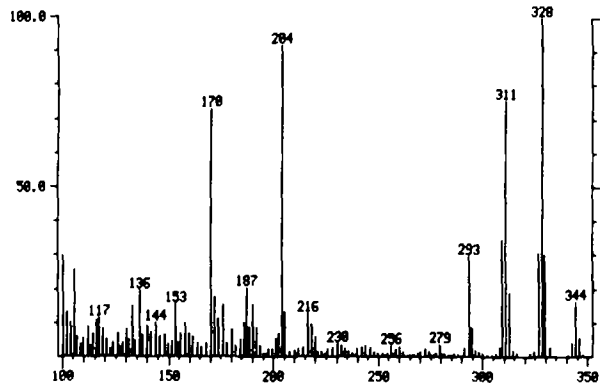

FIG. 9. Ammonia CI-MS of methyl 9-hydroperoxy-*trans*-10,-*cis*-12-octadecadienoate by direct insertion probe.

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Characteristics and Utilization of Dry Roasted Air-Classified Navy Bean Protein Fraction[1]

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ABSTRACT

Navy beans, *Phaseolus vulgaris*, were dry roasted in a particle-to-particle heat exchanger, dehulled by air aspiration, pin-milled and air-classified to yield a high protein fraction. Proximate analyses, nitrogen solubility indices and oligosaccharide contents of this high protein fraction as influenced by processing parameters which affected final product temperature were determined. Farinograms of wheat/bean protein fraction composite flours were run. A high-protein bean flour fraction was selected from these dry and roasted treatments and used in product development. Quality characteristics and consumer acceptability of high-protein prototype products were evaluated. Results of this research indicate that the dry roasting process influences the characteristics of the air-classified protein fraction. Flour color, nitrogen solubility and dough mixing properties were most greatly influenced by roasting time and temperature. Increased roasting resulted in increased browning and decreased nitrogen solubility and dough mixing stability. Wheat flour bread products, substituted with low levels of high-protein bean flour, were of high quality.

INTRODUCTION

The nutritional composition of dry navy beans is ideal for delivery of protein and minerals if properly prepared and positioned in the diet. Dry beans contain various metabolic inhibitors which must be inactivated or eliminated prior to consumption if maximum nutrient potential is to be derived. Increases in nutritional quality have been demonstrated by heating to destroy the heat labile antinutritional protease inhibitors and trypsin inhibitory compounds (1).

Lysine, which accounts for ca. 90% of the free amino groups in the form of epsilon-amino lysl residues, and methionine are highly reactive and limiting amino acids. The loss of epsilon amino groups of lysine occurs by condensation reaction with reducing sugars (2). These Maillard type browning reactions may occur in stored bean products and contribute to a loss of nutritive value and decline in sensory quality.

Heating of foods containing protein results in changes in water status, solubility of the protein and other changes in functionality of protein (3).

Chang and Satterlee (4) produced bean protein concentrates containing 72-81% protein by wet processing using water extraction techniques; Molina and Bressani (5) prepared protein isolates containing ca. 90% protein.

It has been observed, that raw legumes ground without pretreatment develop undesirable odors and flavors which persist after cooking. Lipoxidases have been held responsible for the appearance of off-flavors by catalyzing formation of hydroperoxides from unsaturated fatty acids (6). The highest lipoxidase activity experienced in pulses and oilseeds occurs in soybeans. However, treatment with dry heat for 6-8 min at 104-105 C completely inactivates this enzyme (7).

The objective of this research was to evaluate the effects of selected dry roasting treatments on the composition and functional properties of air-classified navy bean protein. A selected heat treated/bean protein was used in several wheat flour based products.

MATERIALS AND METHODS

Protein Fraction Preparation

Navy beans, *Phaseolus vulgaris*, were dry roasted in a particle-to-particle heat exchanger with control of bead temperature (240 C, 270 C), bean/bead ratio (1/10, 1/15), and roasting time (1 min, 2 min) (8). Roasted navy beans were dehulled

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by air aspiration, pin-milled and air-classified to yield whole, hull, high protein and high starch fractions (9). The high protein fractions were sealed in 2 mil polyethene bags and held at 4 C until analyses were performed.

