Lipid Conversion Factors for Calculating Fatty Acid Contents of Foods[1]

JOHN L. WEIHRAUCH, LINDA P. POSATI, BARBARA A. ANDERSON, and **JACOB EXLER,**
Consumer and Food Economics Institute, ARS, USDA, Hyattsville, Maryland 20782

ABSTRACT AND SUMMARY

The U.S. Department of Agriculture is searching the world literature published since 1960 for data on food lipids and their fatty acid composition. These data are being used to update and expand the national tables of food composition and to establish a computerized nutrient data bank. Customarily, investigators report fatty acid data in terms of weight percent of total methyl esters. For the benefit of users of nutrient tables, relative amounts of component fatty acid esters should be converted to grams fatty acid (as free acid) per 100 grams food. For this purpose, conversion factors, defined as the weight of fatty acids in 1 gram of fat, were derived for various food products. Derivation of, and basis for, factors and their application are described for selected food products. Variables affecting factors are also discussed. Investigators should include, in reports on fatty acid composition of foods, information on total lipid content and on the fatty acid content of the lipid. The latter values are readily obtained by a saponification procedure, complete acid hydrolysis, or if desired, by lipid class analysis.

INTRODUCTION

The urgent need for up-to-date information on the fatty acid contents of foods has been intensified by concern over the types and amounts of fat in American diets. The Nutrient Data Research Group of the Consumer and Food Economics Institute, U.S. Department of Agriculture, is responding to this need by conducting a comprehensive search of the world's literature published since 1960 for data on food lipids and their fatty acid composition (1). Tables of fatty acid contents of foods are being developed from this new collation of data and are promptly published in a series of articles entitled "Comprehensive Evaluation of Fatty Acids in Foods" (2-9). Suitable data are being filed in the Nutrient Data Bank which is now being developed (10,11).

When incorporated into the tables of food composition, these data will serve as a reliable standard of reference to all concerned with the nutrient content of food. The tables of fatty acids also provide a valuable tool for those engaged in research on the possible relevance of dietary lipids to the growing incidence of heart disease and atherosclerosis.

An objective in preparing tables of food composition was to provide data on actual content of each fatty acid in the food as g fatty acid per 100 g food. Data on fatty acids are rarely reported in those units, so conversion from customary analytical units became necessary and prompted the work under discussion.

Gas liquid chromatography (GLC) is the method of choice for determining fatty acids. With this method, data are nearly always reported as the weight percent of the methyl ester of each component in the ester mixture obtained by methylation of the lipid sample. Occasionally methanol is replaced by higher alcohols; for instance, butanol is frequently used to quantify the fatty acids of milk fat, particularly butyric and caproic acids (12). Data from such determinations are most frequently given in mole percent. Recent food labeling regulations require that "the amount of fatty acids, calculated as the triglyceride, shall be stated in grams per serving to the nearest gram" (13). Thus far, these units have rarely appeared in the published literature.

The conversion of methyl ester data to amounts of individual fatty acids per 100 grams of food required the establishment of an appropriate factor relating fatty acid content to total lipid. The conversion factor could be obtained by direct determination of the fatty acid content of the total lipid by saponification or by complete acid hydrolysis. Alternatively, the individual lipid classes and fatty acid content of these lipid fractions could be quantified and used to calculate an average value applicable to the total lipid. Since directly-determined conversion factors are usually not provided in the literature, we used the latter method for deriving factors; calculations were based on published information.

Proper quantification of lipid classes requires adequate extraction of total lipid. This requirement is especially important for foods containing low levels of lipid with relatively high amounts of polar lipids. These polar lipids tend to bind to protein and/or starch and are generally not extracted by apolar solvents. Polar solvents or apolar/polar solvent mixtures are needed to ensure complete extraction of polar lipid fractions. Chloroform plus methanol is the solvent of choice for extracting lipids from animal tissues and products (14), but a somewhat more polar solvent mixture, namely water saturated n-butanol, appears more satisfactory for wheat and wheat flour lipids, especially at 70 C (15) and 100 C (16). Acid hydrolysis is unsatisfactory because, depending on the acid concentration and on temperature and duration of digestion, hydrolysis occurs with variable loss of the non-fatty acid portions of the lipid. Barring artifact formation one would expect the total lipid extract by hydrolysis to be lower than nondestructive solvent extracts by the amount of the loss of glycerol, phosphate, amino base, and/or sugar portions of the lipid.

