Chemical Structure-Odor Correlation in Series of Synthetic Methylene Interrupted *n*-Nonadien-1-ols

Yasunobu Sakoda[a], Kenji Matsui[a], Yoshihiko Akakabe[a], Jun Suzuki[b],
Akikazu Hatanaka[c], and Tadahiko Kajiwara[a]

[a] Department of Biological Chemistry, Faculty of Agriculture, Yamaguchi University, Yamaguchi 753, Japan
[b] Research Laboratories, Soda Aromatic CO., LTD, Tokyo, Japan
[c] Department of Life Science, Graduate School of Integrated Arts and Science, University of East Asia, Shimonoseki 751, Japan

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Structure-Odor Relation, Synthesis, Nonadienols, Principal Component Analysis

Chemical structure-odor correlations in the isomers of *n*-C_9-methylene interrupted dienols were explored using synthetic nine isomers of these alcohols. The synthetic dienols were purified by recrystallization or column chromatography of their 3,5-dinitrobenzoate derivatives.

Chemical structure-odor correlations in all the isomers of the purified *n*-nonadien-1-ols were analyzed by treating the data obtained statistically with the principal component analysis method (Sakoda *et al.,* 1995; Cramer *et al.,* 1988) in comparison with those of *n*-nonen-1-ols. The odor profiles of the *n*-nonadien-1-ols were attributable largely to the geometries of the isomers, compared with *n*-nonen-1-ols (Sakoda *et al.*, 1995). With the principal component analysis, the odor profiles of the series of the dienols were successfully integrated into the first and the second principal components. The first component (PC 1) consisted of combined characteristics of fruity, fresh, sweet, herbal and oily-fatty, and the second component (PC 2) leaf or grassy and vegetable-like. Of the methylene interrupted dienol isomers, (2*E*,6*Z*)- and (3*Z*,6*Z*)-nonadien-1-ols which are natural products and have (6*Z*) in the same, deviated markedly from the other isomers as seen in (6*Z*)-nonen-1-ol of *n*-nonen-1-ols. That suggests that the double bond of (ω3*Z*) was an important factor for natural characteristic odor.

Introduction

Recently, the relations between the characteristic odor and position and/or geometry of a double bond in various isomers of *n*-C_6- and C_9-monoenols were successfully evaluated (Hatanaka *et al.,* 1992; Sakoda *et al.,* 1995). With these investigations, it has been revealed that the position and the geometry of double bond in primary alcohol has a significant and regular effect on its odor profile. Interestingly, naturally occurring (3*Z*)-hexen-1-ol, which is known as "leaf alcohol", and naturally occurring (6*Z*)-nonen-1-ol were found to be deviated markedly from the relationship and showed a unique odor profile. These findings indicated that (ω3*Z*)-moiety in a primary alcohol had rather specific interaction with human odor-sensory system.

n-C_9-dien-1-ols and C_9-dienals such as violet leaf aldehyde; (2*E*,6*Z*)-nonadienal, cucumber alcohol; (2*E*,6*Z*)-nonadien-1-ol, and melon alcohol; (3*Z*,6*Z*)-nonadien-1-ol are also known to be characteristic constituents of flavors of vegetables and fruits. With a compound having two double bonds, the odor profile is expected to be largely different from the corresponding compound having only one double bond. Nevertheless, the chemical structure-odor correlation in the compound having two double bonds has not been explored so far. Here, we report unequivocal syntheses of the isomer of *n*-C_9-methylene interrupted dienols analogous to (2*E*,6*Z*)- and (3*Z*,6*Z*)-nonadien-1-ols, and chemical structure-odor correlation of them are reported.

Materials and Methods

IR spectra were recorded on a JIR 100 FT-IR spectrometer (JEOL, Tokyo, Japan). ^1H NMR and ^{13}C NMR spectra were obtained on a JNM-EX

Reprint requests to Prof. Dr. Tadahiko Kajiwara.

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500 spectrometer (JEOL, Tokyo, Japan) at 500 MHz and 125 MHz, respectively.

