

Characterization of Aroma Components in Barley Bran Sauce Using Statistical Analysis

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Abstract A linear correlation was found by stepwise multiple regression analysis between the sensory score of barley bran sauce aroma and the absolute gas chromatogram (GC) data transformed with square root. In spite of highly significant relationship between the quantity of the peak and the sensory score, it is difficult to estimate the aroma quality of barley bran sauce samples on the basis of only one peak. Peak 29 (methyl 9,12,15-octadecatrienoate) contributed most to the aroma of barley bran sauce. This was followed by 27 (methyl 9,12-octadecadienoate), 28 (ethyl 9,12-octadecadienoate), 12 (phenyl acetaldehyde), and 9 (methyl furfural) in terms of absolute value. When it was calculated using absolute value transformed by square root, peak 28 (ethyl 9,12-octadecadienoate) made the highest contribution to the aroma of barley bran sauce of among the peaks. It was followed by 31 (9,12-octadecadienoic acid), 27 (methyl 9,12-octadecadienoate), 12 (phenyl acetaldehyde), and 29 (methyl 9,12,15-octadecatrienoate).

Keywords: barley bran sauce, stepwise multiple regression analysis, contributing proportion

Introduction

Many kinds of conventional and non-conventional sources of fiber are available as commercial food additives. The cereal grains most commonly used as fiber sources are wheat, corn, and oats. Until now, barley bran has not been used extensively because relatively small quantities of barley are milled and peeled to provide bran as a by-product. Recently, the nutritional benefits of barley bran as a useful source of dietary fiber have been investigated. Lupton and Robinson (1) investigated the effect of barley bran on the acceleration of gastrointestinal transit time. Lupton *et al.* (2) and Newman *et al.* (3) showed that barley bran had cholesterol-lowering properties.

Kwon *et al.* (4) reported on the optimum conditions for the taste of barley bran sauce and Lee *et al.* (5) described the characteristics of barley bran sauce. Choi and Park (6) explained that barley bran sauce taste quality could be predicted to 93% accuracy using multiple regression analysis with taste compounds and sensory evaluation scores. However, the effective components responsible for the aroma of barley bran sauce have not yet been investigated.

Fermented food is made through a long and complicated process under the influence of many kinds of microorganisms (7, 8). In experiments on fermented food, the characteristic aroma was dispersed during the fractionation of aroma concentrate. Therefore, the aroma of fermented food should be also considered as the combined effect of many different aroma compounds (9-12).

In this paper, we applied stepwise multiple regression analysis and contributing proportion analysis to gas

chromatographic data on barley bran sauce aroma. This was done in order to investigate the significant chemical factors for aroma quality as measured by gas chromatographic data in relation to quality differentiation by sensory tests.

Materials and Methods

Material and sensory test Forty-two different barley bran sauces made by the method of Choi *et al.* (12) were used. Each barley bran sauce was evaluated on a scale of 1 to 7 according to order of preference by 12 consumer panels using sniff tests according to a completely randomized experimental design (13, 14). The sum of order of preference scores was used as the sensory score for each sample in this study.

Extraction and identification of aroma compounds An improved Nikerson and Likens' simultaneous steam distillation and extraction apparatus was used to extract the aroma compounds of barley bran sauce (15), using purified diethylether as extraction solvent. The samples and solvents were placed in their respective ports. The solvent was circulated and the aroma compounds were then extracted for more than 2 hr by increasing the temperature of the sample port to boiling point. Anhydrous sodium sulfate was added to the extracted fraction at 4°C to dehydrate. The fraction was then concentrated to a final 100 mL using N₂ gas to obtain a sample for gas chromatogram (GC) analysis. The mass spectrum of each aroma compound was obtained by GC with a Hewlett-Packard 5892 and GC-MS using a CENCEPT SERIES-I (Mass-KRATOS Inc., England). Samples were injected on a 60 m × 0.33 μm × 0.2 mm HP-FFAP column at 230°C. The detector temperature was 250°C. The temperature was

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programmed at 45°C for the first 2 min, with increases of 15°C/min to a final temperature of 220°C. This was maintained for 11.4 min. Helium was used to carry the sample at a rate of 5 mL/min. The electron voltage was 1,100 eV at a split ratio of 10:1.

