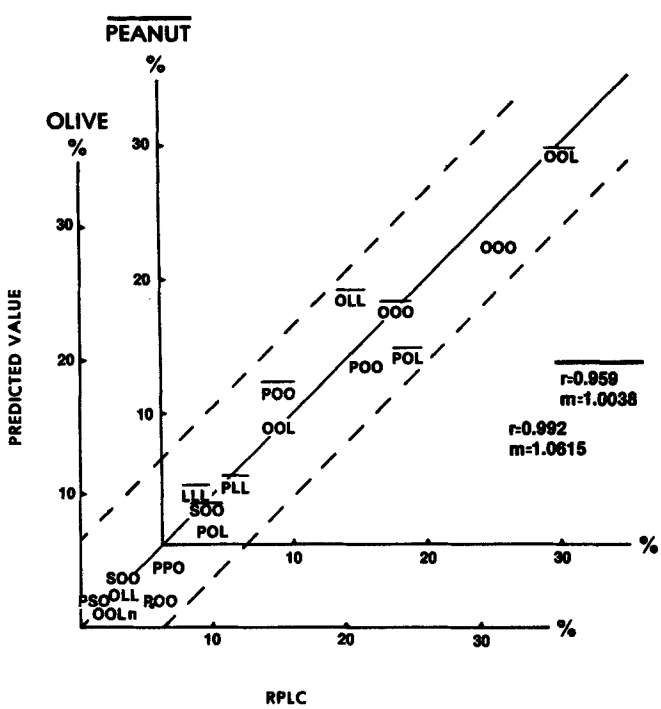

FIG. 9. Composite correlation graph of computer predicted triglyceride composition with reversed-phase liquid chromatographic analyses of peanut and olive oils. Format as in Fig. 6.

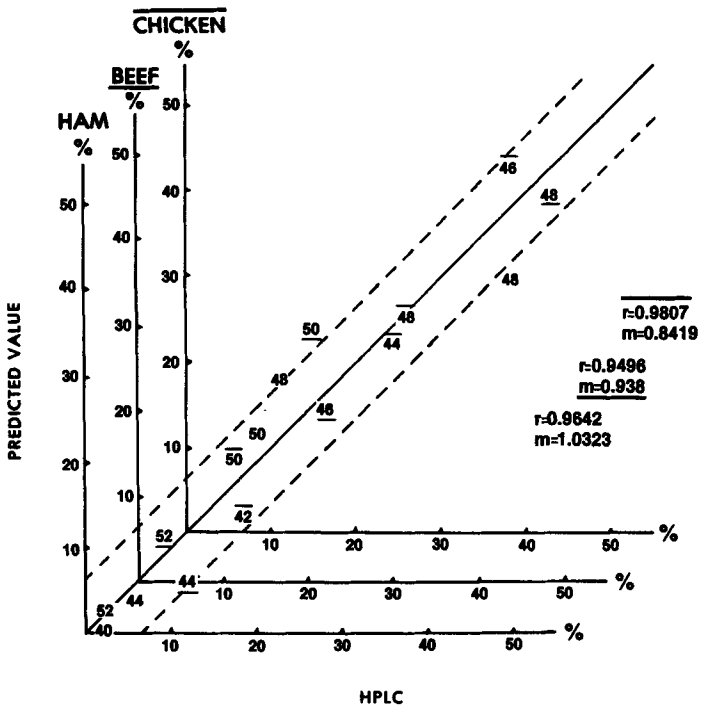

FIG. 10. Composite correlation graph of computer predicted triglyceride composition by equivalent carbon number with liquid chromatographic analyses of certain animal fats. Format as in Fig. 6.