Preparation of (2E,6E)- and (2Z,6E)-nonadien-1-ols

As an α-site counterpart, propargyl alcohol was protected with 3,4-dihydro-2*H*-pyran to give 2-(2-propynyloxy)-tetrahydropyran in 88% yield. On the other hand, as an ω-site counterpart, 3-butyn-1-ol was prepared by coupling of ethylene oxide with sodium acetylide in liquid ammonia. The ynol was protected with 3,4-dihydro-2*H*-pyran to give 2-(3-butynyloxy)-tetrahydropyran in 90% yield. Acetylenic coupling of the tetrahydropyran with ethyl bromide gave 2-(3-hexynyloxy)-tetrahydropyran in 60% yield. The pyranyl ether was converted to 3-hexyn-1-ol with 30% (w/w) phosphoric acid-methanol in 98% yield. Birch reduction of the ynol with sodium in liquid ammonia gave (3*E*)-hexen-1-ol in 84% yield. Bromination of the alcohol with phosphorus tribromide gave (3*E*)-hexenyl bromide in 64% yield. The 2-(2-propynyloxy)-tetrahydropyran was converted to its lithium salt with *n*-butyllithium in tetrahydrofuran (THF) and coupled with (3*E*)-hexenyl bromide in hexamethylphosphoric triamide (HMPA) to give 2-[(6*E*)-nonen-2-ynyloxy]-tetrahydropyran in 33% yield. The pryranyl ether was converted to (6*E*)-nonen-2-yn-1-ol with 30% phosphoric acid in 81% yield. The ynol was hydrogenated over Lindlar catalyst to give (2*Z*,6*E*)-nonadien-1-ol in 98% yield (Lindlar *et al.,* 1966). (2*E*,6*E*)-nonadien-1-ol was obtained by reduction with lithium aluminum hydride (LAH) in ether in 92% yield.

(2*Z*,6*E*)-nonadien-1-ol: b.p. 64.0–66.0 °C/0.27 mmHg; purity 99.6%; m.p. of 3,5-DNB 38.0–40.0 °C; IR (film) cm^{-1}: 3332 (O–H), 3016 (C=C–H), 2962, 2931, 2873 (C–H), 1655 (C=C), 1026 (C–O), 966 (*E*, CH=CH); ^{13}C NMR ($CDCl_3$/TMS): δ = 13.9, 25.6, 27.6, 32.4, 58.6, 128.1, 128.7, 132.4, 133.0 ppm; ^{1}H NMR ($CDCl_3$/TMS): δ = 0.98 (t, 3H, J = 7.6), 1.49 (br s, 1H), 2.17–1.97 (m, 6H), 4.17 (d, 2H, J = 4.4), 5.65–5.34 ppm (m, 4H).

(2*E*,6*E*)-nonadien-1-ol: b.p. 62.0–63.0 °C/0.2 mmHg; purity 99.4%; m.p. of 3,5-DNB 71.0–72.0 °C; IR (film) cm^{-1}: 3336 (O–H), 3028 (C=C), 2964, 2921, 2848 (C–H), 1670 (C=C), 1092 (C–O), 968 (*E*, CH=CH); ^{13}C NMR ($CDCl_3$/TMS): δ = 14.0, 25.6, 32.2, 32.3, 63.8, 128.3, 129.2, 132.6, 132.8 ppm; ^{1}H NMR ($CDCl_3$/TMS): δ = 0.96 (t, 3H, J = 7.3), 1.56 (br s, 1H), 2.13–1.96 (m, 6H), 4.08 (d, 2H, J = 3.4), 5.49–5.39 (m, 2H), 5.69–5.64 ppm (m, 2H).

Preparation of (2E,6Z)- and (2Z,6Z)-nonadien-1-ols

As an ω-site counterpart, 3-hexyn-1-ol was hydrogenated over Lindlar catalyst to give (3*Z*)-hexen-1-ol in 98% yield. (3*Z*)-hexen-1-ol was tosylated with tosyl chloride (Ts–Cl) to give (3*Z*)-hexenyl tosylate in 90% yield. Bromination of the tosylate with sodium bromide gave (3*Z*)-hexenyl bromide in 70% yield. The 2-(2-propynyloxy)-tetrahydropyran was converted to its lithium salt with *n*-butyllithium in tetrahydrofuran (THF) and coupled with (3*Z*)-hexenyl bromide in hexamethylphosphoric triamide (HMPA) to give 2-[(6*Z*)-nonen-2-ynyloxy]-tetrahydropyran in 25% yield. The pyranyl ether was converted to (6*Z*)-nonen-2-yn-1-ol with 30% phosphoric acid in 83% yield. The ynol was hydrogenated over Lindlar catalyst to give (2*Z*,6*Z*)-nonadien-1-ol in 93% yield. (2*E*,6*Z*)-nonadien-1-ol was obtained by reduction with lithium aluminum hydride in ether in 91% yield.

(2*Z*,6*Z*)-nonadien-1-ol: b.p. 51.0–53.0 °C/0.1 mmHg; purity 99.9%; m.p. of 3,5-DNB 20.1–22.3 °C; IR (film) cm^{-1}: 3342 (O–H), 3010 (C=C–H), 2962, 2933 (C–H), 1654 (C=C), 1026 (C–H), 721 (*Z*, CH=CH); ^{13}C NMR ($CDCl_3$/TMS): δ = 14.3, 20.6, 27.0, 27.6, 58.5, 128.0, 128.9, 132.3, 132.6 ppm; ^{1}H NMR ($CDCl_3$/TMS): δ = 0.96 (t, 3H, J = 7.3), 1.62 (br s, 1H), 2.02–2.15 (m, 6H), 4.17 (d, 2H, J = 6.4), 5.29–5.66 ppm (m, 4H).

