Odor-Structure Relationships in *n*-Hexenols and *n*-Hexenals

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The relationships between the chemical structures and the odor characteristics were examined on a series of highly purified *n*-hexenols and *n*-hexenals (14 isomers). The C_6-enals and the corresponding alcohols resembled in odor characteristics each other. However, the odor strength of the aldehydes was 100–1000 times higher than those of the alcohols. In the principal components analysis, the position of carbon-carbon double-bond in the C_6-compounds was closely related to the scores of the first principal component, whereas the functional groups, hydroxy and formyl groups, were related to those of the second principal component except for (*Z*)-3-hexenol.

Introduction

n-Hexenols and *n*-hexenals, which are responsible for "green odor" of green leaves, have been demonstrated to be biosynthesized from C_{18}-unsaturated fatty acids in plants [1]. Bedoukian reported the odor characteristics of all 7 isomers of the hexenols [2]. On the other hand, Meijboom and Jongenotter examined the odor threshold values and characteristics of the 4 isomers of the hexenals [3]. We synthesized a series of 14 isomers of the hexenols and hexenals, and explored the chemical structure – odor characteristic relations statistically.

Materials and Methods

IR spectra were recorded on a JIR 100 FT-IR spectrometer (JEOL, Tokyo, Japan). ^{1}H NMR and ^{13}C NMR spectra were obtained on a JNM-GX 500 spectrometer (JEOL, Tokyo, Japan). MS spectra were taken on a JMS-DX 303 spectrometer (JEOL, Tokyo, Japan). Melting points were recorded on Mettler FP-1 combined with Mettler FP-21. Melting points of 3,5-dinitrobenzoate derivatives (3,5-DNB) of the hexenols and 2,4-dinitrophenylhydrazone derivatives (2,4-DNPH) of the hexenals, are uncorrected.

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Materials

(*Z*)-2-Hexenal was purchased from Chisso Co., Ltd. (Tokyo, Japan) and 3-hexynol from Kanto Chemicals Co., Ltd. (Tokyo, Japan).

Preparation of (E)-2-hexenol and (Z)-2-hexenol

Tetrahydropyranyl ether of propargyl alcohol was treated with metallic sodium in liquid ammonia and then 1-bromopropane. The resulting hexynol was converted by Birch reduction to (*E*)-2-hexenol. (*Z*)-2-Hexenol was obtained by catalytic (*Z*)-selective hydrogenation of the hexynol using Lindlar catalyst.

(*E*)-2-Hexenol: b.p. 71.5–72.0 °C/20 mmHg; purity 99.5%; m.p. of 3,5-DNB 64.8–65.5 °C; IR (NaCl): $\nu = 3329$ (O–H), 1670 (C=C), 970 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 13.7$, 22.4, 34.4, 63.7, 129.2, 133.2; ^{1}H NMR ($CDCl_3$/TMS): $\delta = 0.91$ (t, 3H, $J = 7.36$), 1.41 (m, 2H), 2.02 (m, 2H), 2.15 (br, 1H), 4.07 (d, 2H, $J = 5.54$), 5.59–5.71 (m, 1H); MS (70 eV): m/z (%) = 100 (M^+, 18), 41 (100).

(*Z*)-2-Hexenol: b.p. 69.0–69.5 °C/20 mmHg; purity 99.3%; m.p. of 3,5-DNB 50.2–51.3 °C; IR (NaCl): $\nu = 3327$ (O–H), 1657 (C=C), 706 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 13.7$, 22.8, 29.5, 58.5, 128.8, 132.7; ^{1}H NMR ($CDCl_3$/TMS): $\delta = 0.91$ (t, 3H, $J = 7.36$), 1.39 (2H), 2.05 (2H), 2.10 (br, 1H), 4.18 (d, 2H, $J = 6.30$), 5.49–5.55 (m, 1H), 5.57–5.63 (m, 1H); MS (70 eV): m/z (%) = 100 (M^+, 3), 57 (100).

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Preparation of (E)-3-hexenol and (Z)-3-hexenol

3-Hexynol was converted to the corresponding (*Z*)- and (*E*)-3-hexenols described in 2-hexenols, respectively.