TABLE VI

Comparison of Predictive Composition of Triglycerides in Ham Fat

Equivalent carbon no.	b	TG	Abundance Random	Abundance Exclusive[a]
44	↓	OLL	1.7	2.0
		P_oOL	1.0	1.1
46		OOL	7.4	8.5
		POL	7.3	8.3
48		OOO	10.0	
		SOL	3.0	3.9
		POO	15.0	17.8
		PPO	7.0	8.7
		PSL		1.9
50		SOO	7.3	8.4
		PSO	7.2	8.2
		PPS	1.8	2.0

[a]Assumes no simple triglycerides.
[b]Order of elution.

probe method of sample introduction has been shown (9) to provide an analysis of the triglyceride composition of fats and oils, and the analyses gave reasonably good correlation with predicted values. EI spectra, however, exhibit low abundance of the molecular ions and variable abundance ratios of key ions in the spectrum (e.g., M-RCOO, M-RCO). Quantitative results for mixtures of triglycerides are difficult to obtain from such spectra. More suitable spectra are provided by desorption chemical ionization (10,11) using ammonia as reagent gas in which the M + 18 ion is the most abundant ion in the individual triglyceride spectra and is proportional to the amount of triglyceride in the mixture. NH_3/DCI spectra for the various oils are shown in Figure 12.

The relative abundances of the M + 18 ions corresponding to the individual triglycerides in the various oils are given in Table VII. Using the MS data and the computer predictions of composition, correlations similar to those made for chromatographic analyses (vide supra) are shown in Figure 13.

A summary of the regression analysis based on the entire population of LC and DCI measurements is given in Table VIII.

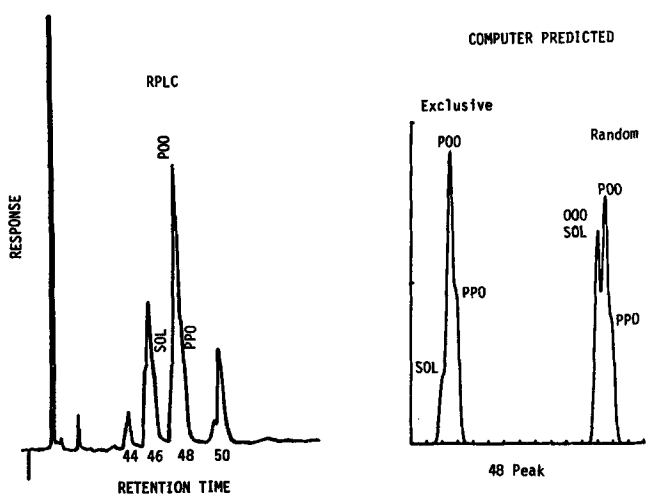

FIG. 11. Comparison of the reversed-phase liquid chromatogram of ham fat (left) with the computer generated chromatographic peak equivalent for carbon number 48 using, respectively, algorithms for a random distribution and an exclusive distribution.