(2*E*,6*Z*)-nonadien-1-ol: b.p. 54.0–56.0 °C/0.25 mmHg; purity 99.3%; m.p. of 3,5-DNB 21.6–23.0 °C; IR (film) cm^{-1}: 3334 (O–H), 3006 (C=C–H), 2962, 2933 (C–H), 1670, 1652 (C=C), 1092 (C–O), 968 (*E*, C=C), 715 (*Z*, C=C); ^{13}C NMR ($CDCl_3$/TMS): δ = 14.3, 20.6, 26.8, 32.3, 63.7, 128.2, 129.3, 132.2, 132.7 ppm; ^{1}H NMR ($CDCl_3$/TMS): δ = 0.96 (t, 3H, J = 7.6), 1.55 (br s, 1H), 2.15–2.00 (m, 6H), 4.08 (d, 2H, J = 4.9), 5.42–5.29 (m, 2H), 5.72–5.66 ppm (m, 2H).

Preparation of (3E,6E)- and (3Z,6E)-nonadien-1-ols

As an ω-site counterpart, acetylenic coupling of the 2-(2-propynyloxy)-tetrahydropyran with ethyl bromide gave 2-(2-pentynyloxy)-tetrahydropyran in 90% yield. The pyranyl ether was converted to 2-pentyn-1-ol with 5% (w/w) PTS-methanol in 90% yield. (2*E*)-penten-1-ol was obtained by Birch reduction in 85% yield. Bromination of the (2*E*)-penten-1-ol with phosphorous tribromide gave (2*E*)-pentenyl bromide in 74% yield. 2-[(6*E*)-nonen-3-ynyloxy]-tetrahydropyran was prepared by Grignard coupling of 2-(3-butynyloxy)-tetrahydropyran with (2*E*)-pentenyl bromide in 86% yield. The pyranyl ether was converted to (6*E*)-nonen-3-yn-1-ol with 5% PTS-methanol in 81% yield. The ynol was hydrogenated over Lindlar catalyst to give (3*Z*,6*E*)-nonadien-1-ol in 97% yield. (3*E*,6*E*)-nonadien-1-ol was obtained by Birch reduction in 98% yield.

(3*Z*,6*E*)-nonadien-1-ol: b.p. 60.0–61.0 °C/0.8 mmHg; purity 97.0%; IR (film) cm^{-1}: 3334 (O–H), 3040 (C=C–H), 2980, 2950, 2898 (C–H), 1660 (C=C), 1045 (C–H), 965 (*E*, C=C), 723 (*Z*, CH=CH); ^{13}C NMR ($CDCl_3$/TMS): δ = 13.8, 25.5, 30.4, 30.8, 62.2, 125.6, 127.0, 131.2, 132.6 ppm ^{1}H NMR ($CDCl_3$/TMS): δ = 0.96 (t, 3H, J = 7.3), 1.76 (br s, 1H), 2.03–1.97 (m, 2H), 2.38–2.29 (m, 2H), 2.77 (t, 2H, J = 7.3), 3.64 (t, 2H, J = 6.7), 5.63–5.33 ppm (m, 4H).

(3*E*,6*E*)-nonadien-1-ol: b.p. 66.0–69.0 °C/0.8 mmHg; purity 99.1%; m.p. of 3,5-DNB 38.0–41.0 °C; IR (film) cm^{-1}; 3335 (O–H), 3030 (C=C–H), 2998, 2945, 2880 (C–H), 1665 (C=C), 1034 (C–H), 963 (*E*, CH=CH); ^{13}C NMR ($CDCl_3$/TMS): δ = 14.3, 26.0, 36.1, 36.5, 62.6, 126.9, 127.6, 132.8, 133.5 ppm; ^{1}H NMR ($CDCl_3$/TMS): δ = 0.97 (t, 3H, J = 7.3), 1.72 (br s, 1H), 2.04–1.98 (m, 2H), 2.31–2.26 (m, 2H), 2.71 (t, 2H, J = 6.1), 3.63 (t, 2H, J = 6.4), 5.62–5.36 ppm (m, 4H).

Preparation of (3Z,6Z)-nonadien-1-ol

As an ω-site counterpart, bromination of the 2-pentyn-1-ol with phosphorus tribromide gave 2-pentynyl bromide in 80% yield. 2-[(3,6)-nondiynyloxy]-tetrahydropyran was prepared by Grignard coupling of 2-(3-butynyloxy)-tetrahydropyran with 2-pentynyl bromide in 74% yield. The pyranyl ether was converted to (3,6)-nonadiyn-1-ol with 5% PTS-methanol in 93% yield. The ynol was hydrogenated over Lindlar catalyst to give (3*Z*,6*Z*)-nonadien-1-ol in 96% yield.

