# Information on the Composition of Fats from Their High-Resolution $^{13}C$ Nuclear Magnetic Resonance Spectra

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**Based on the interpretation of the high-resolution $^{13}C$ nuclear magnetic resonance spectra of 15 spreading fats, baking fats, vegetable creams and an infant formula, it is possible to decide whether the sample contains butterfat, lauric oils, partially hydrogenated fat, linoleic acid or linolenic acid. The data have been interpreted in a semi-quantitative manner, and this provides an insight into the nature of the material present in each sample.**

KEY WORDS: Baking fats, butterfat, hydrogenated fat, infant formula, lauric oils, linoleic acid, linolenic acid, spreading fats, vegetable creams.

We have examined the high-resolution $^{13}C$ nuclear magnetic resonance (NMR) spectra of butter, two vegetable creams, four baking fats, seven spreading fats and one infant formula. Each spectrum, collected in 20–40 min of instrument time, showed 30–70 signals. This number can be increased by resolution enhancement of the spectrum or by collecting it over a longer period of time, but we only found this to be necessary in one case. We have assigned most of the signals—completely or partially—and have thereby obtained useful information on the nature of the fats.

The more important signals are listed in Tables 1 and 2, from which we have excluded the glycerol carbon signals (68.9 and 62.1 ppm) and the methylene envelope (29.1–29.8 ppm). The glycerol signals show that in most samples triacylglycerols are the only components. In a few products 1,3-diacylglycerols are present as a minor component. We discuss first the general significance of each group of signals and then indicate the conclusion for each type of fat examined.

## MATERIALS AND METHODS

Samples were purchased in local shops. They will not be named specifically, but they include one sample of butter (sample number 1), a single (sample 4) and a whipping vegetable cream (sample 5), one infant formula (sample 15), four baking fats (samples 6, 7, 9, 14) and seven spreading fats (samples 2, 3, 8, 10–13).

Anhydrous fat was recovered from most of the samples by extraction with diethyl ether. This method was suitable even with reduced fat spreads. The Roese-Gottlieb extraction procedure was employed (1) for the two vegetable creams.

The spectra were measured in $CDCl_3$ solution with a Brucker AM 300 spectrometer (Burlington, Ontario, Canada). The pulse angle was $51^0$, the pulse repetition time 1.82 s and resolution was 1.22 Hz per data point. Chemical shifts are related to the signal for tetramethylsilane (= 0).

## RESULTS AND DISCUSSION

*C1–C3 carbon atoms.* Most samples had two signals at about 173.2 and 172.8 ppm (difference 0.40–0.43) corresponding to the C1 (acyl) carbon atoms in the $\alpha$ and $\beta$ chains of triacylglycerols, respectively. In sample 9 the $\alpha$ signal split into two (173.28 and 173.24 ppm) for saturated and unsaturated acyl chains. This would probably have been apparent with other samples on resolution enhancement. A signal at 173.02–173.06, apparent only in samples 1, 3 and 4, relates to the presence of butanoic acid in an $\alpha$-chain. Lie Ken Jie *et al.* (2) give values of 173.14 and 172.74 ppm for the $\alpha$- and $\beta$-chains of glycerol tributanoate.

The major C2 signals at 34.2 and 34.05 (difference 0.16–0.17 ppm), corresponding to the $\beta$- and $\alpha$-chains, respectively, are sometimes accompanied by signals at 35.91–35.94 (samples 1–5) and at 34.74, 34.45 and 33.87 ppm (each signal only appears once). The signal at 35.9 ppm belongs to butanoic acid in the $\alpha$-chain. Lie Ken Jie *et al.* (2) give values of 35.94 and 36.09 for glycerol tributanoate.

The major C3 signal at 24.87–24.90 ppm sometimes splits into two (difference 0.02) for the $\alpha$- and $\beta$-chains. Four of the first five samples also have a signal at 24.55–24.57, which arises from the presence of hexanoate esters. Lie Ken Jie *et al.* (2) give values of 24.56 and 24.59 for the C3 signals of glycerol trihexanoate. Sample 14 shows four minor peaks between 24.34 and 24.54 ppm. These signals, associated with butanoic (C1 and C2) and hexanoic esters (C3), will be used later in the discussion to indicate the presence of butterfat.