The derivation of appropriate conversion factors is reported for different food samples that illustrate the considerations which were weighed in developing the factors. The bases for derivation and application of factors for the lipids from eggs, beef, pork, fish, cereal grains (wheat), and milk will be discussed.

TABLE I

Derivation of Conversion Factor (F) for Egg Lipid[a]

Lipid fraction	Wt % of total lipid	g Fatty acid/ g lipid fraction	g Fatty acid/ g total lipid
Triglyceride	65	0.956	0.62
Lecithin	24	0.708	0.17
Cephalin	6	0.756	0.04
Cholesterol	5	0	0

F = (.65 x 0.956) + (.24 x 0.708) + (.06 x 0.756)
F = 0.62 + 0.17 + 0.04
F = 0.83

[1] Presented at the AOCS Meeting in Cincinnati, September 1975.

[a] Adapted from Posati et al. (4).

TABLE II

The Fatty Acid Composition of Egg Yolk[a]

Total Lipid = 33.5%
Factor = 0.83

	Fatty acids				
	Saturated		Unsaturated		
Units	16:0	18:0	16:1	18:1	18:2
Wt % FAME[b]	26	9.3	3.9	43	13
g/100 g FAT	22	7.7	3.3	37	11
g/100 g FOOD	7.4	2.6	1.1	12	3.7
If Factor = 0.956 g/100 g FOOD	8.3	3.0	1.2	14	4.2

[a]A comparison of the fatty acid content calculated by the present and former factor, 0.83 vs. 0.956.

[b]FAME = Fatty Acid Methyl Ester.

contents of lysolecithin separated from lecithin, or for sphingomyelin, plasmalogen, and inositol phosphatide. The latter three components comprise only about 1.2% of the phospholipid fraction and were ignored in deriving the conversion factor.

GLC analysis of the fatty acids in the major lipid fractions—i.e., triglyceride, lecithin, and cephalin—shows that average molecular weights of these fatty acids correspond to acids of carbon chain lengths of 17, 17, and 18 carbons, respectively. Fatty acids of the aforementioned chain lengths would contribute 95.6, 70.8, and 75.6% of the weight of the respective fractions. The last column in Table I gives the grams of fatty acids in 1 gram of egg lipid which were contributed by the respective lipid fractions. The sum of the last column is the total grams of fatty acids in 1 gram of egg lipid; this figure, 0.83, is the conversion factor. The remainder of the lipid consists of glycerol, phosphate, choline, ethanolamine, and sterols.

TABLE III

Derivation of Conversion Factor (F) for the Lipid from Beef, Separable Lean

Lipid fraction	Wt % of total lipid	g Fatty acid/ g lipid fraction	g Fatty acid/ g total lipid
Triglyceride	87	0.956	0.832
Phosphatidyl ethanolamine	3.8	0.750	0.029
Phosphatidyl choline	7.1	0.719	0.051
Phosphatidyl serine	0.6	0.718	0.004
Sphingomyelin	0.5	0.717	0.004

F = (.87 x .956) + (.038 x .750) + (.071 x .719) + (.006 x .718) + (.005 x .717)
F = 0.832 + 0.029 + 0.051 + 0.004 + 0.004
F = 0.92

Egg

The derivation of a conversion factor for egg lipid is outlined in Table I (4). Compositional studies published since 1960 indicate that the average lipid content of egg yolk is 33.5%. Triglyceride content of the lipid varies from 62.0 to 68.6% with a mean value of 65.3%. Phospholipid content ranges from 25.6 to 33.2% with a mean of 29.9%. Of the major phospholipid components, lecithin content ranges from 22.4 to 25.5% with a mean of 24.0%; cephalin ranges from 4.7 to 6.7% with a mean of 5.6%. Few of the reports examined presented quantitative data for the

Application of the conversion factor is demonstrated in Table II. The calculations shown here are generally applicable to most foods and have been incorporated into a computer program for routine calculations. Three items of information are needed to perform the calculations: total lipid = 33.5%; the factor = 0.83; and the methyl ester composition (first line of Table II). The factor, 0.83, is applied directly to these data to convert weight percent fatty acid methyl esters to grams of each fatty acid per 100 g lipid. The data are then multiplied by the lipid content of the food item as a decimal to express results as grams per 100 g food.

