Triticale and Wheat Flour Studies: Compositions of Fatty Acids, Carbonyls, and Hydrocarbons

Klaus Lorenz* and Joseph Maga

A comparison of the chemical composition of wheat and triticale flours demonstrated that their composition of fatty acids, carbonyl compounds, and hydrocarbons is quite similar qualitatively but differed quantitatively. The spring triticale flours contained higher percentages of stearic and linolenic acids and lower amounts of linoleic acid compared to corresponding wheat flours. The spring triticale flours were lower in butanal, 2-butanone, and heptanal, but higher in pentanal than the spring wheat flours. A higher percentage of short-chain hydrocarbons was found in spring triticale flours.

The development of triticale, a polyploid hydrid cereal produced by cross-breeding wheat and rye, has been discussed in an excellent review by Briggle (1969). Early triticale varieties had large but shrivelled seeds, resulting in poor flour yield and high protein content (MacDonald, 1968). As the grain type improved, the protein approached that of hard spring wheat. Triticales have a better balanced amino acid composition than wheat (Villegas *et al.*, 1968). Comparisons of protein nutritive value between wheat and triticale grains indicated a higher value for the triticale grains (Kies and Fox, 1970a,b).

Triticale grains have been considered as feed grains only (Pomeranz, 1971a) because of the poor baking characteristics of flours milled from triticale (Unrau and Jenkins, 1964; Rooney *et al.*, 1969). However, recently it was shown that excellent quality bread can be produced with certain varieties of triticale making only minor modifications in dough mixing procedure (Lorenz *et al.*, 1972).

The fatty acid composition of wheat and flour-milling products shows linoleic acid to be the major component (Morrison, 1963; Nelson *et al.*, 1963). The content of palmitic and oleic acid varies the most between milling fractions. While only trace amounts of odd-chain fatty acids have been reported in wheat products, higher amounts have been reported to be present in rye (Klyushkina *et al.*, 1970).

Carbonyl compounds, especially aldehydes, contribute to the flavor and taste of baked products (Wiseblatt, 1961). Headspace vapor analyses of wheat, triticale, and rye show similar carbonyl compositions differing mainly in the amounts of 2-methyl propanal and pentanal (Hougen *et al.*, 1971).

Hydrocarbons are present in wheat flour in only very small amounts (Youngs and Gilles, 1970). The distribution of hydrocarbons includes normal and isomeric hydrocarbons with a chain length between C-9 and C-33. Some of these compounds have a beneficial effect in bread baking when used in concentrations higher than those found in wheat flour, as demonstrated by Ponte *et al.* (1963) and Elton and Fisher (1968).

This investigation was undertaken to compare the chemical composition, fatty acids, carbonyl compounds, and hydrocarbons, between wheat and triticale flours grown in the same general area. These observed differences in composition might help to explain differences in baking characteristics and final product quality.

MATERIALS AND METHODS

Eight samples of grain, all grown on irrigated sites at Fort Collins and Center, Colorado, 1971, were selected for this investigation. The two winter wheats (Scout and Caprock), two spring wheats (Inia Res. and Ciano Sib.), two spring hexaploid triticales (6TA204 and 6TA206), and two winter hexaploid triticales (TR385 and TR386) were properly tempered and milled on a Brabender Quadrumat Junior mill.

Moisture and ash of the samples were determined by AOAC (1960) procedures and protein content by the Udy Protein Analyzer method (AACC, 1962).

FATTY ACID COMPOSITION

Fatty acids were extracted with a mixture of 60:40 petroleum ether–diethyl ether. The ether extracts were treated and analyzed by glc conditions as described by Lorenz and Maga (1971). Identification of individual fatty acids was made by measuring relative retention times of commercial fatty acids separated under the same glc conditions. Results were expressed as percent of total glc area. Glc area for each component was measured with a Hewlett-Packard Model 3370 B Integrator.