*$\omega$1–$\omega$3 carbon atoms.* Except for short chains, the $\omega$1–$\omega$3 signals are not affected by being in $\alpha$- or $\beta$-chains. However, these shifts are affected by the ester group in acyl chains of short and medium chainlength and by the presence of nearby double bonds. It is not easy to distinguish n-9 from saturated chains, but n-6 and n-3 unsaturated systems give distinct $\omega$1–$\omega$3 signals. Some of these also vary with the *cis* or *trans* configuration of the double bond (3 and Gunstone, unpublished data).

Seven different $\omega$1 signals were apparent in this series of fats. Two (14.03 and 13.98 ppm) have not been assigned. The remainder were allocated as: 14.29 (n-3), 14.12 (n-9 and saturated), 14.09 (n-6), 13.90 ($C_6$) and 13.63 ppm ($C_4$). The signals at 14.12 and 14.09 were not always completely resolved. The five $\omega$2 signals were completely assigned. Typical chemical shifts were 22.72 (n-6), 22.61 (n-9 and saturated), 22.32 ($C_6$), 20.58 (n-3) and 18.37 ($C_4$). The six $\omega$3 signals were assigned as: 31.96 (n-9 and saturated), 31.83 (n-7), 31.70 ($C_8$), 31.57 (n-6, *cis*), 31.44 (n-6, *trans*) and 31.28 ppm ($C_6$). The $\omega$3 carbon atom in n-3 acids is olefinic and is discussed along with other olefinic signals.

*Allylic signals.* The most important allylic signals in these spectra are at 32.6, 27.2 and 25.6 ppm. The first of these (32.63–32.64) comes from $CH_2$ groups adjacent to a *trans* double bond. The signal at 27.2 ppm, related to $CH_2$ groups $\alpha$ to a *cis* double bond, sometimes appears as two signals (difference 0.04 ppm) because the two allylic carbon atoms, *e.g.,* C8 and C11 in oleic esters, are not identical. This is more likely when oleate is the predominant unsaturated acyl chain. The signal at 25.6 ppm comes