Stepwise regression analysis N sensory scores corresponding to each barley bran sauce sample could be described as $Y = (y_1, y_2, \dots, y_i, \dots, y_n)$ (16). If the gas chromatogram of each flavor concentrate showed m peaks, each gas chromatogram could be described as $(x_{i1}, x_{i2}, \dots, x_{ij}, \dots, x_{im})$, and consequently the gas chromatograms for whole samples could be shown as the matrix described below,

$$\begin{pmatrix} X_{11} & X_{12} & \dots & X_{1j} & \dots & X_{1m} \\ \vdots & \vdots & & \vdots & & \vdots \\ X_{i1} & X_{i2} & \dots & X_{ij} & \dots & X_{im} \\ \vdots & \vdots & & \vdots & & \vdots \\ X_{n1} & X_{n2} & \dots & X_{nj} & \dots & X_{nm} \end{pmatrix}$$

where, $n = 1$ to 42, $m = 1$ to 34 in this study. The multiple regression model is generally shown as follows

$$Y = \alpha_1 X_1 + \alpha_2 X_2 + \dots + \alpha_j X_j + \dots + \alpha_m X_m + \beta + \varepsilon \quad (1)$$

α_j = regression coefficient

β = intercept

ε = random error

Y = dependent variable

X_j = independent variable

Variables α_j and β are calculated by the linear least squares methods, and the equation is validated in $n > m$. The correlation coefficient between the real Y and estimated Y obtained from the computed multiple regression model is designated as multiple correlation (R). R^2 , the variance ratio of Y explained by the regression model, is called the coefficient of multiple determination.

Smaller numbers of independent variables are desirable for easier estimation of Y when using the multiple regression model for quality tests or controls in the manufacturing process. Recently, many kinds of multivariate analysis methods have been developed for this purpose, but stepwise regression analysis (SRA) is considered to be the most adequate method for selecting a subset of variables. According to Draper and Smith (17), several different algorithms have been developed for selecting the variables in SRA. However, the increasing and decreasing method is regarded as having the greatest efficiency of calculation and accuracy of analysis. Therefore, the relationships between GC-patterns and sensory scores were analyzed by the increasing and decreasing SRA method. The SRA is performed by trial and error peak selection for obtaining the most suitable subset of the variables. This is done on the basis of the F-values from analysis of variance on each independent variable at each step, because the significance degree of an entered variable is changed by entry of another variable. Therefore, the entry of a variable that is not yet included

Table 1. Transformation of independent variables

	Absolute values	Relative values
1	X_i	$X'_i = X_i / \sum X_j \times 100$
2	$\ln(X_i + 1.0)$	$\ln(X'_i + 1.0)$
3	$\sqrt{(X_i + 10^{-10})}$	$\sqrt{(X'_i + 10^{-10})}$

on the regression, and the removal of variables that are already included in the regression, are determined from the preset conditions of the F-value for each variable.

The variable having the highest F-value was selected for entry among variables not yet included in the regression. If F-value of any variable already included in the regression was under 0.005, the variable was removed from the regression model. If all the variables that were not included had F-values under 0.1, the SRA was stopped at that step. The maximum number of steps was set at forty. The SRA was carried out using the SPSS 7.5 program.

In this report, GC data was analyzed after transformation as shown in Table 1. The 1.0 was added to original data at transformation with logarithm for obtaining 0 by transformation when analyzing non-existing samples and 1×10^{-10} was added to the original data at transformation with square roots to avoid calculating the square root of 0.

Contributing proportion Contributing proportion (P_i), the relative importance of each component to aroma quality, was calculated by Barylko-Pikielna and Metelski's methods (18), shown as in Equation (2):

$$P_i = \frac{|\beta_i \cdot r_{iy} \cdot S_i|}{\sum |\beta_i \cdot r_{iy} \cdot S_i|} \times 100 \quad R^2 \quad (2)$$

S_i represents standard deviation of each component and r_{iy} is the correlation coefficient between each variable and sensory score. β_i and R^2 were partial regression coefficient and coefficient of multiple determination. This analysis was performed by using a SPSS 7.5 program.