(*E*)-3-Hexenol: b.p. 72.5–73.0 °C/20 mmHg; purity 99.6%; m.p. of 3,5-DNB 46.5–47.3 °C; IR (NaCl): $\nu = 3334$ (O–H), 966 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 13.8$, 25.7, 36.0, 62.2, 124.9, 135.7; ^1H NMR ($CDCl_3$/TMS): $\delta = 0.98$ (t, 3H, $J = 7.46$), 2.03 (m, 2H), 2.16 (br, 1H), 2.26 (m, 2H), 3.61 (t, 2H, $J = 6.43$), 5.38 (m, 1H), 5.59 (m, 1H); MS (70 eV): m/z (%) = 100 (M^+, 18), 41 (100).

(*Z*)-3-Hexenol: b.p. 73.5–74.3 °C/20 mmHg; purity 99.2%; m.p. of 3,5-DNB 73.5–74.3 °C; IR (NaCl): $\nu = 3336$ (O–H, 1655 (C=C), 719 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 14.3$, 20.7, 30.8, 62.3, 124.6, 134.9; ^1H NMR ($CDCl_3$/TMS): $\delta = 0.97$ (t, 3H, $J = 7.56$), 2.08 (m, 2H), 2.21 (br, 1H), 2.32 (q, 2H), 3.62 (m, 2H), 5.33 (m, 1H), 5.54 (m, 1H); MS (70 eV): m/z (%) = 100 (M^+, 14), 67 (100).

Preparation of (E)-4-hexenol and (Z)-4-hexenol

Tetrahydrofurfuryl alcohol was reacted with thionyl chloride in pyridine and the chloride thus obtained was converted to 4-pentynol by treatment with sodium amide in liquid ammonia. The pentynol was protected with 2,3-dihydropyrane, and the pyranyl ether was treated with butyllithium in THF and then the lithium acetylide was converted to 4-hexynol by addition of methyl iodide in the presence of HMPA followed by hydrolysis. (*E*)-4-Hexenol and (*Z*)-4-hexenol were obtained from 4-hexynol as above.

(*E*)-4-Hexenol: b.p. 74.5–75.5 °C/20 mmHg; purity 99.6%; m.p. of 3,5-DNB 33.1–33.8 °C; IR (NaCl): $\nu = 3336$ (O–H), 966 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 17.9$, 28.9, 32.5, 62.5, 125.5, 130.8; ^1H NMR ($CDCl_3$/TMS): $\delta = 1.58–1.68$ (m, 5H), 2.06 (m, 2H), 2.27 (br, 1H), 3.62 (m, 2H), 5.39–5.49 (m, 2H); MS (70 eV): m/z (%) = 100 (M^+, 18), 67 (100).

(*Z*)-4-Hexenol: b.p. 73.5–74.2 °C/20 mmHg; purity 98.8%; m.p. of 3,5-DNB 24.8–25.6 °C; IR (NaCl): $\nu = 3336$ (O–H), 1655 (C=C), 700 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 12.7$, 23.3, 32.5, 62.6, 124.6, 130.0; ^1H NMR ($CDCl_3$/TMS): $\delta = 1.60–1.66$ (m, 5H), 2.13 (m, 2H), 2.38 (br, 1H), 3.64 (t, 2H, $J = 6.58$), 5.37–5.43 (m, 1H), 5.44–5.50 (m, 1H); MS (70 eV): m/z (%) = 100 (M^+, 17), 67 (100).

Preparation of 5-hexenol

Tetrahydropyran-2-methanol was converted to 5-hexynol as described above. 5-Hexynol was hydrogenated under Lindlar catalyst to 5-hexenol.

5-Hexenol: b.p. 73.5–74.0 °C/20 mmHg; purity 99.8%; m.p. of 3,5-DNB 49.8–50.5 °C; IR (NaCl): $\nu = 3346$ (O–H), 1641 (C=C), 993, 910 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 25.1$, 32.2, 33.5, 62.7, 114.6, 138.7; ^1H NMR ($CDCl_3$/TMS): $\delta = 1.46$ (m, 2H), 1.58 (m, 2H), 2.08 (m, 2H), 2.29 (br, 1H), 3.63 (2H), 4.94–5.03 (m, 2H), 5.81 (m, 1H); MS (70 eV): m/z (%) = 100 (M^+, 0.4), 67 (100).