**TABLE 1**

**$^{13}C$ Nuclear Magnetic Resonance Signals: Chemical Shift (ppm) and Intensity**

| Sample no. | | 1 | | 2 | | 3 | | 4 | | 5 | | 6 | | 7 | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C1 | $\alpha$ | 173.26 | 3.04 | 173.17 | 4.29 | 173.21 | 3.28 | 173.23 | 4.28 | 173.21 | 4.64 | 173.20 | 3.93 | 173.22 | 3.98 |
| | $C_4$ | 173.06 | 0.57 | — | | 173.02 | 0.39 | 173.03 | 0.18 | — | | — | | — | |
| | $\beta$ | 172.85 | 1.84 | 172.77 | 2.28 | 172.79 | 1.79 | 172.83 | 1.79 | 172.81 | 2.48 | 172.79 | 2.41 | 172.80 | 2.56 |
| C2 | $C_4$ | 35.91 | 1.51 | 35.92 | 0.29 | 35.92 | 0.70 | 35.94 | 0.52 | 35.94 | 0.29 | — | | — | |
| | — | — | | — | | — | | 34.45 | 0.19 | — | | — | | — | |
| | $\beta$ | 34.22 | 3.90 | 34.21 | 4.79 | 34.21 | 4.03 | 34.24 | 5.01 | 34.24 | 5.98 | 34.20 | 4.88 | 34.21 | 5.33 |
| | $\alpha$ | 34.05 | 5.73 | 34.04 | 9.12 | 34.05 | 7.28 | 34.08 | 9.71 | 34.07 | 11.11 | 34.04 | 8.63 | 34.04 | 8.87 |
| | — | — | | — | | — | | 33.87 | 0.21 | — | | — | | — | |
| | | | | | | | | | | | | 24.89 | 11.18 | 24.89 | 12.06 |
| C3 | $\alpha\beta$ | 24.88 | 7.25 | 24.88 | 11.74 | 24.89 | 9.93 | 24.91 | 12.55 | 24.90 | 12.87 | 24.87 | 10.86 | 24.87 | 11.75 |
| | $C_6$ | 24.55 | 0.81 | — | | 24.56 | 0.33 | 24.57 | 0.33 | 24.57 | 0.28 | — | | — | |
| $\omega1$ | n-3 | — | | — | | 14.29 | 0.42 | 14.29[a] | 0.35 | — | | — | | — | |
| | n-9 | 14.14 | 8.51 | 14.12 | 13.63 | 14.13 | 10.72 | 14.13 | 11.76 | 14.12 | 12.42 | 14.12 | 8.48 | 14.13 | 8.89 |
| | n-6 | — | | — | | — | | — | | — | | 14.09 | 7.69 | 14.09 | 9.03 |
| | — | 14.03 | 0.35 | — | | — | | — | | — | | — | | — | |
| | — | — | | 13.98 | 0.47 | 13.96 | 0.28 | — | | — | | — | | — | |
| | $C_6$ | 13.91 | 0.71 | 13.90 | 0.30 | 13.90 | 0.30 | 13.90 | 0.21 | — | | — | | — | |
| | $C_4$ | 13.63 | 1.26 | 13.62 | 0.32 | 13.63 | 0.58 | 13.64 | 0.39 | 13.62 | 0.33 | — | | — | |
| $\omega2$ | n-6 | 22.72 | 9.17 | 22.72 | 12.46 | 22.72 | 10.93 | 22.73 | 13.75 | 22.71 | 13.50 | 22.71 | 8.33 | 22.71 | 8.19 |
| | n-9,S | — | | 22.61 | 1.34 | 22.61 | 1.69 | 22.62 | 1.32 | 22.63 | 1.86 | 22.60 | 7.90 | 22.60 | 8.26 |
| | $C_6$ | 22.32 | 0.73 | — | | 22.32 | 0.35 | 22.33 | 0.22 | 22.32 | 0.26 | — | | — | |
| | n-3 | — | | — | | 20.58 | 0.34 | — | | — | | — | | — | |
| | $C_4$ | 18.36 | 1.50 | 18.36 | 0.31 | 18.37 | 0.64 | 18.38 | 0.34 | 18.37 | 0.30 | — | | — | |
| $\omega3$ | n-9,S | 31.96 | 8.34 | 31.95 | 11.90 | 31.95 | 9.04 | 31.96 | 12.18 | 31.96 | 13.22 | 31.94 | 6.29 | 31.95 | 6.41 |
| | n-7 | 31.79 | 0.65 | 31.81 | 1.21 | 31.81 | 0.73 | 31.83 | 0.51 | — | | — | | — | |
| | $C_8$ | 31.69 | 0.41 | — | | — | | 31.70 | 0.81 | 31.69 | 1.46 | — | | — | |
| | n-6*c* | — | | 31.56 | 1.09 | 31.56 | 1.50 | 31.57 | 0.86 | — | | 31.55 | 6.72 | 31.55 | 8.47 |
| | n-6*t* | — | | 31.44 | 0.45 | — | | — | | — | | — | | — | |
| | $C_6$ | 31.26 | 0.67 | — | | 31.28 | 0.33 | 31.28 | 0.36 | 31.28 | 0.37 | — | | — | |