CARBONYL COMPOSITION

The carbonyl compounds were extracted with carbonyl-free chloroform and converted to their 2,4-dinitrophenylhydrazones. The mixtures of hydrazones were separated by glc as outlined by Lorenz and Maga (1972). To identify the carbonyl compounds, hydrazones of known carbonyl compounds were prepared, and their retention times were measured and compared with those of compounds in the unknown mixture. Results were expressed as percent of total glc area. Glc area for each component was measured with a Hewlett-Packard Model 3370 B Integrator.

HYDROCARBON COMPOSITION

The hydrocarbons were separated and analyzed by a modified procedure of Youngs and Gilles (1970). Flour lipids were extracted by shaking 10 g of flour in 100 ml of petroleum ether on a Burrell shaker for 45 min. The crude lipid extracts were concentrated by rotary vacuum evaporation at 5°C and were streaked on thick-layer plates (750 μ of Silica Gel G) and developed in carbon tetrachloride. The hydrocarbon band was scraped from the plates, eluted from the silica gel with petroleum ether–ethyl ether 1:1, and the volume of the eluant reduced to 2 ml. Five-microliter samples were injected into the glc. Resolution and identification was accomplished using a

---

Department of Food Science and Nutrition, Colorado State University, Fort Collins, Colorado 80521.

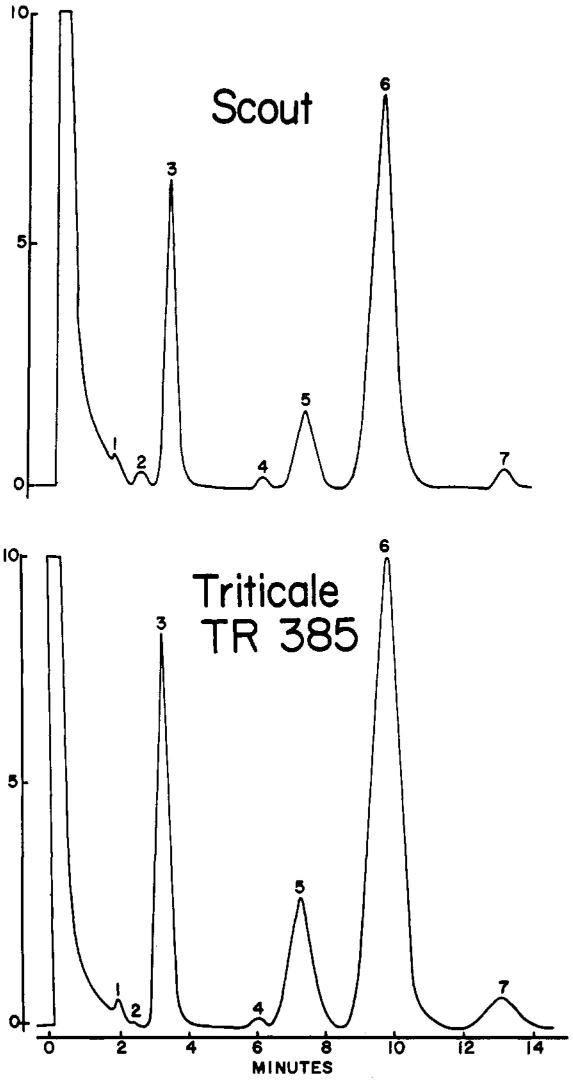

Figure 1. Typical glc fatty acid compositions of wheat and triticale flours. Peak identity: 1, myristic, 2, pentadecanoic, 3, palmitic, 4, stearic, 5, oleic, 6, linoleic, 7, linolenic

Table I. Proximate Analyses of Samples

Spring varieties		Grain protein, %[a]	Flour protein, %[a]	Flour ash, %[a]
Wheat	Inia Res.	12.7	12.4	0.46
	Ciano Sib.	13.2	12.5	0.48
Triticale	6TA204	14.6	11.3	0.53
	6TA206	14.5	11.7	0.54
Winter varieties				
Wheat	Scout	12.0	11.6	0.43
	Caprock	11.2	11.0	0.41
Triticale	TR385	12.0	8.7	0.47
	TR386	10.8	8.6	0.47

[a] On a 14% moisture basis: (N × 6.25), grain protein; (N × 5.7), flour protein.