(3*Z*,6*Z*)-nonadien-1-ol: b.p. 54.0–56.0 °C/0.2 mmHg; purity 96.7%; IR (film) cm^{-1}: 3340 (O–H), 3025 (C=C–H), 2975, 2940 (C–H), 1658 (C=C), 1042 (C–H), 720 (*Z*, CH=CH); ^{13}C NMR ($CDCl_3$/TMS): δ = 14.2, 20.6, 28.5, 30.8, 62.2, 125.4, 126.9, 131.4, 132.1 ppm; ^{1}H NMR ($CDCl_3$/TMS): δ = 0.97 (t, 3H, J = 7.3), 1.72 (br s, 1H), 2.08 (t, 2H, J = 7.3), 2.34–2.32 (m, 2H), 2.82 (t, 2H, J = 7.0), 3.65 (t, 2H, J = 6.4), 5.57–5.28 ppm (m, 4H).

Preparation of (2Z,5Z)-nonadien-1-ol

As an ω-site counterpart, acetylenic coupling of 2-(2-propynyloxy)-tetrahydropyran with propyl bromide gave 2-(2-hexynyloxy)-tetrahydropyran in 79% yield. The pyranyl ether was converted to 2-hexyn-1-ol with 5% (w/w) PTS-methanol in 91% yield. Bromination of the 2-hexyn-1-ol with phosphorous tribromide gave 2-hexynyl bromide in 66% yield. 2-[(2,5)-nonadiynyloxy]-tetrahydropyran was prepared by Grignard coupling of 2-(2-propynyloxy)-tetrahydropyran with 2-hexynylbromide in 73% yield. The pyranyl ether was converted to (2,5)-nonadiyn-1-ol with 5% PTS-methanol in 92% yield. The ynol was hydrogenated over Lindlar catalyst to give (2*Z*,5*Z*)-nonadien-1-ol in 95% yield.

(2*Z*,5*Z*)-nonadien-1-ol: b.p. 67.0–69.0 °C/0.8 mmHg; purity 97.3%; IR (film) cm^{-1}: 3345 (O–H), 3032 (C=C–H), 2975, 2870 (C–H), 1655 (C=C), 1045 (C–H), 700 (*Z*, CH=CH); ^{13}C NMR ($CDCl_3$/TMS): δ = 14.2, 23.2, 26.4, 29.8, 59.0, 127.7, 129.2, 131.1, 131.6 ppm; ^{1}H NMR ($CDCl_3$/TMS): δ = 0.91 (t, 3H, J = 7.6), 1.43–1.34 (m, 2H), 1.76 (br s, 1H), 2.03 (q, 2H, J = 5.2), 2.83 (t, 2H, J = 6.4), 4.22 (d, 2H, J = 6.1), 5.47–5.33 (m, 2H), 5.67–5.50 ppm (m, 2H).

Preparation of (4Z,7Z)-nonadien-1-ol

As an α-site counterpart, 2-(4-pentynyloxy)-tetrahydropyran was obtained in 44% yield by chlorination of tetrahydrofurfuryl alcohol with thionyl chloride in pyridine, followed by cleavage of tetrahydrofurfuryl chloride with sodium amide in liquid ammonia and subsequent protection (4-pentyn-1-ol) with 3,4-dihydro-2*H*-pyran. On the other hand, as an ω-site counterpart, 2-(2-propynyloxy)-tetrahydropyran was converted to its lithium salt with *n*-butyllithium in tetrahydrofuran (THF) and coupled with methyl iodide in hexamethylphosphoric triamide (HMPA) to give 2-(2-butynyloxy)-

tetrahydropyran in 57% yield. The pyranyl ether was converted to 2-butyn-1-ol with 5% (w/w) PTS-methanol in 98% yield. Bromination of the 2-hexyn-1-ol with phosphorous tribromide gave 2-butynyl bromide in 78% yield. 2-[(4,7)-nonadiynyloxy]-tetrahydropyran was prepared by Grignard coupling of 2-(4-pentynyloxy)-tetrahydropyran with 2-butynyl bromide in 63% yield. The pyranyl ether was converted to (4,7)-nonadiyn-1-ol with 5% PTS-methanol in 90% yield. The ynol was hydrogenated over Lindlar catalyst to give (4*Z*,7*Z*)-nonadien-1-ol in 97% yield (Lindlar, *et al.,* 1966).

(4*Z*,7*Z*)-nonadien-1-ol: b.p. 61.0–65.0 °C/0.8 mmHg; purity 96.9%; IR (film) cm^{-1}: 3352 (O–H), 3035 (C=C–H), 2945, 2875 (C–H), 1660 (C=C), 1054 (C–H), 695 (*Z*, CH=CH); ^{13}C NMR ($CDCl_3$/TMS: δ = 12.7, 23.6, 25.3, 32.6, 62.4, 124.1, 128.7, 129.2 ppm; ^1H NMR ($CDCl_3$/TMS): δ = 1.76–1.62 (m, 6H), 2.78–2.12 (m, 2H), 2.80 (t, 2H, J = 6.0), 3.65 (t, 2H, J = 6.4), 5.46–5.53 ppm (m, 4H).