Results and Discussion

Sensory test and GC analysis The sensory evaluation was made by 12 consumer panels using a sniff test. The results showed that the sensory score of the most favored sample was 72 and the least popular sample was rated at 29. One sample received more than 72, 6 samples scored 48-60, 22 samples were between 36 and 48, and 9 samples were evaluated within the 24-36 range. The mean value of these samples was 43.3 and their standard deviation was 10.5.

As shown in Table 2, most of the barley bran sauce samples showed about 34 peaks, in which the content of methyl 9,12-octadecanoate (18.74±23.65 area%) was highest, followed by that of 2-furanmethanol (8.75±16.02 area%) and 2-furancarboxaldehyde (8.67±18.62 area%). Among the 34 aroma components, there were 11 kinds of esters, 5 kinds of phenols and esters, 4 kinds of aldehydes, 2 kinds of alcohols and hydrocarbons, 1 furan, and 4 other minor compounds.

Correlation between sensory scores and the content of

Table 2. Composition of aroma compounds and sensory evaluation values in barley bran sauce

No.	Aroma components	Mean	SD ¹⁾	Max. ²⁾	Min. ³⁾
Aldehydes (4)					
X ₁	3-Furaldehyde	6.70	16.93	69.39	0
X ₃	2-Furancarboxaldehyde	8.67	18.61	61.16	0
X ₉	Methyl furfural	3.81	4.89	29.65	0
X ₁₂	Phenyl acetaldehyde	4.18	4.94	20.11	0
Alcohols (2)					
X ₂	2-Furanmethanol	8.75	16.02	57.24	0
X ₁₄	Phenylethyl alcohol	0.39	0.38	1.44	0
Hydrocarbones (2)					
X ₅	7-Cyclopropane	0.38	1.78	11.63	0
X ₈	5-Methyl-2-(1-methylethyl) cyclohexane	0.06	0.08	0.45	0
Furan (1)					
X ₇	2-Ethyl-5-methylfuran	0.03	0.09	0.48	0
Acids (5)					
X ₄	4-Pentanoic acid	2.39	10.64	54.26	0
X ₁₁	Benzeneacetic acid	2.23	4.85	22.96	0
X ₂₁	Tetradecanoic acid	0.05	0.05	0.21	0
X ₂₄	Hexadecanoic acid	7.73	6.48	27.47	0
X ₃₁	9,12-Octadecadienoic acid	0.15	0.18	0.84	0
Phenols (5)					
X ₁₃	4-Methoxyphenol	0.11	0.09	0.52	0
X ₁₅	4-Mercaptophenol	0.23	0.48	2.05	0
X ₁₆	4-Vinyl-2-methoxy-phenol	2.60	3.19	18.57	0
X ₁₇	2-Methoxy-4-(1-propenyl)phenol	0.04	0.14	0.89	0
X ₁₈	2,6-Bis(1,1-dimethylethyl)-4-methyl phenol	0.80	1.28	7.52	0
Esters (11)					
X ₂₀	Ethyl tetradecanoate	0.14	0.40	2.30	0
X ₂₂	Methyl hexadecanoate	0.05	0.05	0.23	0
X ₂₃	Ethyl hexadecanoate	1.77	3.33	13.92	0
X ₂₅	Dibutyl 1,2-benzenedicarboxylate	0.11	0.29	1.82	0
X ₂₆	Ethyl 9-octadecenoate	2.45	4.30	19.06	0
X ₂₇	Methyl 9,12-octadecadienoate	18.74	23.65	75.23	0
X ₂₈	Ethyl 9,12-octadecadienoate	18.73	21.06	78.84	0
X ₂₉	Methyl 9,12,15-octadecatrienoate	6.11	10.45	37.90	0
X ₃₀	9-Octadecenyl 9-octadecenoate	0.06	0.11	0.52	0
X ₃₃	Phenyl methyl octadecanoate	0.08	0.13	0.70	0
X ₃₄	Bis(2-ethylhexyl) 1,2-benzenedicarboxylate	0.25	0.77	4.56	0
Others (4)					
X ₁₉	1-Furfuryl-2-formyl pyrrole	0.18	0.44	2.83	0
X ₆	Trimethylphosphine	0.12	0.11	0.43	0
X ₁₀	4-Acetyl heptanenitrile	0.45	2.86	18.51	0
X ₃₂	Unknown	0.07	0.14	0.81	0
Y	S.E.V. ⁴⁾	43.26	10.48	72.00	29.00