Hewlett-Packard Model 5750 gas chromatograph equipped with a dual column flame ionization detector. The 6-ft × 1/8-in. o.d. stainless steel columns were packed with 20% SE 30 on 80–100 mesh Gas Chrom Q. The injection port was 230°C, the flame detector was 250°C, and the column temperature was programmed from 60 to 235°C at 8°C per min. The carrier gas was nitrogen with a flow rate of 73 ml/min. The sensitivity was 4×10^2 with a chart speed of 0.5 in./min. Identification of individual hydrocarbons was made by measuring relative retention times of standards separated under the same glc conditions and by comparison with retention times of hydrocarbons reported by Youngs and Gilles (1970). Results were expressed as percent of total glc area. Glc area for each component was measured with a Hewlett-Packard Model 3370 B Integrator.

RESULTS AND DISCUSSION

Analytical data of the cereal grains and of the flours milled from these grains are presented in Table I. The spring varieties, both wheat and triticale, had a higher protein content than the winter varieties. The protein content of the spring triticale grains was higher than that of the wheat samples, but the protein content of the flours of these wheat samples was higher than that of the flours milled from the triticale samples on a 14% moisture basis. The winter varieties, both wheat and triticale, had approximately the same grain protein. However, the flour protein of the triticale samples was lower than that of the wheat samples. The triticale flours had a higher ash content than the corresponding wheat flours.

Fatty Acid Composition. Fatty acid separations of wheat and triticale flours are illustrated in Figure 1. Myristic, pentadecanoic, palmitic, stearic, oleic, linoleic, and linolenic acid were identified. Arachic acid was not separated with our separation technique. The major fatty acid percentage composition of each of the wheat and triticale flours is presented in Table II. Besides the predominant fatty acids (C-14:0, C-16:0, C-18:0, C-18:1, C-18:2, C-18:3, and C-20:0), various trace amounts of short-chained and branched fatty acids have been reported in wheat flour (Pomeranz, 1971b).

Rye flour was found to contain also small amounts of unsaturated C-13, C-14, C-15, C-17 and C-20 (Klyushkina *et al.*, 1970). None of these trace fatty acids were found in either the wheat or triticale flours.

The percentage composition of the flours was quite similar except for the C-18 acids, both saturated and unsaturated. The spring triticale flours contained higher percentages of stearic and linolenic acid and slightly lower amounts of linoleic acid in comparison with the spring wheat flours. The winter triticale flours also contained slightly higher percentages of linolenic acid compared to the corresponding wheat flours. The total percentage of unsaturated fatty acids, however, was approximately the same in both the spring and winter wheat and triticale flours. The differences in fatty acid composition between triticale and wheat flours reported here are small. The percentage composition is likely to change slightly from one crop year to the other due to variations in climate, soil, and variety.

Carbonyl Composition. The carbonyl percentage composition of each of the wheat and triticale flours is presented in Table III. Wheat and triticale flours were found to have the same qualitative carbonyl composition, which agrees with the work of Hougen *et al.* (1971). However, they differ slightly quantitatively. The spring triticale flours were lower in butanal, 2-butanone, and heptanal, but higher in pentanal in comparison with their corresponding wheat flours. The winter triticale flours were lower in 2-butanone than the winter wheat flours. Since the contribution of individual carbonyl compounds to baking quality and final baked product characteristics is not completely understood, an explanation of the significance of some of the differences in carbonyl composition was not attempted.