| Sample no. | | 8 | | 9 | | 10 | | 11 | | 12 | | 13 | | 14[b] | | 15 | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C1 | $\alpha$ | 173.21 | 4.88 | 173.28 | 2.93 | 173.24 | 4.50 | 173.21 | 3.44 | 173.26 | 3.03 | 173.23 | 3.19 | 173.27 | 2.84 | 173.23 | 3.73 |
| | $C_4$ | — | | 173.24 | 4.20 | — | | — | | — | | — | | 173.10 | 0.19 | — | |
| | $\beta$ | 172.80 | 3.12 | 172.83 | 2.89 | 172.83 | 3.05 | 172.80 | 2.11 | 172.83 | 1.83 | 172.81 | 1.33 | 172.86 | 1.24 | 172.80 | 2.05 |
| C2 | $C_4$ | — | | — | | — | | — | | — | | — | | — | | — | |
| | — | — | | — | | — | | — | | — | | — | | 34.74 | 0.31 | — | |
| | $\beta$ | 34.20 | 5.93 | 34.20 | 5.56 | 34.20 | 5.74 | 34.21 | 4.57 | 34.21 | 4.13 | 34.20 | 3.07 | 34.21 | 2.64 | 34.21 | 4.70 |
| | $\alpha$ | 34.04 | 10.74 | 34.03 | 9.44 | 34.03 | 10.21 | 34.05 | 8.16 | 34.05 | 7.17 | 34.04 | 7.00 | 34.05 | 6.12 | 34.06 | 8.89 |
| | — | — | | — | | — | | — | | — | | — | | — | | — | |
| | | 24.89 | 12.50 | | | | | | | | | | | | | | |
| C3 | $\alpha\beta$ | 24.87 | 13.06 | 24.87 | 11.26 | 24.87 | 11.77 | 24.89 | 10.56 | 24.89 | 9.87 | 24.87 | 8.92 | 24.88[b] | 7.68 | 24.89 | 12.48 |
| | $C_6$ | — | | — | | — | | — | | — | | — | | — | | — | |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ω1 | n-3 | — | — | — | | 14.30 | 0.44 | 14.30 | 0.36 | 14.30 | 0.42 | — | | 14.28 | 0.34 |
| | n-9,S | 14.13 | 9.72 | 14.14 | 8.73 | 14.15 | 9.61 | 14.13 | 11.74 | 14.14 | 11.10 | 14.14 | 10.26 | 14.15[e] | 8.26 | 14.12 | 12.56 |
| | | 14.09 | 9.71 | 14.11 | 9.15 | 14.11 | 9.65 | — | | — | | — | | — | | — | |
| | — | — | | — | | — | | — | | — | | 14.02 | 0.52 | 14.03 | 0.68 | — | |
| | — | — | | — | | — | | — | | — | | — | | 14.00 | 0.54 | — | |
| | $C_6$ | — | | — | | — | | — | | — | | — | | — | | — | |
| | $C_4$ | — | | — | | — | | — | | — | | — | | 13.67 | 0.34 | — | |
| ω2 | n-6 | 22.71 | 9.29 | 22.71 | 8.15 | 22.72 | 8.87 | 22.72 | 11.42 | 22.71 | 10.42 | 22.71 | 9.66 | 22.72[f] | 8.22 | 22.71 | 14.00 |
| | n-9,S | 22.60 | 9.06 | 22.60 | 8.19 | 22.60 | 7.82 | 22.61 | 2.12 | 22.60 | 1.67 | 22.60 | 2.00 | 22.60 | 1.00 | 22.60 | 2.02 |
| | $C_6$ | — | | — | | — | | — | | — | | 22.21 | 0.26 | 22.21 | 0.31 | — | |
| | n-3 | — | | — | | — | | — | | 20.57 | 0.27 | 20.56 | 0.25 | 20.53 | 0.19 | — | |
| | $C_4$ | — | | — | | — | | — | | — | | — | | — | | — | |
| ω3 | bp9,S | 31.94 | 7.21 | 31.94 | 6.62 | 31.94 | 7.37 | 31.95 | 9.90 | 31.95 | 8.66 | 31.94 | 7.96 | 31.95 | 6.96 | 31.95 | 12.12 |
| | n-7 | — | | 31.78 | 0.48 | — | | 31.83 | 0.67 | 31.79 | 0.62 | 31.81 | 1.02 | 31.81[h] | 1.08 | 31.82 | 0.53 |
| | $C_8$ | — | | — | | — | | — | | — | | — | | — | | 31.69 | 0.79 |
| | n-6*c* | 31.55 | 8.81 | 31.54 | 8.62 | 31.54 | 8.44 | 31.56 | 1.89 | 31.56 | 1.62 | 31.54 | 1.83 | 31.55 | 0.66 | 31.56 | 1.81 |
| | n-6*t* | — | | — | | — | | 31.44 | 0.26 | — | | 31.43 | 0.39 | 31.43 | 0.39 | — | |
| | $C_6$ | — | | — | | — | | — | | —[g] | | — | | — | | — | |