Purification of commercial (E)-2-hexenal

The commercial (*E*)-2-hexenal was rectified through washing with aqueous sodium hydrogen carbonate solution and distillation under reduced pressure.

(*E*)-2-Hexenal: b.p. 48 °C/20 mmHg; purity 99.3%; m.p. of 2,4-DNPH 147.2–147.6 °C; IR (NaCl): $\nu = 2733$ (C–H of CHO), 1695 (C=O), 1637 (C=C), 976 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 13.5$, 21.2, 34.7, 133.2, 158.7, 194,1; ^1H NMR ($CDCl_3$/TMS): $\delta = 0.97$ (t, 3H, $J = 7.39$), 1.56 (m, 2H), 2.33 (q, 2H, $J = 7.16$), 6.13 (dd, 1H, $J = 7.84$, 15.60), 6.87 (dt, 1H, $J = 6.86$, 15.60), 9.51 (d, 1H, $J = 7.92$); MS (70 eV): m/z (%) = 98 (M^+, 100).

Preparation of (Z)-2-hexenal

(*Z*)-2-Hexenol was oxidized with activated manganese dioxide in *n*-hexane and the resulting mixture was rectified by distillation to give (*Z*)-2-hexenal.

(*Z*)-2-Hexenal: b.p. 46 °C/20 mmHg; purity 98.7%; m.p. of 2,4-DNPH 142.2–142.7 °C; IR (NaCl): $\nu = 1684$ (C=O), 1625 (C=C), 742 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 13.6$, 22.5, 29.9, 130.4, 153.2, 191,0; ^1H NMR ($CDCl_3$/TMS): $\delta = 0.98$ (t, 3H, $J = 7.39$), 1.56 (m, 2H), 2.60 (m, 2H), 5.97 (m, 1H), 6.64 (m, 1H), 10.08 (d, 1H, $J = 8.17$); MS (70 eV): m/z (%) = 98 (M^+, 58), 83 (100).

Preparation of (E)-3-hexenal and (Z)-3-hexenal

1-Butynyllithium was prepared by introducing 1-butyne into a hexane solution of butyllithium under dry nitrogen atmosphere. The hexane was replaced with toluene and HMPA mixture (1:1). To a suspension of 1-butynyllithium was added bromoacetaldehyde dimethyl acetal and the mixture was heated to 60 °C for 1 h. Resulting 3-hexynal dimethyl acetal was converted to (*E*)-hexenal by Birch reduction followed by hydrolysis with an aqueous solution of oxalic acid at room temperature. (*Z*)-3-Hexenal was obtained *via* catalytic hydrogenation of 3-hexynal dimethyl acetal followed by hydrolysis.

(*E*)-3-Hexenal: b.p. 35 °C/20 mmHg; purity 99.0%; m.p. of 2,4-DNPH 99.2–99.6 °C; IR (NaCl): $\nu = 2723$ (C–H of CHO), 1730 (C=O), 970 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 13.5, 25.8, 47.3, 118.3, 138.4, 200.3$; ^1H NMR ($CDCl_3$/TMS): $\delta = 1.01$ (t, 3H, $J = 7.51$), 2.09 (m, 2H,), 3.11 (dd, 2H, $J = 0.90, 6.86$), 5.50 (dt, 1H, $J = 6.85, 15.45$), 5.67 (dt, 1H, $J = 6.29, 15.44$), 9.65 (1H); MS (70 eV): m/z (%) = 98 (M^+, 34), 41 (100).

(*Z*)-3-Hexenal: b.p. 36 °C/20 mmHg; purity 99.0%; m.p. of 2,4-DNPH 102.3–103.1 °C; IR (NaCl): $\nu = 2723$ (C–H of CHO), 1728 (C=O), 1652 (C=C), 723 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 13.9, 21.0, 42.5, 117.5, 137.0, 199.7$; ^1H NMR ($CDCl_3$/TMS): $\delta = 0.99$ (t, 3H, $J = 7.56$), 2.06 (m, 2H), 3.18 (d, 2H, $J = 7.27$), 5.51 (m, 1H), 5.70 (m, 1H), 9.67 (1H); MS (70 eV): m/z (%) = 98 (M^+, 34), 41 (100).