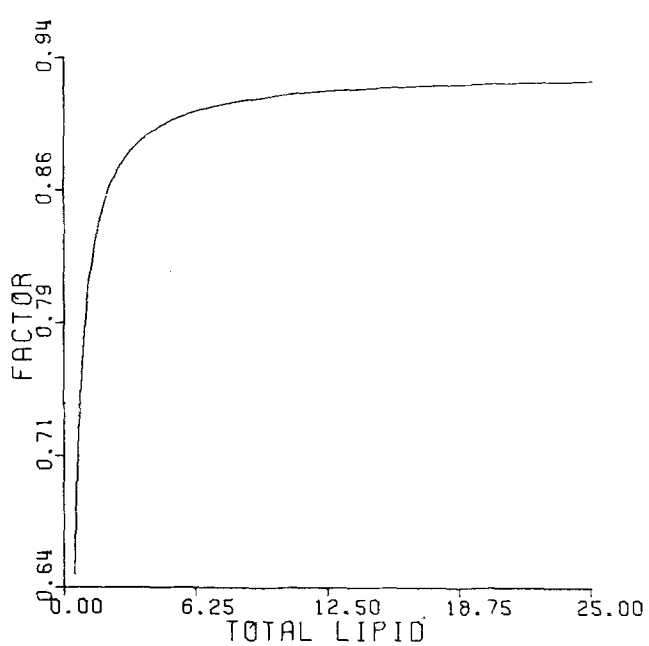

FIG. 1. Change of fatty acid factor with change in total lipid content of finfish.

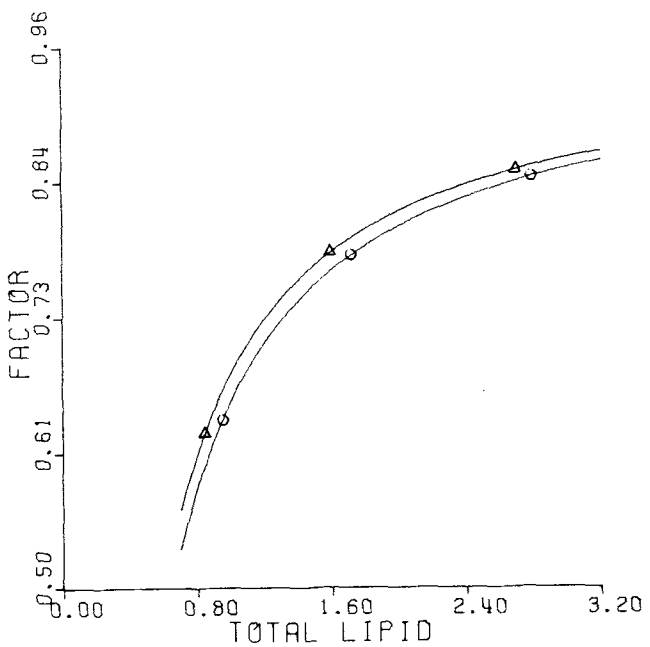

FIG. 2. Change of fatty acid factor with change in total lipid content of mollusks (○) and crustaceans (△).