¹⁾SD: standard deviation. ²⁾Max.: maximum value. ³⁾Min.: minimum value. ⁴⁾S.E.V.: sensory evaluation values indicates the sum of the score in the range from 1 (dislike intensely) to 7 (greatly enjoy) that 12 panels recorded. Each value is the average of 42 replications.

aroma compounds The correlation coefficients between each sample's sensory score and the quantity of each peak are shown in Table 3. A negative correlation coefficient at each peak means that compound makes a negative contribution to sauce quality, and a the positive correlation coefficient represents a chemical that makes a positive contribution. Peaks 9, 12, 21, 29, and 31 showed a significant relationship with the sensory score. Among them, the correlation coefficients of peak 9 (methyl furfural) and 29 (methyl 9,12,15-octadecatrienoate) were very significant at the 1% level at every transformation. However, in spite of the highly significant relationship between the quantity of the peak and the sensory score, it is difficult to estimate the aroma quality of barley bran sauce samples on the basis of only one peak.

Stepwise multiple regression analysis. Stepwise multiple regression analysis was computed using independent variables that were not expected to lower accuracy of the estimation. Peaks that had values of practically zero contributing proportion, and those that represented typical peaks because of strong similarity between peaks, were excluded from analysis. Four regression models computed at the 6th and 15th steps from an absolute value and its square root are shown in equation (3-6). According to equation (3-6), the significance of the regression coefficients was examined on the basis of the F-value.

In the case of absolute value, the regression coefficient at step 6 was significant for 4 variables: 29 (methyl 9,12,15-octadecatrienoate), 7 (2-ethyl-5-methylfuran), 6 (trimethylphosphine), and 8 [5-methyl-2-(1-methylethyl) cyclohexane]. At step 15, it was significant for nine variables: 29 (methyl 9,12,15-octadecatrienoate), 7 (2-ethyl-5-methylfuran), 6 (trimethylphosphine), 2 (2-furanmethanol), 8 [5-methyl-2-(1-methylethyl)-cyclohexane], 24 (hexadecanoic acid), 16 (hexadecanoic acid), 19 (1-furfuryl-2-formyl pyrrole), and 18 [2,6-bis(1,1-dimethylethyl)-4-methyl phenol]. The F-value of these 2 multiple regression models were significant at the 1% level. The standard error of estimation was 5.66 at step 15, smaller than the value of 6.65 seen at step 6. The multiple regression coefficient was 0.815 at step 15, which was smaller than the 0.656 observed at step 6. Thus, both the standard error and the multiple regression coefficient showed an increase in detailed estimation.

In the case of absolute values transformed with square roots, the regression coefficient was significant for every variable at step 6. The F-value of these two multiple regression models was significant at the 1% level. The data at step 6 could explain 60.5%, and step 15 could account for 74.6%, of the aroma of barley bran sauce.

The multiple correlation (R), the coefficient of the multiple determination (R²), and the increase in R at each step are shown in Fig. 1. In terms of absolute value, the R-value (0.571 with entry of peak 29 at the first step) increased with the step number, and it exceeded 0.9 with the entry of peak 31 (9,12-octadecadienoic acid) at step 14. The coefficient of determination was 0.815 at step 15, indicating that 81.5% of the variance of the sensory score could be explained by 15 components. The R-value of 0.947 at step 34 and the coefficient of determination of 0.897 indicated that over 89.7% of the variance of the sensory score could be explained by the regression model.