Preparation of (E)-4-hexenal and (Z)-4-hexenal

4-Hexynal dimethyl acetal was prepared from 1-propynyllithium and 3-bromopropionaldehyde dimethyl acetal in a similar manner as above, except that the coupling reaction was conducted at room temperature. 4-Hexynal dimethyl acetal was led to (*E*)-4-hexenal and (*Z*)-4-hexenal by the similar methods as above.

(*E*)-4-Hexenal: b.p. 37 °C/20 mmHg; purity 99.5%; m.p. of 2,4-DNPH 122.7–123.1 °C; IR (NaCl): $\nu = 2723$ (C–H of CHO), 1728 (C=O), 968 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 17.8, 25.2, 43.5, 126.4, 129.0, 202.3$; ^1H NMR ($CDCl_3$/TMS): $\delta = 1.64$ (dd, 3H, $J = 1.13, 5.95$), 2.32 (m, 2H), 2.48 (m, 2H), 5.39–5.52 (m, 2H), 9.75 (1H); MS (70 eV): m/z (%) = 98 (M^+, 79), 41 (100).

(*Z*)-4-Hexenal: b.p. 38 °C/20 mmHg; purity 99.0%; m.p. of 2,4-DNPH 99.5–99.8 °C; IR (NaCl): $\nu = 2723$ (C–H of CHO), 1726 (C=O), 1657 (C=C), 700 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 12.7, 19.8, 43.7, 125.5, 128.1, 202.2$; ^1H NMR ($CDCl_3$/TMS): $\delta = 1.63$ (m, 3H), 2.38 (m, 2H), 2.49 (m, 2H), 5.33–5.39 (m, 1H), 5.47–5.54 (m, 1H), 9.77 (t, 1H, $J = 1.59$); MS (70 eV): m/z (%) = 98 (M^+, 68), 41 (100).

Preparation of 5-hexenal

5-Hexenol was oxidized to give 5-hexenal with pyridinium chlorochromate (PCC) in dichloromethane at room temperature.

5-Hexenal: b.p. 35 °C/20 mmHg; purity 97.7%; m.p. of 2,4-DNPH 102.9–103.2 °C; IR (NaCl): $\nu = 2723$ (C–H of CHO), 1726 (C=O), 1641 (C=C), 997, 914 cm^{-1}; ^{13}C NMR ($CDCl_3$/TMS): $\delta = 21.2, 33.0, 43.1, 115.6, 137.6, 202,4$; ^1H NMR ($CDCl_3$/TMS): $\delta = 1.74$ (m, 2H), 2.10 (m, 2H), 2.45 (m, 2H), 4.98–5.05 (m, 2H), 5.77 (m, 1H), 9.77 (1H); MS (70 eV): m/z (%) = 98 (M^+, 6), 54 (100).

Purification of n-hexenols

All *n*-hexenols were converted to the corresponding 3,5-dinitrobenzoates, which were purified by recrystallization of the derivatives from ethanol followed by hydrolysis with a base and steam distillation.

Purification of n-hexenals

All hexenals were purified by fractional distillation using spinning band type distillating apparatus (40 theoretical plates) under reduced pressure.

Determination of the odor threshold values

All samples were diluted with dipropylene glycol in brandy glass. They were sniffed by trained flavorists.

Determination of the taste threshold values

All samples were diluted with 95% ethanol at first and then with distilled water. They were tested by keeping in their mouths of trained flavorists.

Sensory evaluation

Five trained flavorists sniffed paper strips dipped in 1% ethanolic solution hexenols or hex-

enals. They were asked to describe the sensory characteristics using the seven sensory descriptors listed below, in which the term of green odor was further classified into four descriptive terms.

1. Green
   - 1−1 Leafy green: an image of leaves of trees.
   - 1−2 Grassy green: an image of grasses and stems.
   - 1−3 Insect-like green: reminiscent of an image of insect-odor, *i.e.* beetles, bugs etc.
   - 1−4 Vegetable-like green: an image of vegetable, *i.e.* tomatoes, green peppers, cabbages etc.
2. Fruity: an image of fruits, *i.e.* apples, berries, pears etc.
3. Sweet: degree of sweetness.
4. Fresh: degree of freshness.
5. Spicy: an image of pepper, nutmeg, cinnamon etc.
6. Oily-fatty: oily-fatty, waxy, rancid.
7. Herbal: an image reminiscent of bitterness of crude drugs.