TABLE IV

Derivation of a Wheat Flour Fatty Acid Conversion Factor

Lipid class	Wt. % of[a] total lipid	Average molecular weight	Average[a] molecular weight per fatty acid moiety	No. of fatty acid moieties	Contribution of fatty acids to average molecular weight	g Fatty acid/ g lipid class	Weight (g) of fatty acids derivable from 100 g lipid
Nonpolar Lipids							
Steryl ester	7.5	658	261	1	261	0.397	2.975
Triglyceride	20.8	866	276	3	828	0.956	19.887
1,2-diglyceride	6.2	610	277	2	554	0.908	5.631
1,3-diglyceride	6.0	608	276	2	552	0.908	5.447
Free sterol	2.1	415	---	---	---	0	---
Free fatty acid	7.0	275	275	1	275	1.0	7.000
Monoglyceride	1.3	349	275	1	275	0.788	1.024
Total	50.9						41.964
Glycolipids[b]							
6-0 Acyl–MGDG	3.6	1022	274	3	822	0.804	2.896
6-0 Acyl steryl glucoside	1.6	822	263	1	263	0.320	0.512
MGDG	4.9	776	279	2	558	0.719	3.523
Steryl glucoside	1.8	574	---	---	---	0	---
MGMG	0.4	549	277	1	277	0.505	0.202
DGDG	13.5	934	277	2	554	0.593	8.001
Cerimade diglycoside	0.03	---	---	---	---	0	---
DGMG	0.6	675	277	1	277	0.410	0.246
Total	26.4					0.583	15.380
Phospholipids							
N-Acyl phosphatidyl ethanolamine	4.9	998	279	3	837	0.839	4.110
N-Acyl lyso phosphatidyl ethanolamine	2.9	735	278	2	556	0.756	2.194
Phosphatidyl ethanolamine	0.8	727	274	2	548	0.754	0.603
Phosphatidyl choline	5.8	772	275	2	550	0.712	4.132
Lyso phosphatidyl ethanolamine	0.9	469	272	1	272	0.580	0.522
Lyso phosphatidyl choline	7.1	511	271	1	271	0.530	3.765
Phosphatidyl inositol	0.1	851	276	2	552	0.649	0.065
Phosphatidyl serine	0.2	775	276	2	552	0.712	0.142
Total	22.7					0.684	15.533

$$\text{Total Conversion Factor} = \frac{41.964 + 15.380 + 15.533}{100} = 0.729 \text{ g FA/g Wheat Flour Lipid}$$

[a]Taken from Morrison et al. (16).

[b]MGDG = Monogalactosyldiglyceride, MGMG = Monogalactosylmonoglyceride, DGDG = Digalactosyldiglyceride, DGMG = Digalactosylmonoglyceride.

TABLE V

Wheat Products—Conversion Factors

Product	Factor	Lipid[a]
Starch	0.60	0.9
Flour	0.67	1.4
Whole grain	0.72	2.6
Bran	0.82	4.6
Germ	0.93	10.9
Germ oil	0.95	100.0

[a]At 14% moisture (except germ oil).

TABLE VI

Equation for Converting FAME to FA Data fro Dairy Products[a]

Wt. % FAME x F x (g Lipid/g Food) = g FA/100 g Food

F = (g FA/g FAME) x 1.005

1.005 = Ratio of 3x Mol. Wt. of FAME to Average Mol. Wt. of Lipid (Triglyceride)

[a]FAME = Fatty Acid Methyl Ester; FA = Fatty Acid.

TABLE VII

Conversion Factors for Fatty Acids of Milk Lipids[a]

Fatty acid	Conversion factor
4:0	0.867
6:0	0.897
8:0	0.916
10:0	0.929
12:0	0.939
14:0	0.947
16:0	0.953
18:0	0.958
14:1	0.946
16:1	0.953
18:1	0.958
18:2	0.957
18:3	0.957
other[b]	0.952

[a]Adapted from Posati et al. (2).

[b]Other includes 15:0 and 17:0.

Before we researched the literature only two factors had been used to calculate fatty acid contents of foods. A general factor, 0.956, was used for all foods except dairy products for which the factor was 0.945 (17). Results for egg lipids, by use of both factors, are compared in Table II; results calculated with factor 0.956 appear in the last line. Palmitic acid is overestimated by about 12%, oleic by 17%, and linoleic by about 13%.

Beef and Pork

Data from numerous analyses of beef fatty acids were statistically compared (3). Except for internal depot fat, such as kidney fat, the fatty acid profiles for separable fat of meat cuts were alike for all anatomical locations of the animal; likewise, the fatty acid profiles of separable lean were alike for the various locations in the carcass. Beef separable fat is 98% triglyceride which would provide a factor of 0.95.

The total lipid in separable lean of beef was 87% triglyceride (3). The lipid class composition and conversion factor derivation for separable lean are shown in Table III. The factor, 0.92, was used to compute the fatty acid concentration of separable lean per 100 g of lipid. From the amount of separable lean and separable fat in various cuts of beef, the fatty acid content for 100 g of these cuts can be calculated.

The method for deriving a factor for the fatty acids of pork lean was similar to that shown for beef. Pork skeletal muscle lipid contains on the average 84% triglyceride and 15% phospholipid (8). The conversion factor for the separable lean of pork was 0.91.