Table 3. Correlation coefficients (R) between sensory scores and contents of aroma compounds¹⁾

No.	R	No.	R	No.	R	No.	R	No.	R	No.	R
X ₁	-0.04	X ₇	0.30	X ₁₃	0.22	X ₁₉	-0.46	X ₂₅	-0.09	X ₃₁	-0.30*
X ₂	0.12	X ₈	-0.05	X ₁₄	-0.21	X ₂₀	-0.14	X ₂₆	-0.19	X ₃₂	0.06
X ₃	0.01	X ₉	0.42**	X ₁₅	0.12	X ₂₁	0.36*	X ₂₇	-0.27	X ₃₃	0.06
X ₄	0.15	X ₁₀	0.01	X ₁₆	0.15	X ₂₂	0.05	X ₂₈	-0.29	X ₃₄	0.09
X ₅	-0.13	X ₁₁	-0.15	X ₁₇	-0.01	X ₂₃	-0.08	X ₂₉	0.57**		
X ₆	0.32*	X ₁₂	0.33*	X ₁₈	-0.20	X ₂₄	0.20	X ₃₀	-0.15		

¹⁾X₁, 3-furaldehyde; X₂, 2-furanmethanol; X₃, 2-furancarboxaldehyde; X₄, 4-pentanoic acid; X₅, 7-cyclopropane; X₆, trimethylphosphine; X₇, 2-ethyl-5-methylfuran; X₈, 5-methyl-2-(1-methylethyl) cyclohexane; X₉, methyl furfural; X₁₀, 4-acetyl heptanenitrile; X₁₁, benzenoacetic acid; X₁₂, phenyl acetaldehyde; X₁₃, 4-methoxyphenol; X₁₄, phenylethyl alcohol; X₁₅, 4-mercaptophenol; X₁₆, 4-vinyl-2-methoxy-phenol; X₁₇, 2-methoxy-4-(1-propenyl)phenol; X₁₈, 2,6-bis(1,1-dimethylethyl)-4-methyl phenol; X₁₉, 1-furfuryl-2-formyl pyrrole; X₂₀, ethyl tetradecanoate; X₂₁, tetradecanoic acid; X₂₂, methyl hexadecanoate; X₂₃, ethyl hexadecanoate; X₂₄, hexadecanoic acid; X₂₅, dibutyl 1,2-benzenedicarboxylate; X₂₆, ethyl 9-octadecenoate; X₂₇, methyl 9,12-octadecadienoate; X₂₈, ethyl 9,12-octadecadienoate; X₂₉, methyl 9,12,15-octadecatrienoate; X₃₀, 9-octadecenyl 9-octadecenoate; X₃₁, 9,12-octadecadienoic acid; X₃₂, unknown; X₃₃, phenyl methyl octadecanoate; X₃₄, bis(2-ethylhexyl) 1,2-benzenedicarboxylate.

* $p < 0.05$, ** $p < 0.01$.