[a]This sample differs from the others in several respects, and assignments in the left-hand column may not apply to the signals of lower intensity in column 14.
[b]24.54 0.21, 24.48 0.21, 24.38 0.22, 24.35 0.25. Abbreviations: *c, cis; t, trans;* S, saturated.
[c]14.35 0.18.
[d]14.41 0.24.
[e]22.91 0.22.
[f]30.91 0.34.
[g]31.85 0.92.

from allylic groups between two *cis* double bonds, *e.g.*, C11 in linoleate and linolenate (25.65) and C14 in linolenate (25.55). Allylic signals at 35.6 (between two *trans* double bonds) and 30.3–30.4 (between one *cis* and one *trans* double bond) were not observed in these spectra.

*Olefinic signals.* The olefinic signals are the most complex group of signals in these spectra (2–17 signals), but they provide valuable information. In the tables they are presented in two groups. The first group contains two, five or ten signals, corresponding to oleate, oleate and linoleate, and oleate, linoleate and linolenate, respectively. The intensities of these signals indicate the relative proportions of these three natural acids present in each sample. The second group are signals corresponding to *trans* 18:1 isomers (8*t*–11*t*), such as are expected in hydrogenated fats (Gunstone, unpublished data). The 11*c* isomer may be of natural origin or a product of partial hydrogenation. Conclusions derived from the olefinic signals should be confirmed, at least in part, by those obtained from the allylic signals.

*Butter (sample 1).* Butterfat contains several signals that distinguish it from the other fats and which can be used to identify its presence in other fats. In particular, it is easy to identify butanoate (by the four signals for C1, C2, ω1 and ω2 carbon chains), hexanoate (by the four signals for C3, ω1, ω2 and ω3 carbon chains) and octanoate ester (by the signal for the ω3 carbon atom). The intensity values for these several signals indicate the presence of these three acids at levels of 13, 6 and 3% (mole basis) in this sample of butterfat.

The olefinic signals show the presence of oleate and *trans*-vaccenate. Linoleate was not indicated from the olefinic signals, but a small allylic signal at 25.63 ppm suggests that this acid may be present.

*Spreading fats containing butter (samples 2 and 3).* Of the seven spreading fats we examined, two (samples 2 and 3) clearly contained butterfat. From the $^{13}C$ spectra of these two samples we noted the following: (i) Both samples contain butterfat. This is indicated by signals for $C_4$ and $C_6$ acids as discussed in the previous section. The two samples contained approximately 15 and 30% of butterfat, respectively. (ii) Olefinic and allylic signals show the presence of partially hydrogenated fat, with sample 2 containing the higher level. (iii) Sample 2 contains oleic and linoleic acids in a ratio of about 16:1, but sample 3 also contains linolenic acid (ratio about 10:3:1).

These two fats differ from the other spreading fats we examined in that they contain butterfat, but they differ from one another in the amount. Both contain hydrogenated fat, sample 2 is derived from oils not containing linolenic acid (probably sunflower), whereas sample 3 incorporates a linolenic acid containing oil (such as soybean or rapeseed). Further consideration of the olefinic signals indicates that less hydrogenated fat is present in sample 3.

*Vegetable creams (samples 4 and 5).* The whipping cream (sample 5) gives a simpler set of olefinic and allylic signals. They suggest that oleic acid at a low level is the only olefinic acid present, though the small allylic signal at 32.63 ppm indicates some *trans* unsaturation. The ω3 signals show the presence of $C_8$ and $C_6$ acyl chains, and the ω1, ω2, C1 and C2 signals indicate a $C_4$ chain. We conclude that this cream contains some butterfat and a fully hydrogenated lauric oil.