Purification of n-nonadien-1-ols

A C_9-unsaturated alcohol (10.0 g, 70.4 mmol) synthesized as above was added into a solution of 3,5-dinitrobenzoyl chloride (17.8 g, 77.4 mmol) in benzene (100 ml). Pyridine (6.1 ml) was added into the mixture and stirred at room temp. The reaction mixture was extracted with ether. The extract was washed with sat. $NaHCO_3$ soln. and brine, dried over Na_2SO_4 (anhydrous), and evaporated *in vacuo* to give a crude 3,5-dinitrobenzoate. It was repeatedly recrystallized from ethanol to give pure 3,5-dinitrobenzoate derivatives in 89–99% yield.

The purified 3,5-dinitrobenzoate derivative (4.0 g, 11.9 mmol) was added into 10% NaOH soln. (150 ml) and then stirred at room temp. The mixture was extracted with ether and washed with brine. The extract was dried over Na_2SO_4 (anhydrous) and concentrated *in vacuo* to give highly pure *n*-nonadien-1-ols (over 96.9% purity) in 82–92% yield (1.4–1.6 g, 97.5–11.0 mmol).

Odor characteristics

Sensory evaluation

Paper strips dipped in 1% triethyl citrate solutions of the synthesized alcohols were sniffed by three trained flavorists. They were asked to describe the sensory characteristics using eight sensory descriptive terms: leaf or grassy green an image of grasses, stems, and leaves; vegetable-like an image of vegetable, i.e., tomatoes, green peppers, cabbages etc.; fruity an image of fruits, i.e. apples, berries, pears etc.; sweet degree of sweetness; fresh degree of freshness; spicy an image of pepper, nutmeg, cinnamon etc.; oily-fatty, waxy, rancid; herbal an image reminiscent of bitterness of crude drugs. Score sheets with four-point scale ranging from threshold to very intense: i.e. 0 = threshold, 1 = very weak, 2 = intense, 3 = very intense, were used for the evaluation of the test samples. The average scores of three panellers were adopted as the odor-strength of the sensory attributes.

Statistical analysis

We applied the average scores from sensory evaluation to principal component analysis using 'ANALYST' (analyzer programs for statistical data, Fujitsu, Tokyo, Japan) on a FACOM M-308 computer (Fujitsu, Tokyo, Japan).

The data from sensory evaluation were statistically analyzed using principal component analysis, one of the multivariate analyses, to characterize the odor profiles of the tested nine compounds using the eight explanatory variables.

Results and Discussion

In this study, nine isomers of *n*-nonadien-1-ols were synthesized in odor to analyze their odor-structure relationship. Because there could be as much as 52 isomers possible, we selected these nine methylene-interrupted diene isomers such as analogous to naturally occurring isomers, i.e., (2*E*,6*Z*)-nonadien-1-ol (cucumber alcohol) and (3*Z*,6*Z*)-nonadien-1-ol.

Odor specificity analysis: odor characteristic of each *n*-nonadien-1-ol was described by using the eight sensory descriptive terms of leaf or grassy, vegetable-like, fruity, sweet, fresh, spicy, oily and herbal. The odor strength in each descriptive term was scored as 0 threshold; 1 very weak; 2 intense; 3 very intense. The average of three trained flavorists was plotted on the radar chart (Figs. 1 and 2). This analysis showed that, if the geometry of double bond was different, the odor characteristic was quite different. The position of each double