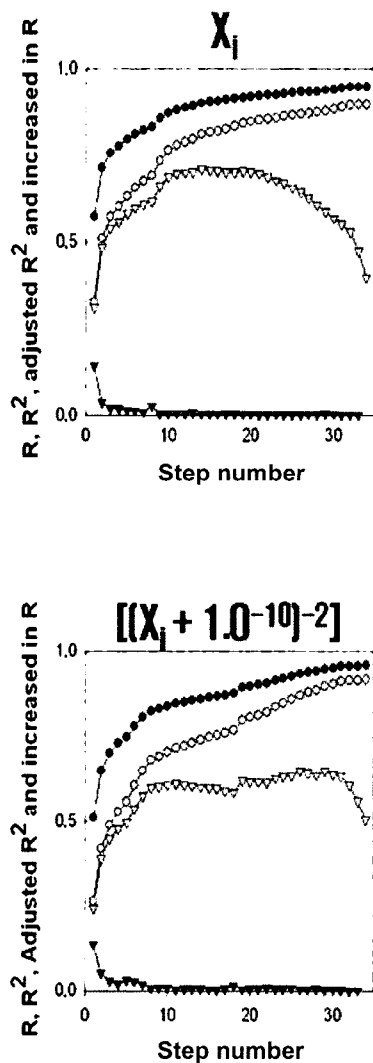


Fig. 1. Multiple correlation coefficient (R), coefficient of multiple determination (R²), adjusted R², and increase in R of aroma at each step computed from the absolute value (X_i) and the absolute value transformed with square root [(X_i+1.0)⁻¹]. ● - ●, multiple correlation coefficient (R); ○ - ○, coefficient of multiple determination (R²); ▼ - ▼, adjusted R²; ▽ - ▽, increase in R.

The results derived from absolute values transformed with square roots showed a similar tendency.

A) Step 6 calculated with X_i

$$Y = 32.013 + 0.583X_{29} + 47.645X_7 + 38.301X_6 + 0.136X_2 - (14.368^{**}) (5.354^{**}) (3.662^{**}) (3.359^{**}) (1.974) \\ 33.068X_8 + 0.268X_{24} \\ (-2.111^*) (1.557) \quad (3)$$

¹⁾R=0.810, ²⁾R₂=0.656, F=11.08**, ³⁾SE=6.65

* $p < 0.05$, ** $p < 0.01$, Numbers in parentheses show *t*-value for each of entered variable.

B) Step 15 calculated with X_i

$$Y = 29.950 + 0.340X_{29} + 27.684X_7 + 50.558X_6 + 0.181X_2 - 64.070X_8 \\ (9.176^{**}) (2.715^*) (2.195^*) (3.809^{**}) (2.699^*) (-2.877^{**}) \\ + 0.449X_{24} + 0.011X_{28} + 2.552X_{16} - 16.662X_{19} - 3.552X_{18} - 4.743X_{14} \\ (-3.398^{**}) (-2.715^*) (-1.653) (-1.570) (1.694) (1.449) \\ - 0.189X_4 + 0.584X_{12} + 16.143X_{31} - 13.373X_{30} \\ (2.860^{**}) (0.176) (3.628^{**}) (-0.830) \quad (4)$$

R=0.903, R²=0.815, F=7.62**, SE=5.66

C) Step 6 calculated with [(X_i+1.0)⁻¹]²

$$Y = 39.562 + 3.738\sqrt{X_{29}} + 63.484\sqrt{X_7} + 27.878\sqrt{X_6} - 2.425\sqrt{X_{28}} + 1.462\sqrt{X_2} \\ (10.972^{**}) (3.885^{**}) (4.029^{**}) (2.430) (-2.614^*) (1.879^*) \\ - 9.032\sqrt{X_{19}} \\ (-1.837^*) \quad (5)$$

R=0.778, R²=0.605, F=8.952**, SE=7.12

D) Step 15 calculated with [(X_i+1.0)⁻¹]²

$$Y = 49.624 + 1.664\sqrt{X_{29}} + 48.448\sqrt{X_7} + 28.196\sqrt{X_6} - 3.348\sqrt{X_{28}} + 2.134\sqrt{X_2} \\ (7.608^{**}) (1.247) (2.717^*) (2.028) (-3.211^{**}) (2.545^*) \\ - 31.957X_{19} - 0.993X_{27} - 1.043X_{26} + 4.810X_{20} + 10.285X_{10} \\ (-2.687^*) (-1.058) (-0.696) (0.869) (1.788)$$

$$+ 12.488X_{33} - 2.407X_{23} - 7.464X_{15} + 27.788X_{21} - 2.113X_{18} \quad (6)$$

(0.986) (-1.461) (-1.330) (0.839) (-0.641)

R=0.864, R²=0.746, F=5.086**, SE=6.63

Standard error of estimation The data on changes in the standard error of estimates for each step are shown in Fig. 2. Accuracy of estimation becomes higher with an increase in the number of the variables entered into the regression model. Consequently, it is assumed that an increase in the number of efficient peaks in the regression models results in a decrease in the standard error of the estimate accompanied by great increase in R. On the contrary, the standard error of the estimate increases despite the increased R value when inefficient peaks enter. Therefore, the selection of adequate peaks as independent variables is very important for the accuracy of the estimation. In this study, the standard error of estimation was minimized at step 15, and then increased at absolute value. This data show that variables for the 15th steps increased the accuracy of the multiple regression model. The introduction of a variable afterward often means lowering the measurement accuracy. Accordingly, the use of 15 compounds was concluded to be useful.