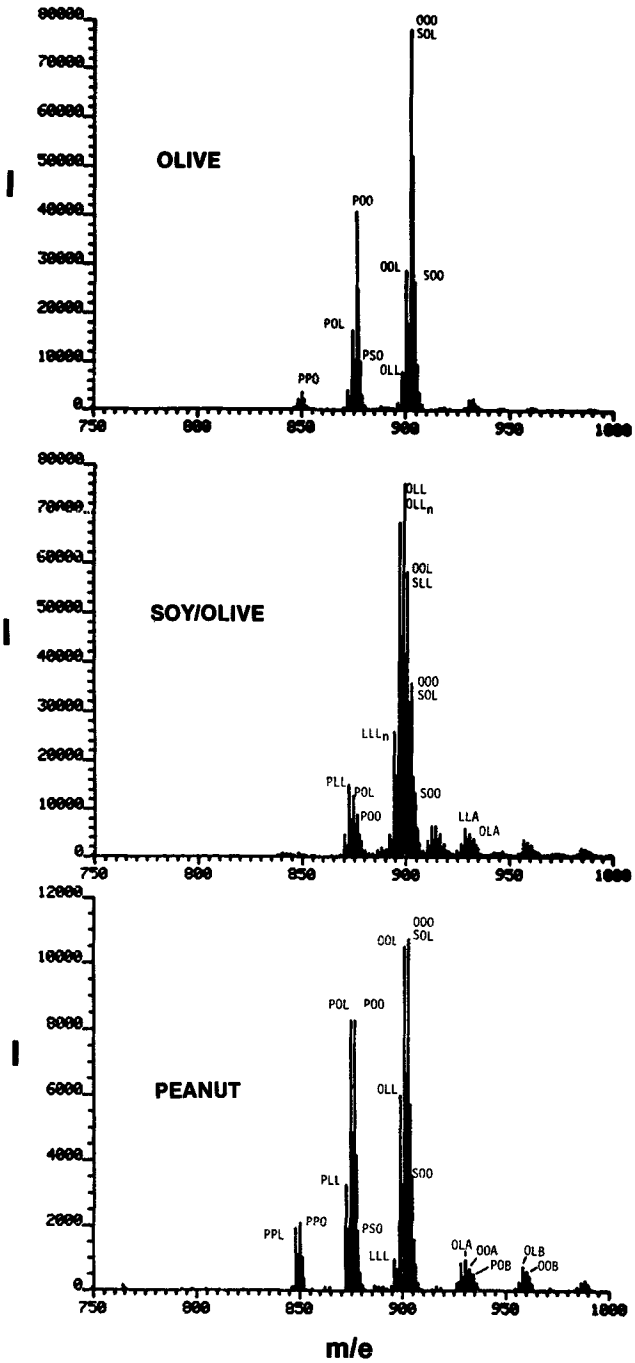

FIG. 12. Desorption chemical ionization spectra (NH_3 as reagent gas) of olive, soy/olive and peanut oils.

ACKNOWLEDGMENT

B.A. Bidlingmeyer of Waters Associates, Inc. provided the triglyceride column and insights concerning its performance characteristics, V.N. Reinhold, Harvard School of Public Health, performed the desorption chemical ionization mass spectra and S.M. Swift of this laboratory made the fatty acid analyses.

REFERENCES

1. Litchfield, C., Analysis of Triglycerides, Academic Press, New York, NY, 1972.
2. Perkins, E.G. (ed.), Analysis of Lipids and Lipoproteins, American Oil Chemists Society, Champaign, IL, 1975.
3. Hitchcock, C., and E.W. Hammond, in Developments in Food Analysis Techniques 2, edited by R.D. King, Applied Science Publishing, Ltd., London, 1980, pp. 199-201.
4. El-Hamdy, A.H., and E.G. Perkins, JAOCS 58:49 (1981).
5. Barber, M., T.O. Merren and W. Kelley, Tetrahedron Lett. 18:1063 (1964).
6. Barber, M., J.R. Chapman and W.A. Wolstenholme, Int. J. Mass Spectrom. Ion Phys. 1:98 (1968).
7. Lauer, W.M., A.J. Aasen, G. Groff and R.T. Holman, Lipids 5:861 (1970).
8. Aasen, A.J., W.M. Lauer and R.T. Holman, Ibid 5:869 (1970).
9. Hites, R.A., Anal. Chem. 42:1736 (1970).
10. Murate, T., Ibid 49:2209 (1977).
11. Schulte, E., M. Höhn and U. Rapp, *Fresenius*, 307:115 (1981).
12. AOAC-IUPAC Gas Chromatographic Method No. 28.057, AOAC Methods, 13th ed., 1980, p. 447.
13. Coleman, M.H., Adv. Lipid Res. 1:1 (1963).
14. Perkins, E.G., and A.V. Hanson, JAOCS 42:1032 (1965).
15. Koman, V., and J. Kotuc, Ibid 54:95 (1977).
16. Koman, V., J. Kotuc and M. Csicsayova, Ibid. 55:629 (1978).
17. Maui, U.V.S., and G. Lakshminarayana, Fette Seifen Anstrichm. 72:434 (1970).
18. Merritt, C., Jr., Presentation at the 11th International Symposium on Advances in Chromatography, Houston, TX, 1976.
19. Merritt, C., Jr., Presented at the 12th International Symposium on Advances in Chromatography, St. Louis, MO, 1977.
20. Bidlingmeyer, B.A., M. Vajdi, S.G. Kayser and C. Merritt, Jr., J. Chromatogr. Sci. (in press).
21. Perkins, E.G., and A. El-Hamdy, Presentation at Am. Oil Chem. Soc. Meeting, San Francisco, June 1979.
22. Snedecor, G.W., and W.G. Cochran, Statistical Methods, 6th edn., Iowa State University Press, Ames, IA, 1967.