Table II. Major Fatty Acid Composition of Wheat and Triticale Flours, % of Total glc Composition

Spring varieties		C-14	C-15	C-16	C-18	C-18:1	C-18:2	C-18:3
Wheat	Inia Res.	0.6	0.5	14.6	0.3	8.0	73.1	2.9
flours	Ciano Sib.	0.7	0.5	19.6	0.2	12.9	63.2	2.9
Triticale	6TA204	1.0	0.9	18.0	0.6	10.0	62.8	6.7
flours	6TA206	0.9	0.4	19.2	0.6	11.7	60.6	6.6
Winter varieties								
Wheat	Scout	1.4	0.4	19.8	1.2	12.4	62.5	2.3
flours	Caprock	0.9	0.4	21.9	1.2	10.1	60.7	4.8
Triticale	TR385	0.7	0.1	19.3	1.3	12.8	59.3	6.5
flours	TR386	0.8	1.1	18.2	1.1	11.5	62.3	5.0

Table III. Short Chain Carbonyl Composition of Wheat and Triticale Flours, % of Total glc Composition

Compound	Inia Res.	Ciano Sib.	6TA204	6TA206	Scout	Caprock	TR385	TR386
Acetaldehyde	5.1	9.7	6.9	16.2	5.9	9.2	7.3	15.0
Propanal	3.9	4.1	2.1	7.5	4.9	4.7	2.3	9.0
Acetone	13.4	22.5	22.4	16.0	12.5	14.4	19.8	12.0
Butanal	12.1	9.9	5.2	8.7	7.2	13.6	11.4	13.8
2-Butanone	29.7	24.8	15.6	12.7	29.0	33.7	19.4	17.0
Pentanal	13.5	9.4	32.0	23.6	9.8	15.6	5.1	15.1
2-Pentanone	5.5	5.8	10.0	3.4	12.1	1.7	6.8	6.6
Hexanal	7.8	5.6	3.8	8.0	10.8	3.8	10.3	7.6
Heptanal	9.0	8.2	2.0	3.9	7.8	3.3	17.6	3.9

Table IV. *n*-Hydrocarbon Composition of Wheat and Triticale Flours, % of Total glc Composition

Compound	Spring varieties				Winter varieties			
	Inia Res.	Ciano Sib.	6TA204	6TA206	Scout	Caprock	TR385	TR386
C-7	2.1	0.2	6.4	4.6	4.5	0.9	3.7	2.8
C-8	3.4	2.2	5.4	3.8	5.3	1.2	4.9	2.6
C-9	4.6	3.1	6.6	5.5	4.4	1.4	4.3	3.3
C-10	2.6	2.2	4.2	4.1	3.3	2.0	4.1	3.8
C-11	0.7	0.4	0.9	0.9	1.1	0.5	0.5	0.4
C-12	1.3	2.5	1.3	1.3	0.8	0.7	1.3	1.2
C-13	5.0	3.4	3.8	3.7	3.6	3.4	1.9	4.3
C-14	9.4	6.7	6.9	6.2	7.9	8.4	6.6	8.2
C-15	5.8	10.9	5.5	7.8	8.0	7.0	7.0	8.2
C-16	15.1	17.3	9.7	10.9	12.4	10.9	11.7	12.4
C-17	13.6	18.2	14.3	15.3	12.9	17.0	13.2	19.2
C-18	9.4	7.5	11.7	12.8	12.2	13.0	14.8	11.4
C-19	6.0	6.7	6.0	9.5	10.8	11.9	6.4	9.0
C-20	8.4	10.1	7.7	6.3	6.8	10.9	8.5	5.2
C-21	6.1	4.3	5.4	4.6	4.1	7.4	6.2	6.1
C-22	6.5	4.3	4.2	2.7	1.9	3.4	4.9	1.9

Total aldehyde content, which was reported to have a direct correlation with the flavor and taste of bread (Wiseblatt, 1961), was slightly higher in the triticale flours. This could be partially responsible for the distinct flavor of bread baked with triticale flour. However, the flavor of baked products is derived not only from the ingredients of the formulation, but also from new compounds formed under the constantly changing conditions of moisture, pH, and temperature of the baking process (Lorenz and Maga, 1972; Niederauer, 1969).