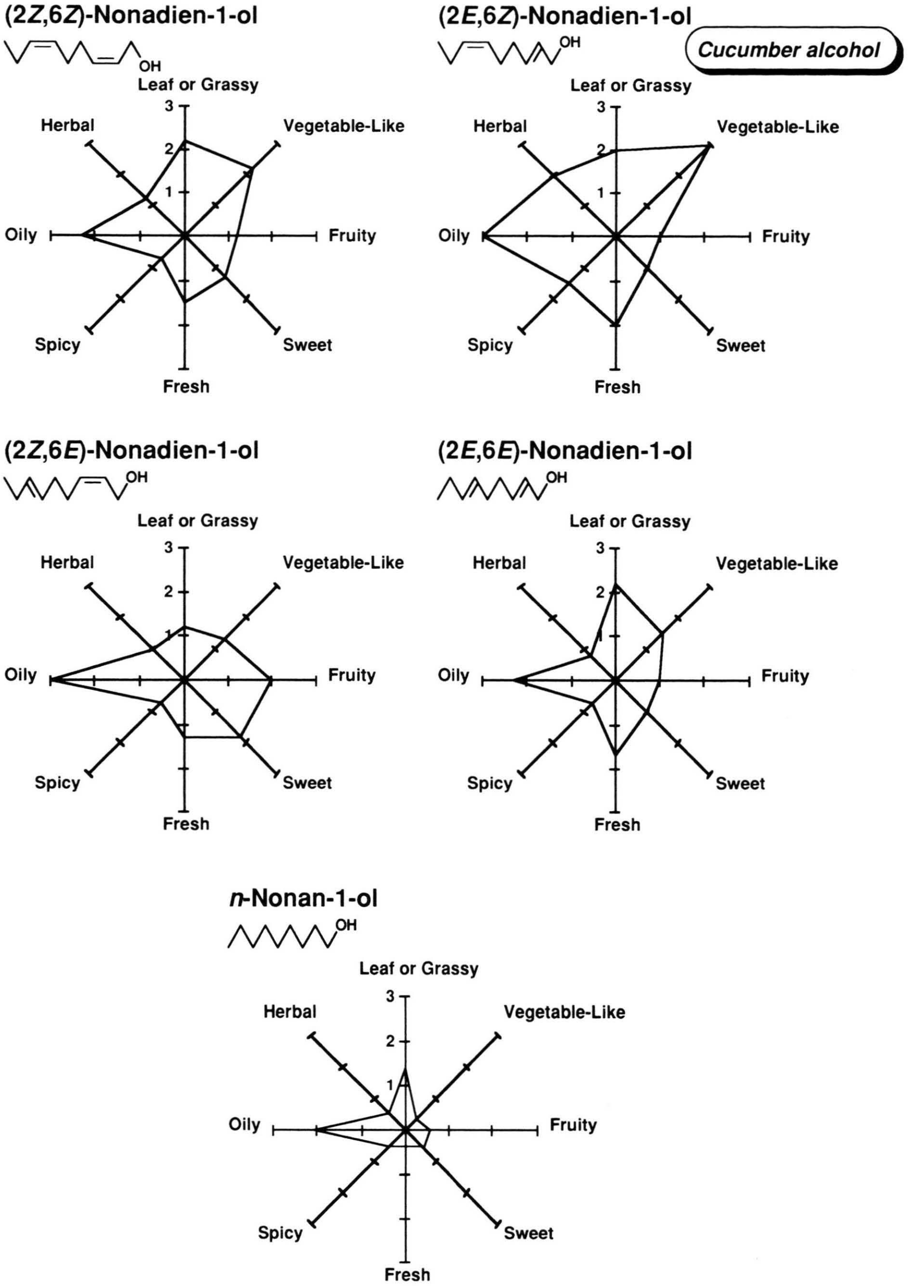
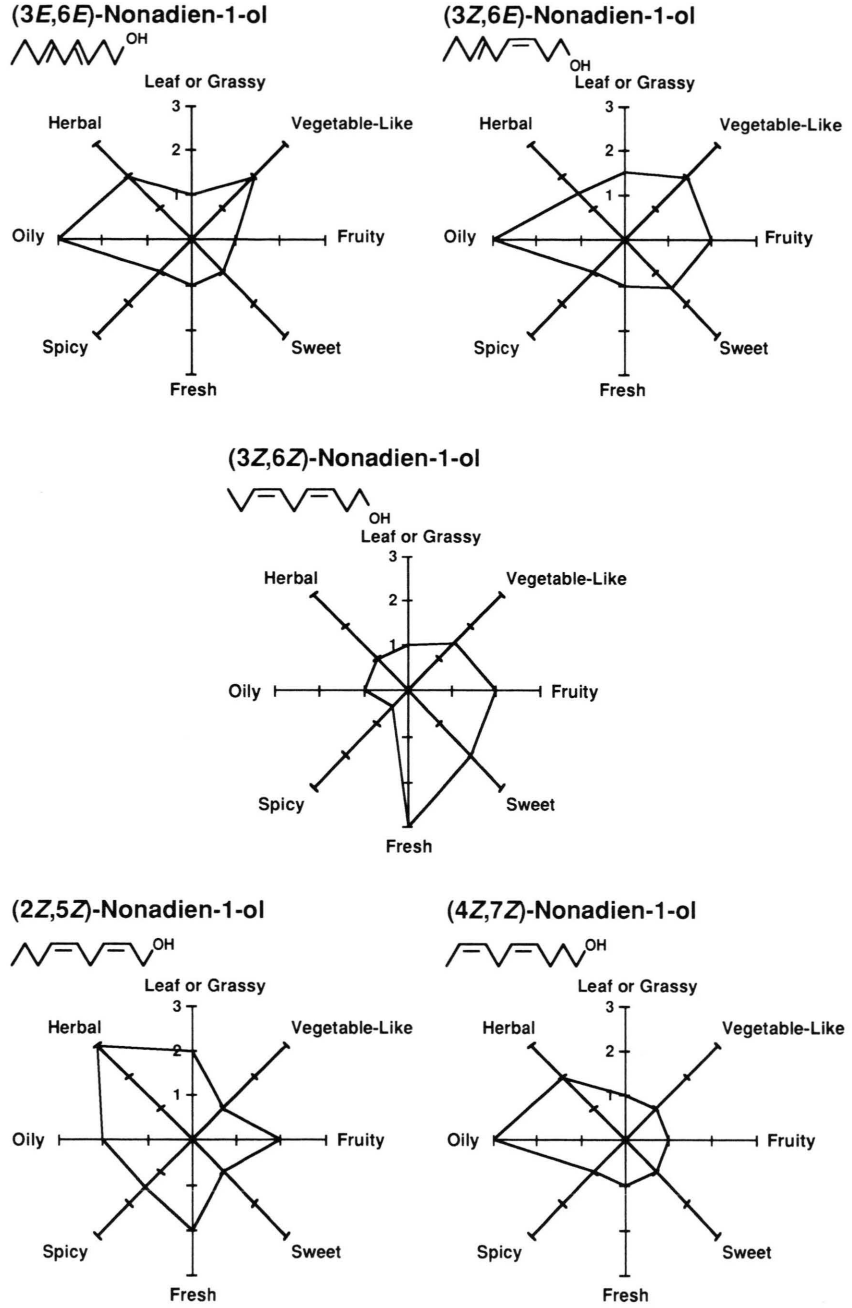