TABLE VII

Relative Abundance of M + 18 Ions in Desorption Chemical Ionization Spectra

TG[a]	M[b]	M + 18	Soy/olive oil	Peanut oil	Olive oil
LLL_n	876	894	3.9	–	–
LLL	878	896	21.4	1.0	
OLL_n	878	896			
PLL_n	852	870	1.5	–	–
OLL	880	898	23.9	10.0	3.6
OOL_n	880	898			
PLL	854	872	4.7	5.3	–
POL_n	854	872		–	–
OOL	882	900	18.4	17.4	13.6
SLL	882	900		–	–
P_OOO	856	874	–	–	
POL	856	874	4.1	13.6	7.7
PPL	830	848	0.4	3.2	–
LLA	910	928	1.7	–	–
OOO	884	902	11.3	17.7	37.1
SOL	884	902		13.6	19.4
POO	858	876	2.8		
PSL	858	876		–	–
PPO	832	850	0.2	3.5	1.6
OLA	912	930	1.5	1.7	–
SOO	886	904	4.3	6.0	12.6
PSO	860	878	–	3.0	4.5
OLB	940	958	–	1.2	–
OOA	914	932	–	1.2	–
OOB	942	960	–	1.0	–
POB	916	934	–	0.8	–

[a]Triglyceride: for abbreviations see Table II.
[b]Molecular ion.

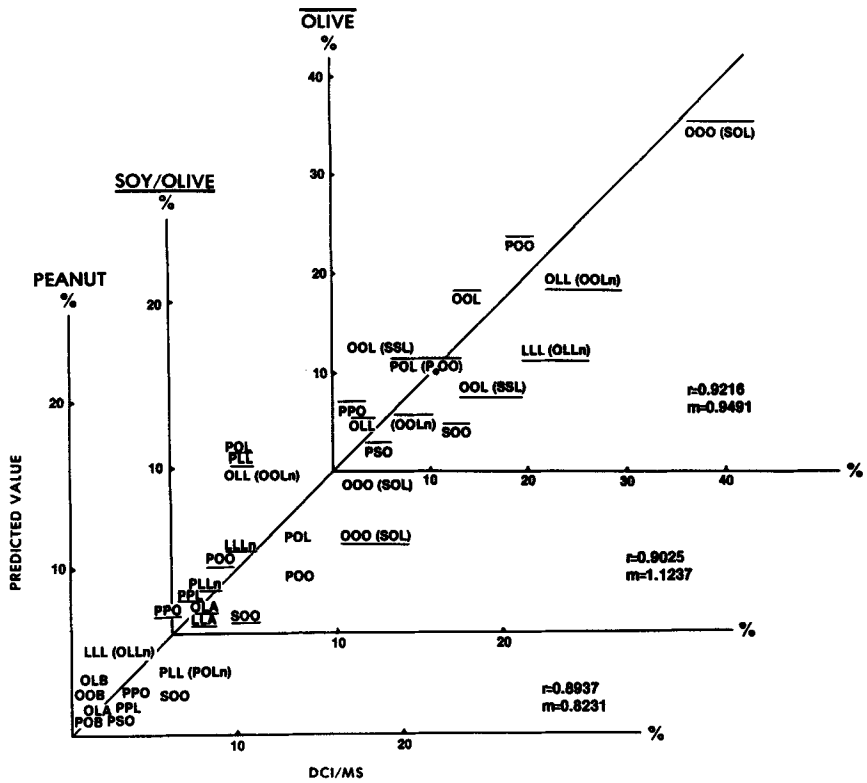

FIG. 13. Composite correlation graph of computer predicted triglyceride composition with NH_3/DCI spectral analyses of peanut, olive and soy/olive oils. Format as in Fig. 6. Values for isometric TG are summed.

TABLE VIII

Regression Analyses Based on the Entire Population of Measurements

	LC	DCI
N	79	38
m	.96	.96
r	.97	.91

23. Dutton, J.J., and J.A. Cannon, JAOCS 33:46 (1956).
24. Scholfield, C.R., and M.A. Hicks, Ibid 34:77 (1957).
25. Scholfield, C.R., and H.J. Dutton, Ibid 35:493 (1958).
26. Scholfield, C.R., J. Nowakowska and H.J. Dutton, Ibid 38:175 (1961).

[Received December 22, 1981]