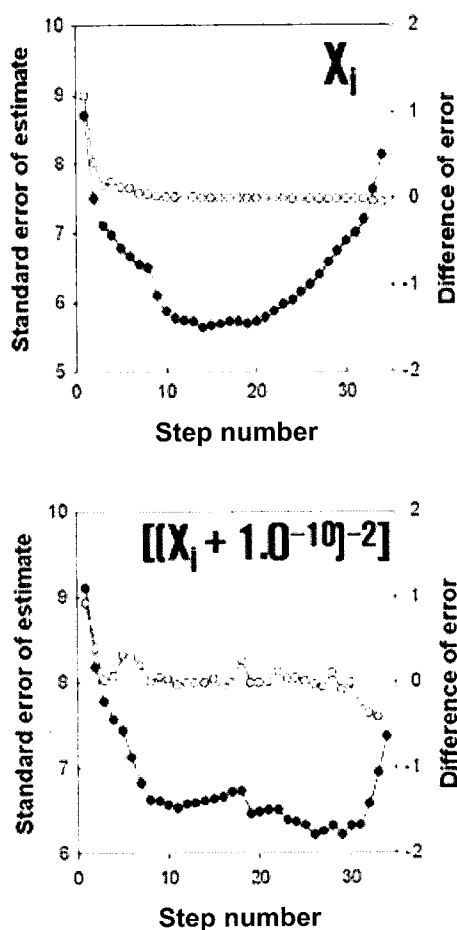


Fig. 2. Change in standard error of estimate of aroma computed for each step from the absolute value (Xi) and the absolute value transformed by square root [(Xi+1.0⁻¹⁰)⁻²]. ●-●, standard error of estimate; ○-○, difference of error.

Contributing proportion The rank of each peak and its contribution to barley bran sauce aroma is shown in Table 4 and Fig. 3. It was found that peak 29 (methyl 9,12,15-octadecatrienoate) contributed the highest proportion to the aroma of barley bran sauce. It was followed by 27 (methyl 9,12-octadecadienoate), 28 (ethyl 9,12-octadecadienoate), 12 (phenyl acetaldehyde), and 9 (methyl furfural) at

Table 4. Contributing proportion (Pi) and the rank of each peak to the aroma of barley bran sauce¹⁾

No.	Pi ²⁾ (%)		
	Xi	ln(Xi+1.0)	$\sqrt{(X_i + 10^{-10})}$
X ₁	1.10(17)	1.03(24)	1.44(19)
X ₂	3.50(6)	0.77(25)	3.74(7)
X ₃	0.29(27)	1.41(21)	1.53(18)
X ₄	1.30(16)	2.2(15)	2.13(13)
X ₅	0.43(24)	1.33(22)	1.08(21)
X ₆	0.52(22)	6.07(2)	0.44(29)
X ₇	0.67(21)	4.32(6)	2.50(12)
X ₈	0.86(20)	0.45(27)	0.15(31)
X ₉	4.81(5)	3.83(10)	0.88(23)
X ₁₀	0.09(31)	0.22(29)	0.01(34)
X ₁₁	1.77(14)	4.24(7)	3.47(9)
X ₁₂	8.70(4)	0.06(34)	7.61(4)
X ₁₃	3.49(7)	0.17(32)	2.79(11)
X ₁₄	0.28(28)	1.87(20)	4.55(6)
X ₁₅	0.22(29)	2.82(13)	0.60(26)
X ₁₆	2.98(9)	2.09(17)	1.67(17)
X ₁₇	0.01(34)	0.09(33)	0.05(33)
X ₁₈	2.08(13)	5.19(3)	0.31(30)
X ₁₉	0.88(19)	3.13(12)	0.92(22)
X ₂₀	0.14(30)	0.71(26)	0.48(28)
X ₂₁	2.33(11)	1.93(19)	0.57(27)
X ₂₂	0.02(33)	0.31(28)	0.14(32)
X ₂₃	0.31(26)	4.41(5)	2.86(10)
X ₂₄	2.87(10)	1.17(23)	0.68(25)
X ₂₅	0.47(23)	0.19(31)	1.90(15)
X ₂₆	1.04(18)	3.23(11)	0.72(24)
X ₂₇	12.73(2)	3.98(9)	9.08(3)
X ₂₈	12.72(3)	8.48(1)	13.22(1)
X ₂₉	15.57(1)	4.00(8)	7.35(5)
X ₃₀	3.14(8)	4.93(4)	3.69(8)
X ₃₁	2.33(11)	2.64(14)	9.93(2)
X ₃₂	0.04(32)	2.13(16)	2.02(14)
X ₃₃	0.34(25)	1.99(18)	1.33(20)
X ₃₄	1.72(15)	0.22(29)	1.71(16)