Score sheets with a 6-point scale ranging from threshold to very intense, *i.e.* 0 = threshold, 1 = very weak, 2 = weak, 3 = medium, 4 = intense, and 5 = very intense, were used for evaluation of test samples. The average scores of five panellers' were adopted as the odor-strenght of the sensory attributes.

Statistical analysis

The average scores from sensory evaluation were subjected to principal component analysis (PCA) [4] using "ANALYST" (analyzer programs for statistical data, Fujitsu, Tokyo, Japan) on a FACOM M-380 computer (Fujitsu, Tokyo, Japan).

Results and Discussion

The threshold values of odor and taste are summarized in Table I. As seen in the table, the effect of geometry in the threshold values of odor and taste was much lower than that of the position of double bond. The values for hexenols were 10 to 1000 times higher than those for the corresponding hexenals having the same position of double bond and geometry.

The olfactory characteristics of the *n*-hexenols and *n*-hexenals are presented using radar charts as in Fig. 1. Although the absolute values of descriptive terms of *n*-hexenals in the chart could not be directly compared with those of *n*-hexenols because of their differences of dilution, close resemblances were found between the hexenols and hexenals having the same position and geometry of double bond.

With 2-hexenols and 2-hexenals, Fruity, Sweet and Fresh were imaged. As shifting the double bond to the ω-end, the odor profiles tended to have Oily-fatty and Herbal images. However characteristics due to the differences in geometry of the double bond were not clearly shown from these charts.

Statistical analysis

The data from sensory evaluation were statistically analyzed using principal component analysis to characterize the odor profiles of the tested compounds. The analysis was carried out with all the 14 compounds using the 10 explanatory variables, *i.e.*, descriptive terms. Table II shows the resulting eigenvalues, eigenvectors and the proportions of the correlation matrics from the first principal component to the sixth. As the cumulative proportion up to the second principal component was

Table I. Threshold values (ppm) of *n*-hexenols and *n*-hexenals in odor and taste.

C_6-Compounds Double bond position Geometry	C-2 (*E*)	 (*Z*)	C-3 (*E*)	 (*Z*)	C-4 (*E*)	 (*Z*)	C-5
Odor							
n-Hexenol	10	10	1	1	0.1	0.1	1
n-Hexenal	0.01	0.01	0.001	0.001	0.001	0.001	0.001
Taste							
n-Hexenol	0.6	2	1	0.03	0.3	0.09	2
n-Hexenal	0.06	0.08	0.006	0.0008	0.008	0.002	0.002