Fig. 1. Odor profiles of *n*-nonadien-1-ols ((2*E*,6*E*)-, (2*E*,6*Z*)-, (2*Z*,6*E*)- and (2*Z*,6*Z*)-nonadien-1-ols) and *n*-nonan-1-ol. Eight sensory descriptive terms were used for the sensory characteristics: leaf or grassy green an image of grasses, stems, and leaves; vegetable-like an image of vegetable, i.e., tomatoes, green pepper, cabbages etc.; fruity an image of fruits, i.e. apples, berries, pears etc.; sweet degree of sweetness; fresh degree of freshness; spicy an image of pepper, nutmeg, cinnamon etc.; oily-fatty, waxy, rancid; herbal an image reminiscent of bitterness of crude drugs. Score sheets with four-point scale ranging from threshold to very intense: i.e. 0 = threshold, 1 = very weak, 2 = intense, 3 = very intense, were used for the evaluation of the test samples. The average scores of three panellers were adopted as the odor-strength of the sensory attributes.


(3*E*,6*E*)-Nonadien-1-ol

(3*Z*,6*E*)-Nonadien-1-ol

(3*Z*,6*Z*)-Nonadien-1-ol

(2*Z*,5*Z*)-Nonadien-1-ol

(4*Z*,7*Z*)-Nonadien-1-ol

Fig. 2. Odor profiles of *n*-nonadien-1-ols ((3*E*,6*E*)-, (3*Z*,6*E*)-, (3*Z*,6*Z*)-, (2*Z*,5*Z*)- and (4*Z*,7*Z*)-nonadien-1-ols).

bond also have quite effects on its odor. Vegetable-like factor was strongest with (2*E*,6*Z*)-nonadien-1-ol. The vegetable-like factor was weakened, in the order of (2*Z*,6*Z*)-, (2*E*,6*E*)- to (2*Z*,6*E*)-nonadien-1-ols. Among the isomers analyzed (3*Z*,6*Z*)-nonen-1-ol showed pleasant flavor having high fruity, sweet and fresh factors, and (2*E*,6*Z*)-nonen-1-ol showed pleasant flavor having high vegetable-like factor. It should be noted that these are both the naturally occurring compounds.