Chemical Analyses

Chemical composition of dry roasted high protein fraction was determined using AACC methods (10). Moisture and ash contents were determined according to procedures described in Methods 44-15 and 08-01, respectively. Protein was analyzed by the standard micro-Kjeldahl Method 46-13. Nitrogen Solubility Index Method 46-23 was modified by placing a 400 mL beaker containing the water-flour mixture on a mechanical stirrer and stirring at 120 rpm for 120 min at 30 C. Crude fat content was determined by Method 30-26. Bean flour protein fraction was evaluated for enzyme neutral detergent fiber (ENDF) by the method described by Robertson and Van Soest (11), with 1 mg of amyloglucosidase included to provide additional digestion of starch.

Soluble sugars were initially extracted from 1 g of protein flour using 10 mL of 80% ethanol in an 80 C water bath shaker for 10 min. The mixture was centrifuged at 2000 rpm (1140 × g) for 3 min and the supernatant was transferred into a new tube. The extraction was repeated two more times with the same procedure, except that 5 mL of 80% ethanol were used the second time. Two mL of 10% lead acetate were added to the supernatant collected from these three extractions. The mixture was shaken and centrifuged to precipitate protein, and the supernatant was transferred to another rube. Two mL of 10% oxalic acid were added to the tube, and again the mixture was shaken and centrifuged to remove the residual lead acetate. The final supernatant was brought to 25 mL volume and was passed through a SEP-PAK C_{18} Certridge (Waters Associates, Inc.) A 30 L aliquot was injected into a high performance liquid chromatograph (HPLC) equipped with the carbohydrate analysis column (Waters Associates, Inc., Model M600A).

Functional Characteristics

Color of bean flours receiving the different heat treatments was evaluated by the Hunter Lab Model D25 Color Difference Meter. Physical dough properties and mixing characteristics of the heat treated protein flour were evaluated using the Farinograph (Brabender Instruments, Inc.) equipped with a 50 g bowl. The constant dough weight procedure of the AACC Method 54-21 (10) was followed, using a 50 g sample composed of 10% bean flour and 90% wheat flour.

Preparation and Evaluation of Bean Protein Substituted Products

The bean protein fraction, dry roasted in 240 C for 1 min with a bean/bead ration of 1/15, was selected for use in the following wheat flour based products: (a) yeast raised doughnut holes; (b) white pan bread and (c) peanut butter cookies.

Raised doughnut holes. Substitution of 25% protein flour for wheat flour was compared with the control. The doughs were mixed in a Kitchen Aid K5-A mixer. Sugar, salt and shortening were creamed at medium speed. The water was heated to 43 C, and the yeast was hydrated for 5 min. The kneading time for the doughs was 3 min at low speed. They were fermented for 1 hr (32 C and 80% RH), rolled to ½" thickness, cut with the 2" doughnut cutter, and proofed for 30 min.

The holes were fried in a Sears fryer/cooker, using 1.4 L of Superfine® all vegetable liquid frying shortening (PVO International, Inc.). They were fried at 190 C for 1 min on each side, being flipped after 30 sec. Doughnut holes were removed and placed on paper towels to drain. A Hunter Color Difference Meter Model D25 was used to determine color, and a Kramer shear press equipped with the 3000 lb transducer operating at a range of 10 with the standard shear compression cell was used to determine tenderness.

Bread. White bread was prepared by substituting 0, 5 and 10% protein flour for a commercial bread flour (bromated and malted), using the straight dough method. Kneading with a dough hook, operating at 120 rpm on a Kitchen-Aid K5-A mixer, was completed in 5 min. The dough was fermented at 30-31 C and a relative humidity of 85-90% until doubled in bulk, before being degassed, rolled and shaped into loaves with a National Manufacture Company Roller and Sheeter. The 225 g loaf was then proofed for 40 min, baked for 30 min in a preheated rotary oven at 204 C, and cooled to room temperature before evaluation.

Volume was determined by rapeseed displacement. Tenderness of breads was measured using Kramer Shear Press equipped with a standard shear compression cell and a 300 lb tranducer operating at a range of 10. Color was determined with the Hunter Color Difference Meter. A 10 member, trained panel evaluated sensory attributes using a 10 cm linear line scale with "10" being optimum.