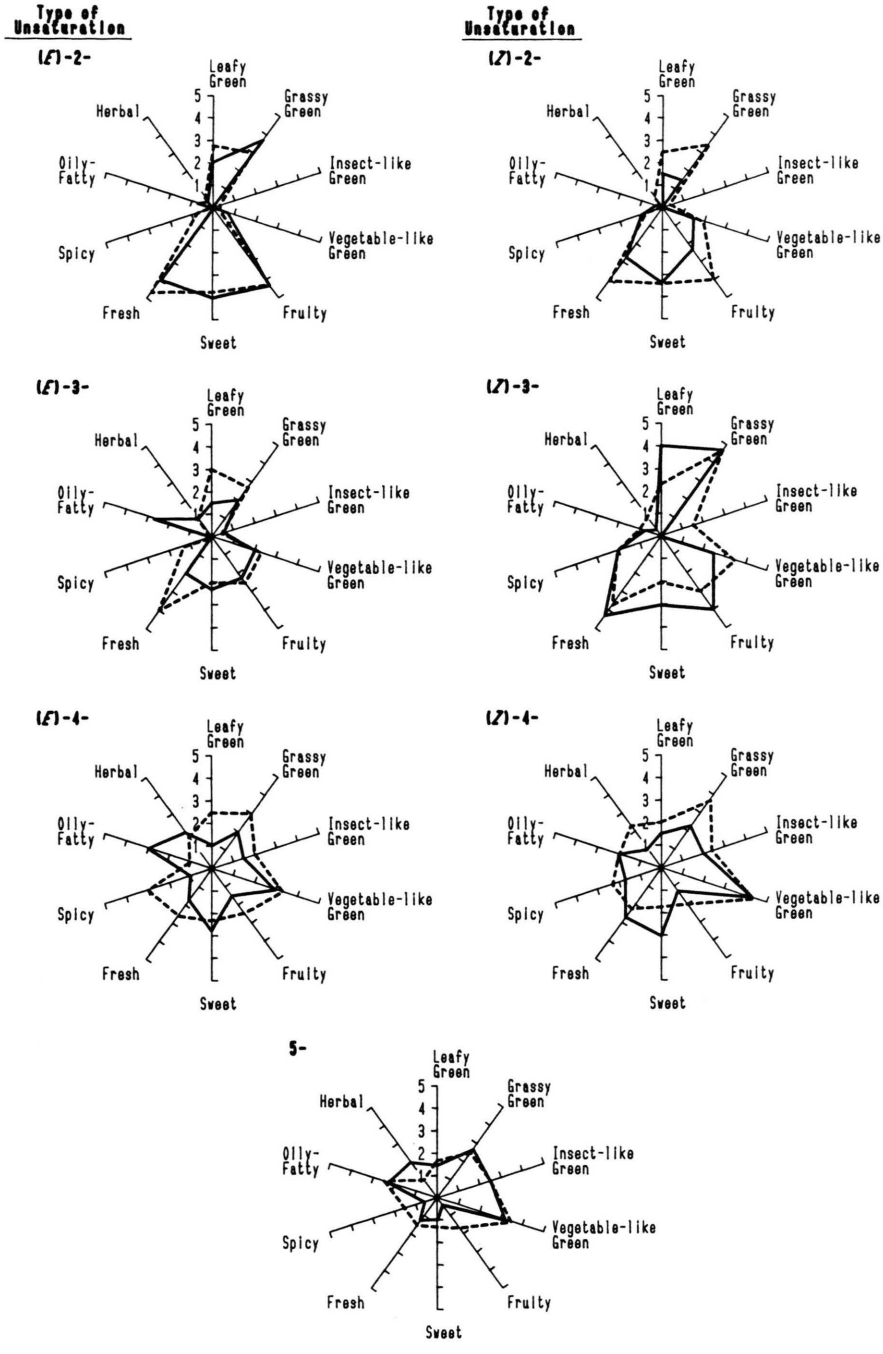

Fig. 1. Odor profiles of *n*-hexenols and *n*-hexenals. ——— for *n*-hexenols; --------- for *n*-hexenals.

over 80% and the proportions after the third principal component were remarkably small, further analysis was made on the first and the second principal components to summarize the odor images.

Fig. 2 shows the plot of the score of each compound as well as the vectorized patterns of the each explanatory variable on the $x-y$ plane, where the x-axis is given for the first principal component

Table II. The principal components analyses of the odor of *n*-hexenols and *n*-hexenals.

Odor description	PC 1	PC 2	PC 3	PC 4	PC 5	PC 6
Leafy green	0.6473	0.6558	0.0226	−0.2643	−0.0111	0.2352
Grassy green	0.3818	0.7667	0.4528	0.1582	−0.1058	−0.1089
Insect-like green	−0.8935	0.2881	0.0149	0.0999	0.0348	−0.2155
Vegetable-like green	−0.7932	0.4983	−0.1188	0.1201	−0.1982	−0.0404
Fruity	0.9281	0.1573	0.1485	0.1830	0.0457	0.0523
Sweet	0.7808	−0.3105	−0.1854	0.4850	0.0649	0.0385
Fresh	0.9243	0.2753	0.0076	0.0292	0.0788	−0.1020
Spicy	−0.2476	0.8235	−0.4590	0.1385	0.0269	0.0991
Oily-fatty	−0.8475	−0.2111	0.2697	0.2315	−0.1675	0.2715
Herbal	−0.8223	0.2401	0.1868	0.0584	0.4618	0.0791
Eigenvalue	5.773	2.326	0.595	0.467	0.306	0.220
Proportion	57.732	23.265	5.947	4.666	3.063	2.196
Cumulative proportion	57.732	80.997	86.944	91.610	94.673	96.869

PC: Principal component.

