Confirmation of *trans* 18:1 Fatty Acid Isomers

Sir,

The aim of our research was to confirm the identity of *trans* 18:1 fatty acid positional isomers, and not to determine fatty acid composition.

In 1995, gas chromatography (GC) peaks for *trans* 18:1 isomers had been correctly identified by comparison with methyl or isopropyl ester standards (1,2). Because some GC peak assignments were at variance with those of two other 1995 publications (3,4), we decided to confirm the identity of *trans* 18:1 positional isomers in a mixture as 4,4-dimethyloxazoline (DMOX) derivatives by GC–mass spectrometry (MS) (5). Unlike esters, DMOX derivatives proved to be an excellent means for discriminating between fatty acid positional isomers by GC–MS (5).

Unfortunately, we did not know about the separation of the Δ13 and 14 pair of *trans* 18:1 positional isomers reported by Professor Randall Wood in a book chapter on "*Sample Preparation, Derivatization and Analysis"* (6). Professor Wood had published a GC chromatogram showing baseline resolution of these Δ13 and 14 *trans* 18:1 fatty acid methyl ester (FAME) isomers on a nonpolar SP-2100 (methyl silicone) 60 m × 0.25 mm borosilicate glass column (6). More recently, partial resolution for this pair of FAME isomers was obtained on a 100-m CP Sil 88 column (7).

We believe that GC separations of fatty acid derivatives with long retention times are not for routine analysis. Inspection of GC chromatograms observed at 140°C for methyl ester and DMOX derivatives (see Fig. 3, reference 5) clearly indicates that the Δ13 and Δ14 *trans* 18:1 DMOX positional isomers were better separated than the corresponding FAME. This resolution allowed us to obtain distinctive mass spectra for these two DMOX isomers. Also at 140°C, the Δ6 and 7 *trans* 18:1 positional isomers were separated only as DMOX derivatives (see Fig. 6, reference 5), but coeluted as FAME even at 125°C (7).

REFERENCES

1. Molkentin, J., and D. Precht, Optimized Analysis of *trans*-Octadecenoic Acids in Edible Fats, *Chromatographia 41*:267–272 (1995).
2. Wolff, R.L., and C.C. Bayard, Improvement in the Resolution of Individual *trans*-18:1 Isomers by Capillary Gas–Liquid Chromatography: Use of a 100-m CP-Sil 88 Column, *J. Am. Oil Chem. Soc. 72*: 1197–1201 (1995).
3. Precht, D., Variation of *trans* Fatty Acids in Milk Fats, *Z. Ernährungswiss. 34*:27–29 (1995).
4. Adlof, R.O., L.C. Copes, and E.A. Emken, Analysis of the Monoenoic Fatty Acid Distribution in Hydrogenated Vegetable Oils by Silver Ion HPLC, *J. Am. Oil Chem. Soc 72*:571–574 (1995).
5. Mossoba, M.M., R.E. McDonald, J.A.G. Roach, D.D. Fingerhut, M.P. Yurawecz, and N. Sehat, Spectral Confirmation of *Trans* Monounsaturated C_{18} Fatty Acid Positional, *Ibid. Chem. Soc. 74*:125–130 (1997).
6. Wood, R., *Sample Preparation, Derivatization and Analysis,* in *Analyses of Fats, Oils and Derivatives*, edited by E.G. Perkins, AOCS Press, Champaign, 1993, pp. 236–269.
7. Precht, D., and J. Molkentin, Comparison of the Fatty Acids and the Isomeric Distribution of *trans*-C18:1 Fatty Acids of Milk Fat, Margarine, Shortenings, Cooking and Dietetic Fats, *Kiel. Milchwirtsch. Forschungsber. 49*:17–34, 1997.

Magdi M. Mossoba
Martin P. Yurawecz
John A.G. Roach
Center for Food Safety and Applied Nutrition
Food and Drug Administration
Mail Stop HFS 717
200 C Street, SW
Washington, DC 20204

[Received August 14, 1997; accepted January 22, 1998]