Finfish

When lipid class composition is given, the calculation of factors for finfish is essentially the same as that for other food groups. When specific data were not available, however, other methods had to be devised.

The total lipid of a given species of finfish may vary widely with season (18). For example, the fat content of whole Atlantic herring ranges from 3.2 g in the spring to a maximum of 20.2 g in early winter (19). We therefore sought a means of relating lipid conversion factors to varying lipid levels.

We suspected that phospholipids (PL) increased with total lipid (TL), but the data on phospholipids were not sufficient for meaningful statistical analysis. However, statistical examination of triglyceride (TG) versus total lipid (TL) values indicated a linear relationship between the two. Equations are shown below with values for total lipid and lipid classes given as weight percent.

$$TG = (0.904 \times TL) - 0.453 \quad (I)$$

Assuming nonsaponifiables (NS) were a constant at 0.05% and substituting different values for total lipid into the equation

$$PL = TL - TG - NS \quad (II)$$

it was confirmed that phospholipids did increase slightly as total lipid increased.

An equation relating factors to total lipid was then derived

$$Factor = 0.933 - 0.143/TL \quad (III)$$

and values for factors for different lipid levels were calculated and plotted on an offline digital plotter (Fig. 1). Factor values increase rapidly up to a total lipid content of ca. 5% after which values approached a limit of 0.93 which approximately equals the fatty acids of triglyceride. For classification of fish for our tables of food composition and for the Nutrient Data Bank, it was convenient to use 5% fat content as a breaking point between lean and fat fish. The graph in Figure 1 has been useful for estimating the fatty acid concentrations in the lipids of lean fish.

Shellfish

The edible portions of mollusks and crustaceans contain very small amounts of lipid with values between 0.75 and 3 g per 100 g of meat. Because total lipid was so low and data to statistically relate total lipid to triglyceride were insufficient, we assumed that nonsaponifiables were present at a constant level of about 0.125% and phospholipid at 0.65% and 0.75% in crustaceans and mollusks, respectively.

Equations relating factors and total lipid were then derived for both mollusks and crustaceans:

$$Factor\ (mollusks) = 0.956 - 0.296/TL \quad (IV)$$

$$Factor\ (crustaceans) = 0.956 - 0.273/TL \quad (V)$$

Representative values were calculated and plots are shown in Figure 2. Changes in the factor were greatest at low values of total lipid.

Wheat Flour

Wheat (products) were chosen from the plant family for discussion here because their lipids have been thoroughly investigated (20) and because the wheat lipids contain relatively high amounts of glycolipids and phospholipids. Table IV summarizes the information for calculating a wheat flour lipid factor.

The work of MacMurray and Morrison (21) served as the basis for the computations. They quantitated the lipid classes of a wheat flour sample by extracting with water saturated n-butanol and by employing a series of column and thin layer chromatographic procedures. We determined the average molecular weight of the fatty acids in each lipid class from analytical values reported by these authors. The average molecular weight of the fatty acids ranged from261 in steryl esters to 279 in monogalactosyl diglycerides and N-acyl phosphatidyl ethanolamines. The average molecular weight of total fatty acids in wheat flour is 276.

The factor for this particular flour was 0.729 g FA/g wheat flour lipid and is of the same magnitude as factors derived via saponification; e.g., Fisher et al. (22) reported a range of 0.69 to 0.76 with a mean of 0.728; Burkwall and Glass (23) found 0.67; and Inkpen and Quackenbush (24) reported 0.704.

Several wheat products and their fat content and factors were tabulated in Table V to demonstrate the difference in fatty acid content of the lipids from various parts of the wheat kernel. The factor for starch is based on a lipid class analysis by Acker (15) who reported 62% lysolecithin in starch lipid. Values for flour, whole grain, and bran are those reported by Burkwall and Glass (23). The value for germ was calculated from data reported by Moruzzi et al. (25). We assumed that refined germ oil would contain primarily triglyceride which would yield about 0.95 g fatty acids per g of oil.

Classes of lipids found in wheat flour area also present in the lipids of other grains, fruits, and vegetables. The individual factors from Table V may be used for estimating fatty acid conversion factors of other foods provided the average molecular weights of the fatty acids from lipid classes of such foods correspond closely to those from wheat flour lipids.