Peanut butter cookies. Two types of peanut butter cookies, wheat flour control and high protein (30% bean protein substituted for flour), were prepared at the Michigan State University Bakery. Dough and cookies from each treatment were evaluated for their physical characteristics. Sensory properties of baked cookies were evaluated by 300 participants at Focus: HOPE, a USDA prescription food distribution center, Detroit, Michigan using a 7-point hedonic scale. Panelists included a wide representation of children, teenagers and adults. The children were approximately equal number of males and females, whereas the other age groups had more females. Black was the predominant race, although some white and other races took part.

RESULTS AND DISCUSSION

Chemical Composition of Protein Flour

Chemical compositions of high protein flours from eight roasting conditions are presented in Table I. Moisture contents ranged from 6.1% to 7.3%, with an average of 6.9%; fat contents ranged from 2.3% to 3.2%, with an average of 2.7%; protein contents ranged from 39.3% to 47.6%, with an average of 43.4%; ash contents ranged from 4.5% to 6.0% with an average of 5.2%; and dietary fiber ranged from 2.4% to 5.0%, with an average of 3.8%. Protein levels obtained from various roasting treatments were somewhat lower than those reported by Patel et al. (12) and Sahasrabudhe et al. (13). Nitrogen solubility indices of protein flours are shown in Figure 1. Results indicated that increases in roasting temperature and time significantly reduced the NSI values.

Data of HPLC sugar analysis of flours are presented in Table II. Roasting of beans did not show adverse effect on the sugar levels of protein flours. Stachyose was found to be the major oligosaccharide in the fraction, with only a trace amount of raffinose detected.

Physical Characteristics of Protein Flour

Table III shows the Hunter lab color values of protein fractions from various roasting treatments. Increasing the heat treatment generally resulted in darker, more red, and more yellow products. Eight protein flours were substituted for 10% bread flour to obtain Farinograph values; the results are shown in Table IV. Increased water absorption accompanied increase in roasting treatment. Arrival time and peak

TABLE I

Chemical Analyses of High-Protein Flour Fractions Air-Classified from Navy Beans Dry Roasted at Various Conditions[a]

Treatment							
Bean/bead ratio	Residence time (min)	Bead temperature (C)	Moisture (% wb)	Ash	Protein	Fat	Dietary Fiber
				(% db)			
1/10	1	240	6.9 ± 0.1^{c}	6.0 ± 0.1^{f}	44.2 ± 1.4^{b}	2.7 ± 0.2^{abc}	2.5 ± 0.1^{a}
		270	7.3 ± 0.0^{d}	5.9 ± 0.0^{e}	44.0 ± 1.9^{b}	3.0 ± 0.2^{bc}	2.4 ± 0.1^{a}
	2	240	7.3 ± 0.0^{d}	5.1 ± 0.0^{d}	44.2 ± 0.9^{b}	2.3 ± 0.3^{a}	5.0 ± 0.1^{e}
		270	7.2 ± 0.0^{d}	5.1 ± 0.0^{d}	43.9 ± 0.9^{b}	2.8 ± 0.3^{abc}	4.5 ± 0.0^{d}
1/15	1	240	7.1 ± 0.1^{c}	4.7 ± 0.1^{b}	41.3 ± 0.3^{ab}	2.5 ± 0.2^{ab}	4.5 ± 0.1^{d}
		270	6.9 ± 0.1^{c}	4.9 ± 0.1^{c}	42.6 ± 0.3^{b}	2.7 ± 0.2^{abc}	3.7 ± 0.2^{c}
	2	240	6.5 ± 0.0^{b}	5.1 ± 0.0^{d}	47.6 ± 0.5^{c}	3.2 ± 0.1^{c}	4.3 ± 0.0^{d}
		270	6.1 ± 0.1^{a}	4.5 ± 0.0^{a}	39.3 ± 1.3^{a}	2.7 ± 0.1^{ab}	3.4 ± 0.0^{b}

[a]Mean values and standard deviations (like letters within each column indicate significant differences at $P < 0.05$ by Tukey mean separation; n = 3).