Hydrocarbon Composition. Hydrocarbon separations of wheat and triticale flours are presented in Figure 2. The hydrocarbon percentage composition of each of the wheat and triticale flours is presented in Table IV. The baseline drift was compensated for by the integrator. Wheat and triticale flours were found to have the same qualitative *n*-hydrocarbon composition, but differing slightly quantitatively. C-11 was present in smallest amounts in all flours, while C-16, C-17, and C-18 together amounted to more than 30% of the *n*-hydrocarbon distribution. The spring triticale flours showed a higher percentage of short-chain *n*-hydrocarbons (C-7–C-11) than the corresponding wheat flours. This was also found with the winter varieties with the exception of Scout, which had a short-chain *n*-hydrocarbon composition as high as that of the corresponding triticale samples. The chromatograms also indicated the presence of *n*-hydrocarbons with a chain length shorter than C-7. These, however, were partially covered by the solvent peak and have, therefore, not been included in the total composition of *n*-hydrocarbons. Youngs and Gilles (1970) reported *n*-hydrocarbons between C-9 and C-33 in flour and wheat milling fractions. Under our conditions *n*-hydrocarbons between C-7 and C-22 could be shown along with iso-, anteiso-, and 1-cyclohexyl derivatives, as discussed by Youngs and Gilles (1970). This accounts for the differences in distribution of the *n*-hydrocarbons reported in this study and that reported by Youngs and Gilles (1970).

Comparing total peak areas of *n*-hydrocarbons of corresponding wheat and triticale flours, it can be concluded that total *n*-hydrocarbon amounts of triticale flours approximately

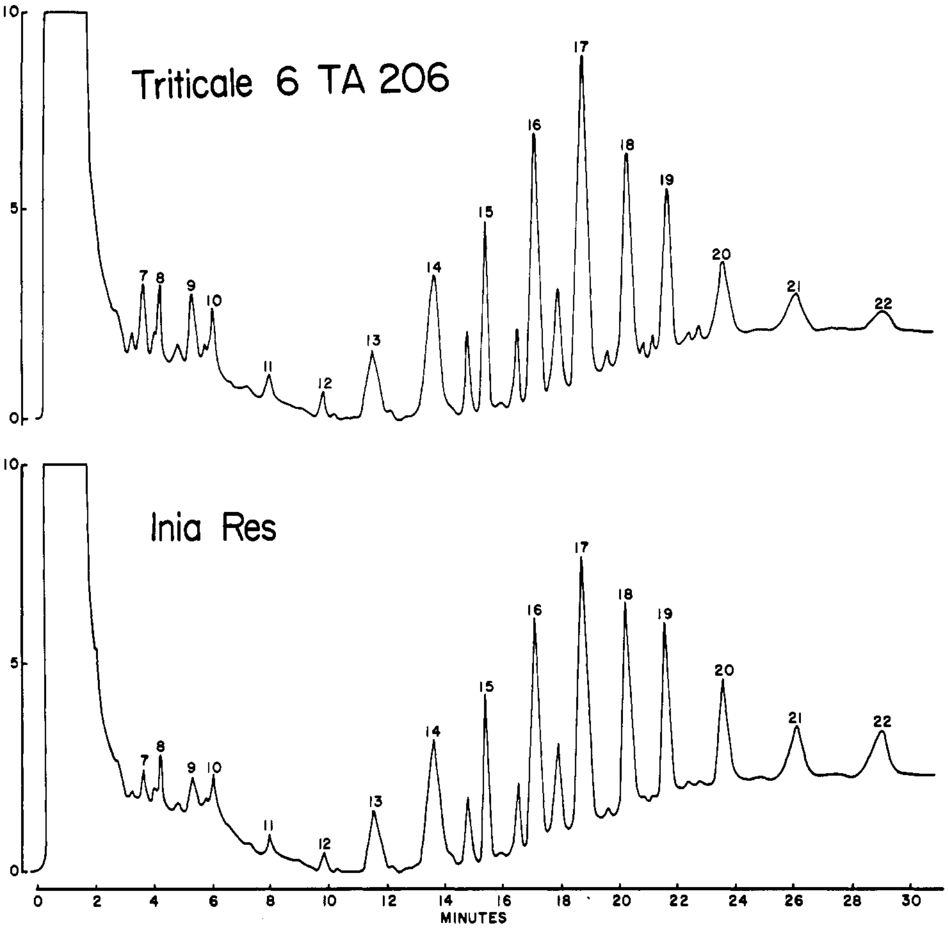

Figure 2. Typical glc hydrocarbon compositions of wheat and triticale flours. Peak identity: number refers to hydrocarbon chain length. The peaks preceding each numbered peak are the iso and anteiso hydrocarbons, while those following the numbered peaks are 1-cyclohexyl derivatives with one less carbon than the numbered peak