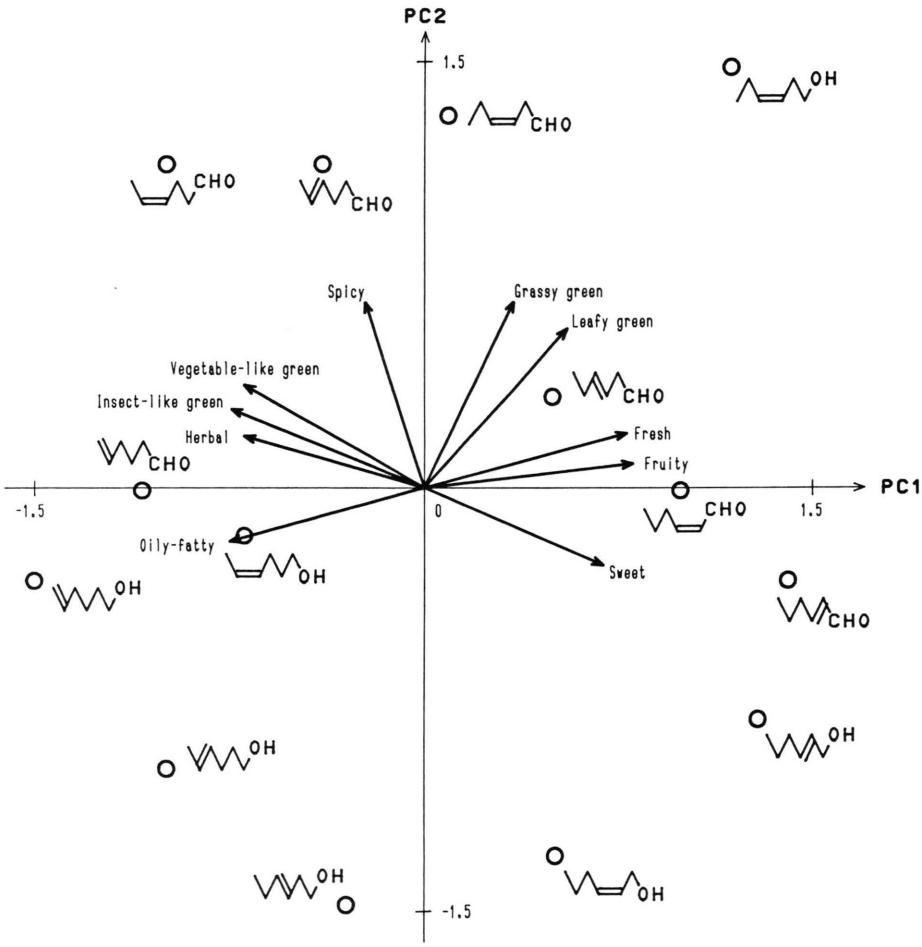

Fig. 2. The Score plots and the vectors of the eigenvalues on the plane of the first principal component *vs.* the second principal component in *n*-hexenols and *n*-hexenals.

and the *y*-axis for the second. Fresh, Fruity and Sweet notes greatly correlated with *x*-axis, whereas Green and Spicy notes correlated with *y*-axis. Each aldehyde having a double bond at C-2 position was located in the right hand of the figure, which indicated that they had a fruity and sweet image. Whereas, the corresponding alcohols were located below, and they showed an image of more sweet but less green than the corresponding aldehydes. (*Z*)-3-Hexenol showed the highest values of the both components, which meant this isomer had a high green and fresh note. The compounds having a double-bond at C-4 or C-5 position, especially 5-hexenol and 5-hexenal, were located to the left side of the figure, that meant they had strong Oily-fatty, Insect-like green and Herbal images. 4-Hexenals located in the left and upper part of the figure and expressed a strong image of Spicy and Vegetable-like green in contrast to the corresponding alcohols located in the left and lower part. (*Z*)-3-Hexenal located on the upper part near the *y*-axis which indicated a strong image of Spicy and grassy green, but it can be distinguished from (*Z*)-3-hexenol which located at the righter side showing an image of Fruity and Fresh. (*E*)-3-Hexenal was weaker in Grassy green and Spicy than (*Z*)-3-hexenal and is located in the lower part of the figure.

It is notable from this analysis that the position of a double bond closely related to the scores of the first principal component and the type of the functional group (alcohol/aldehyde) to those of the second principal component. Only the (*Z*)-3-hexenol deviated from these results and will require an additional study.

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