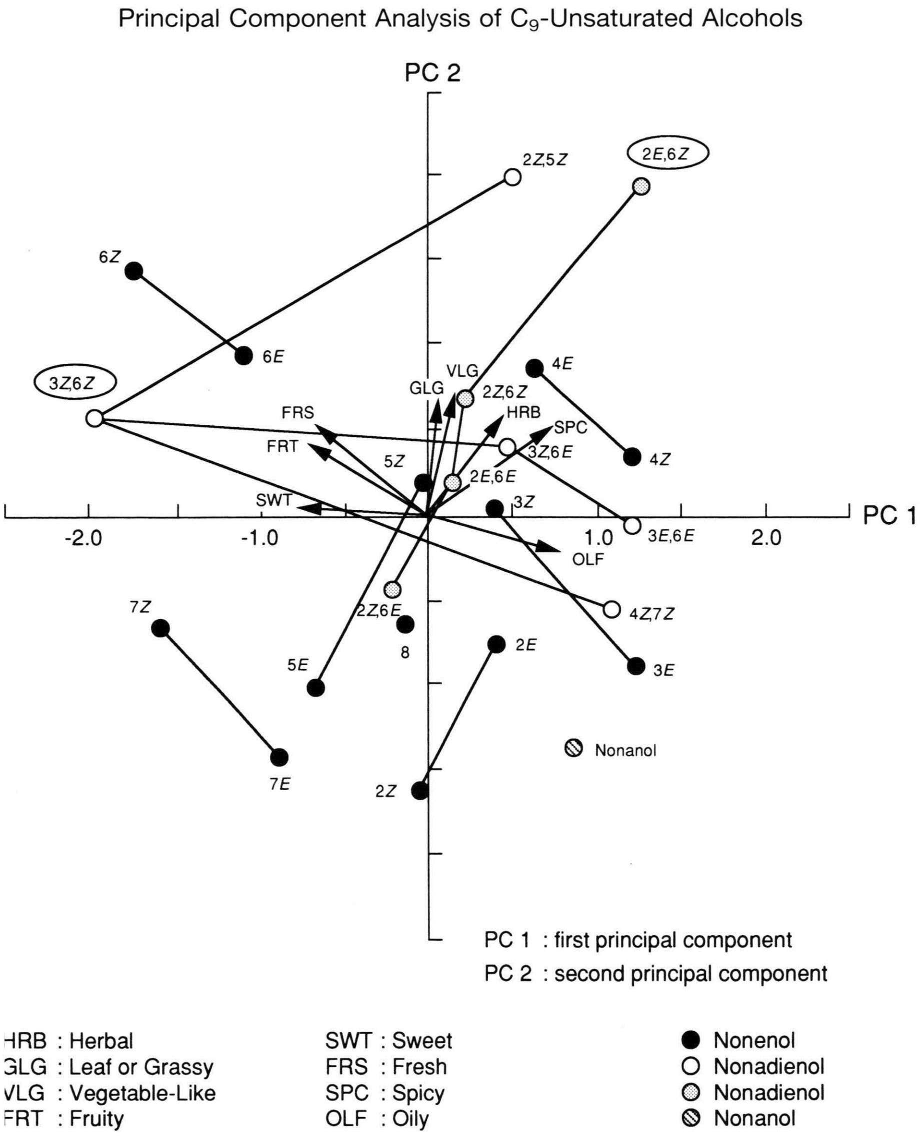


Fig. 3. The score plots and the vectors of the eigenvalues on the plane of the first principal component *vs.* the second principal component in *n*-nonen-1-ols, *n*-nonanol, and isomers of (2*E*,6*Z*)- and (3*Z*,6*Z*)-nonadien-1-ols.

Principal analysis: previous result of principal analyses concerning about C_6-monoenols and monoenals, and C_9-monoenols suggested that this analytical system can be properly used for the odor evaluation (Hatanaka *et al.,* 1992; Sakoda *et al.,* 1995). After the analysis, fresh, fruity and sweet factors were found to inversely contribute to PC 1, on the other hand, herbal, vegetable-like and leaf or grassy were found to positively contribute to PC 2. The contribution of PC 1 and PC 2 summed up to nearly 60% (Table). For convenient comparison, all the data previously obtained in our laboratory are simultaneously plotted. As shown in Fig. 3, it was indicated that 5-, 6- and 7-nonen-1-ols, which contain a double bond in w side had a positive value of PC 1, on the other hand, 2-, 3-, and 4-nonen-1-ols which contain a double bond in the α-terminal functional group side did a negative

Table I. The principal component analyses of the odor of the *n*-nonen-1-ols, *n*-nonanol, and isomers of (2*E*,6*Z*)- and (3*Z*,6*Z*)-nonadien-1-ols.

Odor description	PC 1	PC 2	PC 3
Fresh	−0.674	0.516	0.115
Fruity	−0.697	0.420	0.364
Leaf or grassy	0.069	0.636	−0.509
Herbal	0.459	0.574	0.607
Oily-fatty	0.778	−0.219	0.202
Spicy	0.732	0.506	0.236
Sweet	−0.792	0.025	0.172
Vegetable-like	0.227	0.678	−0.467
Eigenvalue	2.978	1.941	1.118
Proportion	37.2	24.3	14.0
Cumulative proportion	37.2	61.5	75.5

PC: Principal component.

one. In the four geometrical isomers of 2,6-nonadien-1-ols, only (2*E*,6*Z*)-nonadien-1-ol located at especially high point of both PC 1 and PC 2. Both the components gradually decreased from (2*Z*,6*Z*)-, (2*E*,6*E*)- to (2*Z*,6*E*)-nonadien-1-ols. The spatial relationship between (2*Z*) and (2*E*) isomers in the 2,6-dienols highly correlated with that of (2*Z*)- and (2*E*)-nonenols. On the other hand, in the four geometrical isomers of (3,6)-nonadien-1-ols, only (3*Z*,6*Z*)-nonadien-1-ol located apart at negative site of PC 1, while the others located at the positive site. PC 1 increased as number of (*E*)-geometry increased in the 3,6-nonadien-1-ols. Again, the spatial relationship between (3*Z*,6*E*) and (3*E*,6*E*) has high correlation with that of corresponding monoene isomers, i.e., (3*E*)- and (3*Z*)-nonen-1-ols. These analyses showed that, among these *n*-nonadien-1-ols, (2*E*,6*Z*)- and (3*Z*,6*Z*)-nonadien-1-ols, which have a *Z*-double bond at w3 position had specific odor-character of both the first and the second principal components. This was also observed with (3*Z*)-hexen-1-ol and (6*Z*)-nonen-1-ol, which contain an w3*Z* double bond. From those results, that an w3*Z*-moiety in volatile alcohols has specific interaction with a sensory system of human was suggested intensely. This strategy was found to be interested in evaluating chemical structure-oder correlation.

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