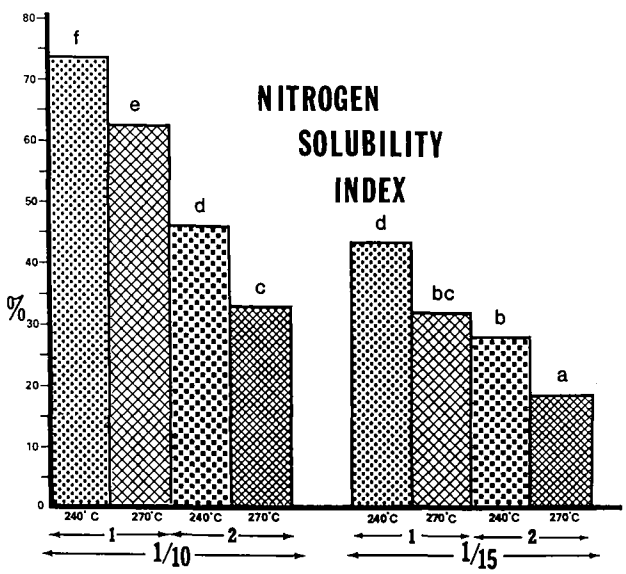

FIG. 1. Mean nitrogen solubility index (%) for protein flour dry roasted under various processing conditions: bean/bead ratio (1/10, 1/15); residence time (1, 2 min); and bead temperature (240, 270 C). Means with similar letters are not significantly different, $P < 0.05$.

TABLE II

HPLC Sugar Analysis of High-Protein Flour Fractions Air-Classified from Navy Beans Dry Roasted at Various Conditions[a]

Treatments						
Bean/bead ratio	Residence time (min)	Bead temperature (C)	Sugar content (% db)			
			Glucose	Sucrose	Raffinose	Stachyose
1/10	1	240	1.4 ± 0.1^{a}	2.9 ± 0.4^{a}	0.3 ± 0.0^{a}	3.4 ± 0.3^{a}
		270	1.5 ± 0.4^{a}	3.2 ± 0.2^{a}	0.3 ± 0.1^{a}	3.4 ± 0.3^{a}
	2	240	1.7 ± 0.3^{a}	2.9 ± 0.2^{a}	0.2 ± 0.0^{a}	3.5 ± 0.2^{a}
		270	1.8 ± 0.3^{a}	3.1 ± 0.2^{a}	0.2 ± 0.0^{a}	3.3 ± 0.2^{a}
1/15	1	240	1.5 ± 0.4^{a}	3.0 ± 0.1^{a}	0.2 ± 0.0^{a}	3.6 ± 0.3^{a}
		270	1.6 ± 0.2^{a}	2.9 ± 0.2^{a}	0.3 ± 0.1^{a}	3.5 ± 0.5^{a}
	2	240	1.8 ± 0.2^{a}	3.2 ± 0.4^{a}	0.3 ± 0.1^{a}	3.6 ± 0.6^{a}
		270	1.3 ± 0.2^{a}	2.9 ± 0.2^{a}	0.3 ± 0.0^{a}	3.4 ± 0.6^{a}

[a]Mean values and standard deviations (like letters within each column indicate no significant differences at $P < 0.05$ by Tukey mean separation; n = 3).

TABLE III

Hunterlab Color Values of High-Protein Flour Fractions Air-Classified from Navy Beans Dry Roasted at Various Conditions[a]

Treatment			Color values		
Bean/bead ratio	Residence time (min)	Bead temperature (C)	L	a_L	b_L
1/10	1	240	87.2 ± 0.1[e]	-2.5 ± 0.1[a]	7.3 ± 0.1[a]
		270	87.5 ± 0.1[fg]	-2.6 ± 0.1[a]	8.0 ± 0.1[b]
	2	240	87.7 ± 0.1[g]	-2.6 ± 0.1[a]	8.2 ± 0.1[c]
		270	86.7 ± 0.1[d]	-2.4 ± 0.1[b]	8.9 ± 0.1[d]
1/15	1	240	87.4 ± 0.1[f]	-2.6 ± 0.1[a]	8.1 ± 0.1[bc]
		270	86.6 ± 0.1[c]	-2.4 ± 0.1[b]	9.1 ± 0.1[e]
	2	240	86.4 ± 0.1[b]	-2.4 ± 0.1[b]	9.8 ± 0.1[f]
		270	85.2 ± 0.1[a]	-2.0 ± 0.1[c]	11.5 ± 0.1[g]

[a]Mean values and standard deviations (like letters within each column indicate no significant differences at $P < 0.05$ by Tukey mean separation; n = 3).
[b]Standardized to a white tile: L = 95.35, a_L = -0.6, b_L = + 0.4.