equal those of wheat flours. Youngs and Gilles (1970) concluded that the small amounts of *n*-hydrocarbons in wheat flour (0.0036%) make it doubtful that they could affect baking quality. The same conclusion can be drawn for the *n*-hydrocarbons in triticale flours. In none of the bread-baking studies reported (Ponte *et al.*, 1963; Elton and Fisher, 1968), which indicated that hydrocarbons can alter bread-baking characteristics of flours considerably, have hydrocarbons been used in such small amounts.

ACKNOWLEDGMENT

The authors acknowledge the assistance of Ronald Normann in obtaining and milling of the cereal grains and performing protein determinations.

LITERATURE CITED

American Association of Cereal Chemists, "Cereal Lab. Methods," 7th ed., Method 46-14, 1962.
Association of Official Agricultural Chemists, "Official Methods of Analysis," 9th ed., 1960, pp 158, 13.003, 13.006.
Briggle, L. W., *Crop Sci.* **9**, 197 (1969).
Elton, G. A. H., Fisher, N., *J. Sci. Food Agr.* **19**, 178 (1968).
Hougen, F. W., Quilliam, M. A., Curran, W. A., J. AGR. FOOD CHEM. **19**, 182 (1971).
Kies, C., Fox, H. M., *Cereal Chem.* **47**, 615 (1970a).
Kies, C., Fox, H. M., *Cereal Chem.* **47**, 671 (1970b).
Klyushkina, Y. F., Denisenko, Y. I., Nechaev, A. P., *Prikl. Biokhim. Mikrobiol.* **6**, 617 (1970).
Lorenz, K., Maga, J., *J. Food Sci.* **36**, 936 (1971).
Lorenz, K., Maga, J., J. AGR. FOOD CHEM. **20**, 211 (1972).
Lorenz, K., Welsh, J., Normann, R., Maga, J., *Cereal Chem.* **49**, 187 (1972).
MacDonald, M. D., *Euphytica Suppl.* **1**, 185 (1968).
Morrison, W. R., *J. Sci. Food Agr.* **14**, 870 (1963).
Nelson, J. H., Glass, R. L., Geddes, W. F., *Cereal Chem.* **40**, 343 (1963).
Niederauer. Th., *Muehle* **41**, 707 (1969).
Pomeranz, Y., "Wheat Chemistry and Technology," American Association of Cereal Chemists, St. Paul, Minnesota, 1971a, p 16.
Pomeranz, Y., "Wheat Chemistry and Technology," American Association of Cereal Chemists, St Paul, Minnesota, 1971b, p 407.
Ponte, J. G., Titcomb, S. T., Cotton, R. H., *Cereal Chem.* **40**, 285 (1963).
Rooney, L. W., Gustafson, C. B., Perez, N., Porter, K. B., Progress Report, Texas A&M Univ., Texas Agr. Exp. Station, Sept 1969.
Unrau, A. M., Jenkins, B. C., *Cereal Chem.* **41**, 365 (1964).
Villegas, E., McDonald, C. E., Gilles, K. A., Res. Bull. No. 10 Intern. Maize and Wheat Improvement Center, Mexico, D. F., Mexico (1968).
Youngs, V. L., Gilles, K. A., *Cereal Chem.* **47**, 317 (1970).
Wiseblatt, L., *Baker's Dig.* **35**(5), 160 (1961).

Received for review December 29, 1971. Accepted March 30, 1972. Published with the approval of the Director of the Colorado State University Experiment Station as Scientific Series Paper No. 1696.