**TABLE 2**

**$^{13}C$ Nuclear Magnetic Resonance Signals: Chemical Shift (ppm) and Intensity[a]**

| Sample no. | 1 | | 2 | | 3 | | 4 | | 5 | | 6 | | 7 | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Allylic | | | | | | | | | | | | | | |
| *t* | 32.64 | 1.04 | 32.64 | 4.52 | 32.64 | 2.05 | 32.64 | 0.69 | 32.63 | 0.49 | 32.63 | 1.63 | 32.63 | 1.92 |
| — | — | | — | | — | | 32.56 | 0.21 | — | | — | | — | |
| — | — | | 32.30 | 0.35 | — | | — | | — | | — | | — | |
| — | — | | 32.18 | 0.29 | — | | — | | — | | — | | — | |
| *c* | 27.24 | 2.44 | 27.24 | 10.36 | 27.25 | 8.39 | 27.25 | 4.83 | 27.25 | 1.56 | 27.22 | 17.40 | 27.22 | 20.42 |
| *c* | 27.19 | 2.32 | 27.20 | 9.88 | 27.21 | 7.73 | — | | 27.21 | 1.36 | — | | — | |
| *cc* | 25.63 | 0.33 | 25.65 | 0.62 | 25.65 | 1.97 | 25.67 | 1.13 | — | | 25.65 | 8.62 | 25.65 | 10.11 |
| *cc* | — | | —[d] | | 25.56 | 0.63[e] | 25.57 | 0.28 | — | | — | | — | |
| Olefinic (oleic, linoleic, α-linolenic) | | | | | | | | | | | | | | |
| Ln | — | | — | | 131.92 | 0.36 | 131.94 | 0.19 | — | | — | | — | |
| L, Ln | — | | 130.17 | 1.31 | 130.19 | 1.87 | 130.21 | 1.03 | — | | 130.20 | 7.23 | 130.21 | 8.81 |
| O L | 130.00 | 1.69 | 130.00 | 7.16 | 130.00 | 5.25 | 130.02 | 3.13 | 130.01 | 0.98 | 129.99 | 7.03 | 130.00 | 8.44 |
| O | 129.70 | 1.43 | 129.69 | 6.38 | 129.70 | 4.49 | 129.72 | 2.40 | 129.70 | 0.90 | 129.70 | 2.87 | 129.71 | 2.99 |
| Ln | — | | — | | 128.29 | 0.48 | 128.30 | 0.24 | — | | — | | — | |
| Ln | — | | — | | 128.24 | 0.48 | 128.25 | 0.21 | — | | — | | — | |
| L | — | | 128.09 | 0.42 | 128.09 | 1.18 | 128.11 | 0.74 | — | | 128.08 | 6.49 | 128.09 | 7.55 |
| L | — | | 127.91 | 0.45 | 127.91 | 1.14 | 127.93 | 0.72 | — | | 127.91 | 6.80 | 127.91 | 8.01 |
| Ln | — | | — | | 127.78 | 0.51 | 127.80 | 0.18 | — | | — | | — | |
| Ln | — | | — | | 127.13 | 0.26 | 127.15 | 0.18 | — | | — | | — | |
| Olefinic (other) | | | | | | | | | | | | | | |
| 8*t* | — | | 130.58 | 0.48 | 130.58 | 0.23 | — | | — | | — | | — | |
| 9*t* | — | | 130.47 | 0.77 | 130.48 | 0.40 | — | | — | | — | | 130.49 | 0.59 |
| 10*t* | — | | 130.42 | 1.03 | — | | — | | — | | — | | — | |
| 11*t* | 130.39 | 0.38 | 130.39 | 1.01 | 130.39 | 0.44 | — | | — | | — | | — | |
| 11*t* | 130.29 | 0.40 | 130.29 | 1.11 | 130.29 | 0.46 | — | | — | | — | | — | |
| 10*t* | — | | 130.23 | 1.04 | — | | — | | — | | — | | — | |
| — | — | | 129.91 | 1.61 | — | | — | | — | | — | | — | |
| 11*c* | — | | 129.82 | 1.40 | 129.82 | 0.67 | 129.84 | 0.37 | — | | — | | 129.83 | 0.63 |