TABLE IV

Farinograph Values of High-Protein Flour Fractions Air-Classified from Navy Beans Dry Roasted at Various Conditions[a,b]

Treatment						
Bean/bead ratio	Residence time (min)	Bead temperature (C)	Water absorption (%)	Arrival time (min)	Peak time (min)	Stability (min)
1/10	1	240	70.4 ± 0.1[a]	4.7 ± 0.3[d]	5.7 ± 0.3[d]	3.3 ± 0.5[a]
		270	70.9 ± 0.4[ab]	4.0 ± 0.0[c]	5.1 ± 0.3[c]	3.4 ± 0.1[a]
	2	240	71.2 ± 0.1[bc]	3.3 ± 0.2[b]	4.5 ± 0.1[b]	3.1 ± 0.2[a]
		270	71.7 ± 0.2[cd]	3.2 ± 0.3[ab]	4.4 ± 0.1[b]	3.0 ± 0.6[a]
1/15	1	240	71.1 ± 0.1[bc]	3.2 ± 0.0[ab]	4.3 ± 0.1[b]	3.0 ± 0.1[a]
		270	72.6 ± 0.1[ef]	3.4 ± 0.2[b]	4.6 ± 0.1[b]	3.2 ± 0.4[a]
	2	240	72.1 ± 0.3[de]	3.2 ± 0.2[ab]	4.3 ± 0.1[b]	2.5 ± 0.5[a]
		270	73.2 ± 0.2[f]	2.8 ± 0.1[a]	3.7 ± 0.0[a]	2.5 ± 0.5[a]

[a]Mean values and standard deviations (like letters within each column indicate no significant differences at $P < 0.05$ by Tukey mean separation; n = 3).
[b]High protein fraction substituted 10% for wheat flour.

time of flours decreased with increased roasting. Mixing stability of flours, although not significantly different from each other, showed a decreasing trend as the bean/bead ratio and roasting time increased.

Baked Products Quality Evaluation

Fogg and Tinklin (14) found that low levels of cottonseed flour (10-15% replacement) in baked products reduced dough stickiness, increased water, binding, benefited machining properties, reduced fat absorption and increased shelf life. In the current study, the shear press values show that, at the 25% substitution level, less force is required to shear the doughnut holes. These results correlate with sensory scores for tenderness (Table V). The taste panel found the control raised doughnut holes to be moderately tender, and sensory values were higher for the doughnut holes with 25% substituted navy bean protein. Exteriors of raised doughnut holes had similar Hunter color values. Moreover, all sensory scores for raised doughnut holes with 25% substituted bean protein were equivalent to the control (Table V). Thus, substitution of bean protein in raised doughnuts is feasible.

Bread. Bean protein substitution in bread was highly successful, and results are presented in Table VI. Volume and crumb color were not adversely affected, even at levels of 10% substitution. Shear values showed that significantly more force was required as the level of bean protein substitution increased; however, sensory panelists did not detect a significant difference in bread tenderness. Flavor scores were not adversely affected. Prior research with other single cell, oil seed and legume flours has indicated that volume, color and flavor are often adversely affected (15,16,17). D'Appolonia (18) reported that roasting of navy beans improved the success of incorporation of whole bean flour; however, color was adversely affected due to heat inactivation of lipoxygenase. In the current study, color was only slightly affected, and roasted bean protein can be successfully incorporated into bread to raise the protein level 10 and 20% by 5 and 10% substitution, respectively.

