

Supporting Information

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Details of the transformations with BAD lyophilisate

Biotransformation of (E)-2-octen-1-ol (1a)

According to the general procedure, **1a** (1 mmol, 152 μ L) was added as a solution in 10 mL of 2-propanol to a lyophilisate of *B. adusta* after 20 min of its rehydration in phosphate buffer. The reaction mixture was stirred for 4 h. Purification of the crude gave 109 mg of (*E*)-2-octenal (**2a**, 87%) as a pale yellow colorless liquid. ^1H and ^{13}C spectra were identical to those of the authentic reference standard.

Biotransformation of (E)-2-hexen-1-ol (1d)

According to the general procedure, **1d** (1 mmol, 119 μ L) was added as a solution in 10 mL of 2-propanol to a lyophilisate of *B. adusta* after 20 min of its rehydration in phosphate buffer. The reaction mixture was stirred for 4 h. Purification of the crude gave 20 mg of (*E*)-2-hexenal (**2d**, 20%) as a colorless liquid. ^1H and ^{13}C spectra were identical to those of the authentic reference standard.

Biotransformation of (E,E)-2,4-hexadien-1-ol (1e)

According to the general procedure, **1e** (1 mmol, 98 mg) was added as a solution in 10 mL of 2-propanol to a lyophilisate of *B. adusta* after 20 min of its rehydration in phosphate buffer. The reaction mixture was stirred for 4 h. Purification of the crude gave 62 mg of (*E,E*)-2,4-hexadienal (**2e**, 65%) as a colorless liquid. ^1H and ^{13}C spectra were identical to those of the authentic reference standard.

Biotransformation of (E,E)-2,4-decadien-1-ol (1f)

According to the general procedure, **1f** (1 mmol, 154 mg) was added as a solution in 10 mL of 2-propanol to a lyophilisate of *B. adusta* after 20 min of its rehydration in phosphate buffer. The reaction mixture was stirred for 4 h. Purification of the crude gave 103 mg of (*E,E*)-2,4-

decadienal (**2f**, 68%) as a yellow liquid. ^1H and ^{13}C spectra were identical to those of the authentic reference standard.

Biotransformation of geraniol (1g)

According to the general procedure, **1g** (1 mmol, 173 μL) was added as a solution in 10 mL of 2-propanol to a lyophilisate of *B. adusta* after 20 min of its rehydration in phosphate buffer. The reaction mixture was stirred for 4 h. Purification of the crude gave 144 mg of citral (**2g**, 68%) as a pale yellow liquid. ^1H and ^{13}C spectra were identical to those of the authentic reference standard.

Biotransformation of nerol (1h)

According to the general procedure, **1h** (1 mmol, 173 μL) was added as a solution in 10 mL of 2-propanol to a lyophilisate of *B. adusta* after 20 min of its rehydration in phosphate buffer. The reaction mixture was stirred for 4 h. Purification of the crude gave 79 mg of citral (**2g**, 68%) as a pale yellow liquid. ^1H and ^{13}C spectra were identical to those of the authentic reference standard.

Biotransformation of (Z)-2-nonen-1-ol (1i)

According to the general procedure, **1i** (1 mmol, 168 μL) was added as a solution in 10 mL of 2-propanol to a lyophilisate of *B. adusta* after 20 min of its rehydration in phosphate buffer. The reaction mixture was stirred for 4 h. Purification of the crude gave 116 mg of (*E*)-2-nonenal (**2b**, 83%) as a colourless liquid. ^1H and ^{13}C spectra were identical to those of the authentic reference standard.

Characterization data of products

(E)-2-octenal (2a): ^1H NMR (400 MHz, CDCl_3 , ppm): $\delta = 9.50$ (d, $J = 7.8$ Hz, 1H), 6.86 (dt, $J = 6.8$, $J = 15.4$ Hz, 1H), 6.11 (ddt, $J = 1.6$, $J = 7.6$, $J = 15.5$ Hz, 1H), 2.36-2.29 (m, 2H), 1.52-1.39 (m, 2H), 1.35-1.19 (m, 4H), 0.89 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): $\delta = 194.33$ (CHO), 159.01 (C=C), 132.99 (C=C), 32.66 (CH_2), 31.26 (CH_2), 27.35 (CH_2), 22.35 (CH_2), 13.87 (CH_3). This compound was previously described. ^[1]