¹⁾X₁-X₃₄; see the legend in Table 3.

²⁾Numbers in parenthesis are rank of the contributing proportion (Pi%) of each peak.

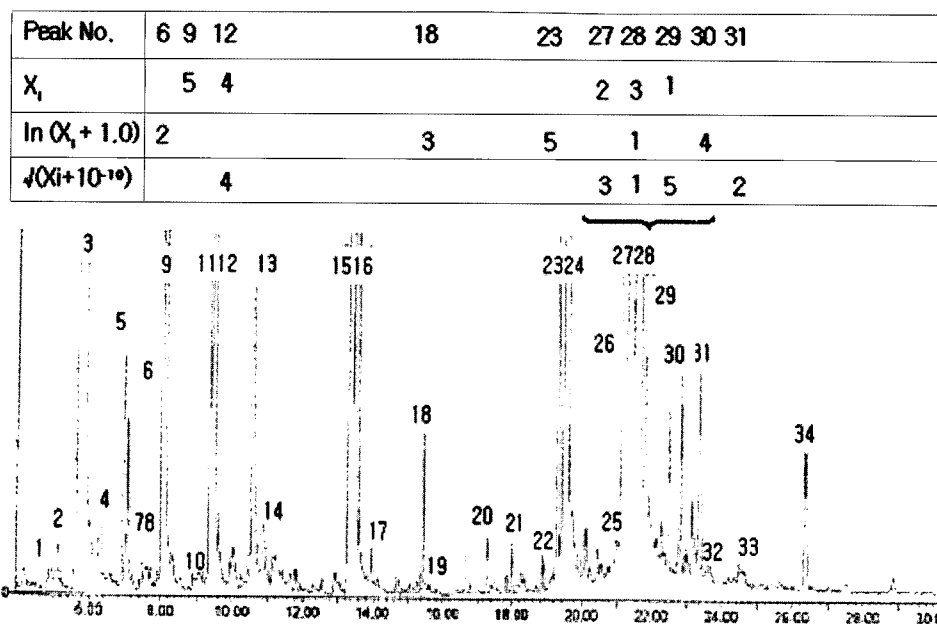


Fig. 3. Total chromatogram of aroma components in barley bran sauce and rank of the contributing proportions ($P_i\%$) of each peak transformed with 3 variables.

absolute value. On the other hand, peaks 10 (4-acetyl heptanenitrile), 32 [unknown], 22 (ethyl hexadecanoate), and 17 [2-methoxy-4-(1-propenyl) phenol] did not contribute to the aroma of barley bran sauce. When contributing portion was calculated using absolute value transformed with square roots, peak 28 (ethyl 9,12-octadecadienoate) made the highest contribution among the peaks to the aroma of barley bran sauce. The next highest values were, in descending order: 31 (9,12-octadecadienoic acid), 27 (methyl 9,12-octadecadienoate), 12 (phenyl acetaldehyde), and 29 (methyl 9,12,15-octadecatrienoate).

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