Milk

Compared to most fat whose fatty acids contain primarily 16 and 18 carbons, milk fat has relatively large amounts of low molecular weight fatty acids. The ratio of three times the molecular weight of fatty acids to the average molecular weight of milk triglyceride would be considerably different for the short chain acids when compared to the acids containing 16 and 18 carbons. Therefore, a different factor was derived for each acid.

The general formula for converting methyl esters to grams fatty acids per 100 g of food is applicable. Factors F were derived as indicated in Table VI. A constant 1.005 converts 100 g methyl esters to 100 g triglycerides. Corresponding constants for ethyl and butyl esters are 1.058 and 1.165 respectively.

The factors for individual acids are presented in Table VII. They range from 0.867 for butyric to 0.958 for stearic and oleic acids. If a single factor were applied to the data—for example, 0.945, which is generally accepted as the average weight percent of fatty acids in milk fat expressed as a decimal—the calculated values for butyric acid would be overestimated by about 9%, and smaller errors would be introduced into the other figures.

ACKNOWLEDGMENTS

This study was conducted with financial assistance received under Interagency Reimbursable Agreement No. 2Y01 HV 40019-01 with the National Heart and Lung Institute, National Institutes of Health, Bethesda, MD 20014. Brucy Gray and Philip Washburn assisted with the statistical analyses and computer programming.

REFERENCES

1. Kinsella, J.E., L.P. Posati, J.L. Weihrauch, and B.A. Anderson, Crit. Rev. Food Technol. 5:299 (1975).
2. Posati, L.P., J.E. Kinsella, and B.K. Watt, J. Amer. Diet. Ass. 66:482 (1975).
3. Anderson, B.A., J.E. Kinsella, and B.K. Watt, Ibid. 67:35 (1975).
4. Posati, L.P., J.E. Kinsella, and B.K. Watt, Ibid. 67:111 (1975).
5. Fristrom, G.A., B.C. Stewart, J.L. Weihrauch, and L.P. Posati, Ibid. 67:351 (1975).
6. Brignoli, C.A., J.E. Kinsella, and J.L. Weihrauch, Ibid. 68:224 (1976).
7. Weihrauch, J.L., J.E. Kinsella, and B.K. Watt, Ibid. 68:335 (1976).
8. Anderson, B.A., Ibid. 69:44 (1976).
9. Exler, J., and Weihrauch, J.L., Ibid. 69:243 (1976).
10. Murphy, E.W., B.K. Watt, and R.L. Rizek, JAOAC 57:1198 (1974).
11. Butrum, R., and S.E. Gebhardt, JAOCS 53:727A (1976).
12. Jensen, R.G., J.G. Quinn, D.L. Carpenter, and J. Sampugna, J. Dairy Sci. 50:119 (1967).
13. Federal Register 38:6961, March 14, 1973.
14. Folch, J., M. Lees, and G.H. Sloane-Stanley, J. Biol. Chem. 226:497 (1957).
15. Acker, L., Getreide Mehl und Brot 28:181 (1974).
16. Morrison, W.R., D.L. Mann, W. Soon, and A.M. Conventry, J. Sci. Food Agr. 26:507 (1975).
17. Willard, C., R.D. Englert, and L.M. Richards, JAOCS 31:131 (1954).
18. Exler, J., J.E. Kinsella, and B.K. Watt, JAOCS 52:154 (1975).
19. Stoddard, J.H., Fisheries Research Board of Canada Technical Report No. 79 (1968).
20. Mecham, D.K., in "Wheat Chemistry and Technology," Edited by Y. Pomeranz, Monograph Series III (Revised), Amer. Assn. Cereal Chem., St. Paul, MN, 1971, p. 393.
21. MacMurray, T.A., and W.R. Morrison, J. Sci. Food Agr. 21:520 (1970).
22. Fisher, N., B.M. Bell, C.E.B. Rawlings, and R. Bennet, Ibid. 17:370 (1966).
23. Burkwall, M.P., Jr., and R.L. Glass, Cereal Chem. 42:236 (1965).
24. Inkpen, J.A., and F.W. Quackenbush, Ibid. 46:580 (1969).
25. Moruzzi, G., R. Viviani, A.M. Sechi, and G. Lenaz, J. Food Sci. 34:581 (1969).

[Received August 2, 1976]