| Sample no. | 8 | | 9 | | 10 | | 11 | | 12 | | 13 | | 14 | | 15 | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Allylic | | | | | | | | | | | | | | | | |
| *t* | 32.63 | 1.91 | 32.64 | 2.18 | 32.64 | 2.40 | 32.64 | 3.28 | 32.64 | 2.96 | 32.63 | 3.53 | 32.64 | 3.75 | — | |
| — | — | | — | | — | | — | | — | | —[b] | | —[c] | | — | |
| — | — | | — | | — | | — | | — | | 32.31 | 0.36 | 32.31 | 0.41 | — | |
| — | — | | — | | — | | — | | — | | 32.18 | 0.54 | 32.19 | 0.59 | — | |
| *c* | 27.22 | 21.89 | 27.21 | 19.90 | 27.21 | 20.60 | 27.25 | 10.56 | 27.24 | 8.86 | 27.22 | 8.17 | 27.23 | 4.51 | 27.25 | 9.94 |
| *c* | — | | — | | — | | 27.21 | 9.72 | — | | — | | 27.20 | 3.79 | 27.21 | 9.38 |
| *cc* | 25.65 | 10.53 | 25.64[f] | 10.00 | 25.64 | 10.03 | 25.66 | 2.21 | 25.65 | 1.96 | 25.63 | 2.16 | 25.63 | 0.75 | 25.66 | 1.93 |
| *cc* | — | | | | — | | 25.56 | 0.47 | 25.55 | 0.41 | 25.54 | 0.42 | — | | 25.56 | 0.29 |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Olefinic (oleic, linoleic, α-linolenic) | | | | | | | | | | | | | | | | | | |
| Ln | — | | — | | — | | 131.93 | 0.27 | 131.94 | 0.34 | 131.92 | 0.33 | | | | | — | |
| L, Ln | 130.19 | 9.78 | 130.21 | 8.67 | 130.21 | 8.96 | 130.19 | 2.62 | 130.20 | 2.24 | 130.18 | 2.29 | 130.21 | 0.96 | 130.20 | 1.69 | | |
| O L | 129.99 | 9.38 | 130.00 | 8.87 | 130.00 | 9.87 | 130.01 | 6.18 | 130.01 | 5.67 | 129.99 | 3.81 | 130.00 | 2.37 | 130.01 | 7.00 | | |
| O | 129.71 | 3.85 | 129.70 | 2.86 | 129.70 | 3.82 | 129.70 | 4.98 | 129.70 | 4.24 | 129.69 | 3.08 | 129.70 | 1.74 | 129.70 | 5.64 | | |
| Ln | — | | — | | — | | 128.29 | 0.38 | 128.29 | 0.42 | 128.27 | 0.44 | — | | 128.30 | 0.27 | | |
| Ln | — | | — | | — | | 128.24 | 0.47 | 128.23 | 0.45 | 128.22 | 0.36 | — | | — | | | |
| L | 128.08 | 8.40 | 128.07 | 7.46 | 128.07 | 7.54 | 128.10 | 1.68 | 128.09 | 1.46 | 128.07 | 1.41 | 128.07 | 0.41 | 128.10 | 1.51 | | |
| L | 127.91 | 8.36 | 127.89 | 7.81 | 127.89 | 7.93 | 127.91 | 1.65 | 127.90 | 1.44 | 127.89 | 1.38 | 127.89 | 0.40 | 127.91 | 1.45 | | |
| Ln | — | | — | | — | | 127.79 | 0.41 | 127.77 | 0.46 | 127.75 | 0.39 | — | | — | | | |
| Ln | — | | — | | — | | 127.14 | 0.27 | 127.12 | 0.36 | 127.10 | 0.31 | — | | — | | | |
| Olefinic (other) | | | | | | | | | | | | | | | | | | |
| 8*t* | — | | 130.58 | 0.26 | 130.58 | 0.36 | 130.58 | 0.36 | 130.58 | 0.54 | 130.56[g] | 0.47 | 130.58[h] | 0.57 | — | | | |
| 9*t* | 130.48 | 0.55 | 130.48 | 0.51 | 130.48 | 0.55 | 130.49 | 0.76 | 130.48 | 0.86 | 130.47 | 0.64 | 130.48 | 0.80 | — | | | |
| 10*t* | — | | 130.43 | 0.36 | 130.42 | 0.53 | 130.43 | 0.66 | 130.43 | 0.68 | — | | — | | | | | |
| 11*t* | — | | — | | — | | — | | — | | 130.38 | 0.91 | 130.39 | 0.85 | — | | | |
| 11*t* | — | | — | | — | | 130.30 | 0.68 | — | | 130.28 | 0.93 | 130.29 | 0.83 | — | | | |
| 10*t* | — | | — | | — | | — | | — | | — | | — | | | | | |
| — | — | | — | | — | | — | | — | | — | | 129.92 | 0.87 | — | | | |
| 11*c* | 129.82 | 0.74 | 129.83 | 0.68 | 129.83 | 0.68 | 129.82[i] | 0.89 | 129.82 | 0.72 | 129.81 | 1.40 | 129.82 | 0.88 | 129.82 | 0.51 | | |