Finally, to test bean protein compatibility with a soft wheat product, peanut butter cookies were prepared with 0 and 30% bean protein substitution. Substituting bean protein for wheat flour had little effect on color of either the dough or baked cookie. Due to the bean protein's increased water holding capacity, cookie spread decreased slightly and cookie tenderness increased (Table VII). Panelists' general comments were favorable. Preliminary scanning of the

TABLE V

Instrumental and Sensory Evaluations of Yeast Raised Doughnut Holes Prepared with 0 and 25% Navy Bean Protein Flour Substitution

Level of substitution (%)	Instrumental evaluation[a]				Sensory evaluation[b]				
	Tenderness (lb/g)	Color values			Tenderness	Texture	Fat absorption	Flavor	Crumb
		L	a_L	b_L					
0	17.9 ± 1.2[b]	28.7 ± 0.2[a]	2.0 ± 0.3[a]	3.4 ± 0.2[a]	3.7 ± 0.3[a]	3.2 ± 0.2[a]	3.6 ± 0.3[a]	3.8 ± 0.6[a]	3.8 ± 0.2[a]
25	14.7 ± 3.0[a]	28.4 ± 0.4[a]	3.5 ± 0.5[a]	3.1 ± 0.4[a]	3.8 ± 0.2[a]	3.4 ± 0.9[a]	4.0 ± 0.0[a]	3.9 ± 1.0[a]	3.7 ± 0.5[a]

[a]Mean values and standard deviations (like letters within each column indicate significant differences at $P < 0.05$ by Tukey mean separation; n = 3).

[b]1 to 5 scale was used with 5 being optimum.

[c]Hunter color values: L = lightness (0 = black, 100 = white); $^{+}a_L$ = red; $^{+}b_L$ = yellow.

TABLE VI

Physical and Sensory Characteristics of Bread Prepared with 0, 5 and 10% Navy Bean Protein Flour Substitution

Level of substitution (%)	Physical characteristics					Sensory characteristics[b]		
	Volume (mL)	Tenderness (lb/g)	Color of crumb[c]			Texture	Tenderness	Flavor
			L	a_L	b_L			
0 (control)	743 ± 2[a]	5.25 ± 0.34[a]	68.2 ± 0.1[a]	8.3 ± 0.0[a]	17.4 ± 0.1[a]	6.0 ± 1.6[a]	7.7 ± 1.4[a]	6.2 ± 1.4[a]
5	734 ± 4[a]	6.78 ± 0.08[b]	65.2 ± 0.1[a]	8.3 ± 0.0[a]	16.1 ± 0.0[a]	6.8 ± 1.1[a]	6.3 ± 1.6[a]	5.5 ± 1.7[a]
10	763 ± 3[b]	7.99 ± 0.11[c]	65.5 ± 1.6[a]	9.1 ± 0.1[a]	16.3 ± 1.2[a]	5.1 ± 1.7[a]	7.1 ± 1.4[a]	6.1 ± 1.4[a]

[a]Mean values and standard deviations (like letters within each column indicate significant differences at $P < 0.05$ by Tukey mean separation; n = 3).

[b]10 cm linear line scale was used with 10 being optimum.

[c]Hunter color values: L = lightness (0 = black, 100 = white); $^{+}a_L$ = red; $^{+}b_L$ = yellow.

TABLE VII

Physical Characteristics of Peanut Butter Cookies Made with Wheat Flour (Control) and 30% Navy Bean Protein Flour[a]

Level of substitution (%)	Moisture (%)	Color values[b]			Baking loss (%)	Spread factor[c] (W/T)	Tenderness (lb/g)
		L	a_L	b_L			
Dough							
0 (Control)	13.5 ± 0.0[a]	37.7 ± 0.1[b]	9.5 ± 0.1[a]	16.8 ± 0.1[b]	–	–	–
30	12.7 ± 0.0[a]	31.7 ± 0.4[a]	10.5 ± 0.1[a]	14.8 ± 0.2[a]	–	–	–
Cookies							
0 (Control)	5.8 ± 0.3[a]	45.2 ± 0.7[a]	13.4 ± 0.4[a]	20.7 ± 0.2[a]	10.7 ± 0.5[a]	10.0 ± 0.3[a]	25.7 ± 0.8[b]
30	7.0 ± 0.2[b]	44.6 ± 0.7[a]	12.9 ± 1.0[a]	20.6 ± 0.4[a]	11.2 ± 0.2[a]	9.1 ± 0.2[a]	21.6 ± 1.6[a]

[a]Mean values and standard deviations (like letters within each column indicate significant differences at $P < 0.05$ by Tukey mean separation; n = 3).

[b]Hunter color values: L = lightness (0 = black, 100 = white); $^{+}a_L$ = red; $^{+}b_L$ = yellow.

[c]W/T = width/thickness of cookies.

data showed that high fiber cookies scored as high as the control, and the high protein cookie scored slightly lower. Mean scores and standard deviations for these variables were: control, 5.9 ± 1.1; high fiber, 5.9 ± 1.2; and high protein, 5.5 ± 1.4. Tests showed significant differences ($P < 0.05$) between control and high protein cookies. Even though statistical differences occurred, all cookies were rated acceptable by the taste panelists.

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⁂Computer Modeling of Theoretical Structures of Monoacid Triglyceride α-Forms in Various Subcell Arrangements

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ABSTRACT

Six theoretical triarachidin space-filling α-form structures were examined using a computer modeling technique that simulated restricted oscillations of carbon zigzag planes in synchronous and nonsynchronous modes. Intermolecular minimization procedures determined best-fit positions around a centralized molecule, which enabled calculation of total lattice energy values for nine different hexagonal subcell arrangements. Subcell arrangement had a greater effect on the energy of the system than did the configuration of the triglyceride. The analysis thus far indicates several equally preferred structure-subcell arrangement combinations for triglyceride α-forms rather than a single crystalline entity.

INTRODUCTION

Knowledge of the molecular conformation and three-dimensional packing of triglycerides in different crystal forms is fundamental to understanding lipid phase behavior. It is obvious that these solid-state structures play a vital role not only in fat processing but also in organized structures of biological systems. Yet after years of research, the molecular conformation is known for only the β-form (highest melting) (1), which represents essentially one-third of the overall picture also involving the α-form (lowest melting) and β′-form (intermediate melting) (2). Although X-ray diffraction (3–5), infrared spectroscopy (6), nuclear magnetic resonance (7) and thermal analysis (4, 8, 9) have contributed substantially to the knowledge of α- and β′-forms, their elusive crystal structures and molecular packing characteristics have escaped these investigations. Computer modeling, an alternative procedure that can provide insight into molecular arrangements, has been applied to lipids primarily for intramolecular conformational analysis of phospholipids (10) and short-chain triglycerides (11, 12). The current study emphasizes intermolecular interactions because they were previously successful in accounting for structural relationships and stabilities among *n*-hydrocarbons (13). Like hexagonal hydrocarbons, α-form triglycerides can be considered the first of several forms in a chain of events leading eventually to stable β-forms. Because of its orthogonal structure and similarity to the triglyceride liquid state (5), the α-form represents a convenient starting point. We thus modeled various theoretical conformers of α-triarachidin for comparative lattice energy information on both the structure and packing arrangements.

On cooling from the melt, most long-chain compounds transform into a hexagonal crystal structure with the chains possessing rotational freedom about longitudinal axes. In triglycerides, the acyl methylene chains are considered to perform restricted rotation or oscillatory motion because of their attachment to the polar glycerol region, but small oscillations take up the same amount of space as complete rotation (7). The α-form melting points (4, 9) and X-ray long spacings (4) of triglycerides do not alternate between even and odd chainlengths, thereby suggesting vertical acyl methylene chains with respect to the end group planes, in contrast to β′- and β-forms with tilted chains. Since β- and/or β′-forms are rapidly made from the α-form, any theoretical α-form structures are likely to be in the tuning-fork type configuration of the β-form and alternate between upright and inverted positions of adjacent molecules (1). An understanding of the configurational and position arrangement possibilities for the α-form and the techniques to obtain them will allow for prediction and validation of structures and pathways to β′- and β-forms and other new forms recently discovered (9).

EXPERIMENTAL

α-Form Structures

A triglyceride model was constructed of trioctanoin using the Minit Model System (Science Related Materials, Inc., Janesville, WI) having a scale of 1.25 cm/Å. By manipulation of the bonds around the glycerol region and, at the same time, maintaining an all *trans* configuration of the acyl chains, a symmetrical tuning-fork conformation was found (Fig. 1A) that allowed the length of the molecule to approximate closely the recorded long spacing for the α-form (4). The atomic coordinates of atoms were determined using bond lengths and angles reported for the single crystal of the trilaurin β-form (1). A distinguishing feature of the molecule is that the carbon zigzag plane of chain 2 is approximately perpendicular, or nonparallel, to the carbon zigzag planes of chains 1 and 3. Also, a plane bisecting the