[a]For details of samples 1–15, see Results and Discussion section. Ln, linolenic; L, linoleic; O, oleic; *c, cis*; *t, trans*. [b]32.74 0.54, 32.50 0.82, 32.39 0.37, 27.42 0.30, 26.92 0.33. [c]32.50 0.84, 32.40 0.33, 27.41 0.28, 26.93 0.28, 26.83 0.27, 26.73 0.21, 26.50 0.21. [d]27.45 0.29, 25.09 0.28. [e]25.12 0.27. [f]26.93 0.28. [g]128.27 0.44. [h]131.84 0.19, 131.05 0.20, 130.72 0.32, 129.58 0.30, 129.40 0.28, 129.34 0.30. [i]128.01 0.25.

The single cream (sample 4) differs from the whipping cream in that it contains a vegetable oil with oleic, linoleic and linolenic acids (ratio 12:4:1) with little evidence of partial hydrogenation. The presence of $C_4$, $C_6$ and $C_8$ chains indicates that the cream contains some butterfat and hydrogenated lauric oil.

*Baking fats (samples 6, 7, 9 and 14).* Sample 14 gave a spectrum that was more complex than any of the others. It probably contains partially hydrogenated fish oil and is a complex mixture. It is not discussed further.

The remaining baking fats (samples 6, 7 and 9) are similar in most respects. There is no evidence of butterfat or lauric oil; all three contain oleic and linoleic acid in a similar ratio (approximately 1:2.6), but no linolenic acid. They are clearly rich in linoleic acid and are probably based on sunflower oil. The small peaks associated with *trans*-allylic and *trans*-olefinic carbon atoms suggest that these fats contain only low levels of partially hydrogenated fat.

*Spreading fats not containing linolenic acid (samples 8 and 10).* Two of the spreading fats are similar to the baking fats just discussed. They contain oleic and linoleic acids in a ratio of about 1:2, but linolenic acid is absent. The level of hydrogenated fat is low. These fats are probably based on sunflower oil.

*Spreading fats containing linolenic acid (samples 11, 12 and 13).* These three spreading fats give more complex spectra. The olefinic signals, supported by allylic signals, show the presence of oleic, linoleic and linolenic acids in a ratio of about 11:4:1. Oleic, and not linoleic, is the dominant unsaturated acid. Olefinic and allylic signals also show the presence of *trans* acids and, therefore, presumably of partially hydrogenated fats. The presence of α-linolenic acid suggests that these samples are based on soybean or rapeseed oil.

*Infant formula (sample 15).* The fat recovered from this sample contained oleic and linoleic acid in the ratio about 3.5:1. α-Linolenic acid was also expected. This was indicated by the small ω1 signal at 14.28 ppm, but appropriate olefinic signals were not observed, even after resolution enhancement. After urea fractionation (4), however, the mother liquor showed ω1, ω2, allylic and olefinic signals appropriate for α-linolenic acid. The fat contained a lauric oil (ω3 signal for $C_8$), but there was no evidence of partially hydrogenated fat.

The high-resolution $^{13}C$ NMR spectra of domestic fats shows the presence or absence of butterfat or lauric oils on the basis of signals related to $C_4$, $C_6$ and $C_8$ chains. They also indicate the presence or absence of oleic, linoleic, linolenic acid and of partially hydrogenated vegetable oil through the olefinic, allylic and ω1–ω3 signals. The baking and spreading fats appear to fall into two groups. One group contains oleic and linoleic acids in the ratio 1:2.0–2.5, have little hydrogenated fat and are probably based on sunflower oil. The other group contains oleic, linoleic and linolenic acids in the ratio about 11:4:1, along with partially hydrogenated fat.

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