(E)-2-hexenal (2d): ^1H NMR (400 MHz, CDCl_3 , ppm): $\delta = 9.48$ (d, $J = 8.1$ Hz, 1H), 7.10 (m, 1H), 6.32 (m, 2H), 6.06 (m, 1H), 1.92 (d, $J = 5.8$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): $\delta = 194.09$ (CHO), 158.77 (C=C), 133.12 (C=C), 34.61 (CH_2), 21.08 (CH_2), 13.56 (CH_3). This compound was previously described. ^[1]

(E,E)-2,4-hexadienal (2e): ^1H NMR (400 MHz, CDCl_3 , ppm): $\delta = 9.54$ (d, $J = 8.0$ Hz, 1H), 6.83 (dt, $J = 6.8$, $J = 15.7$ Hz, 1H), 6.09 (ddt, $J = 1.4$, $J = 7.9$, $J = 15.6$ Hz, 1H), 2.33-2.26 (m, 2H), 1.57-1.47 (m, 2H), 0.94 (t, $J = 7.6$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): $\delta = 194.04$ (CHO), 152.65 (C=C), 141.94 (C=C), 130.13 (C=C), 129.90 (C=C), 18.96 (CH_3). This compound was previously described ^[2].

(E,E)-2,4-decadienal (2f): ^1H NMR (400 MHz, CDCl_3 , ppm): $\delta = 9.53$ (d, $J = 8.2$ Hz, 1H), 7.09 (m, 1H), 6.37-6.24 (m, 2H), 6.07 (dd, $J = 8.2$, $J = 15.3$ Hz, 1H), 2.25-2.18 (m, 2H), 1.51-1.42 (m, 2H), 1.39-1.25 (m, 4H), 0.90 (t, $J = 6.8$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): $\delta = 194.08$ (CHO), 152.88 (C=C), 147.46 (C=C), 130.27 (C=C), 128.72 (C=C), 33.19 (CH_2), 31.35 (CH_2), 28.22 (CH_2), 22.43 (CH_2), 13.97 (CH_3). This compound was previously described ^[3].

Citral (2g): ^1H NMR (400 MHz, CDCl_3 , ppm): $\delta = 9.96$ -9.87 (m, 1H), 5.85 (m, 1H), 5.06 (m, 1H), 2.56 (t, $J = 7.5$ Hz, 1H), 2.21 (m, 3H), 2.14 (d, $J = 1.4$ Hz, 2H), 1.96 (d, $J = 1.4$ Hz, 1H), 1.66 (s, 3H), 1.57 (d, $J = 6.5$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): $\delta = 191.22$ (CHO), 190.68 (CHO), 163.77 (2C=C), 133.61 (C=C), 132.83 (C=C), 128.61 (C=C), 127.38 (C=C), 122.59 (C=C), 122.28 (C=C), 40.55 (CH_2), 32.57 (CH_2), 27.05 (CH_2), 25.71 (CH_2), 25.59 (2 CH_3), 25.03 (CH_3), 17.65 (CH_3), 17.53 (2 CH_3). This compound was previously described ^[4].

(E)-2-nonenal (2b): ^1H NMR (400 MHz, CDCl_3 , ppm): δ = 9.49 (d, J = 7.8 Hz, 1H), 6.83 (dt, J = 6.9, J = 15.6 Hz, 1H), 6.11 (ddt, J = 1.5, J = 8.0, J = 15.6 Hz, 1H), 2.36-2.29 (m, 2H), 1.51-1.47 (m, 2H), 1.37-1.21 (m, 6H), 0.86 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ = 194.33 (CHO), 159.01 (C=C), 133.01 (C=C), 32.76 (CH_2), 31.55 (CH_2), 28.85 (CH_2), 27.84 (CH_2), 22.53 (CH_2), 13.99 (CH_3). This compound was previously described ^[5].

(Z)-2-nonenal (1n): ^1H NMR (400 MHz, CDCl_3 , ppm): δ = 10.08 (d, J = 8.5 Hz, 1H), 6.67 (dt, J = 8.2, J = 11 Hz, 1H), 5.96 (m, 1H), 2.61 (m, 1H), 1.57-1.47 (m, 3H), 1.40-1.19 (m, 6H), 0.92-0.86 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3 , ppm): δ = 191.23 (CHO), 153.64 (C=C), 130.31 (C=C), 31.53 (CH_2), 29.19 (CH_2), 28.75 (CH_2), 28.01 (CH_2), 22.51 (CH_2), 14.00 (CH_3). This compound was previously described ^[6].

NMR spectra of isolated products

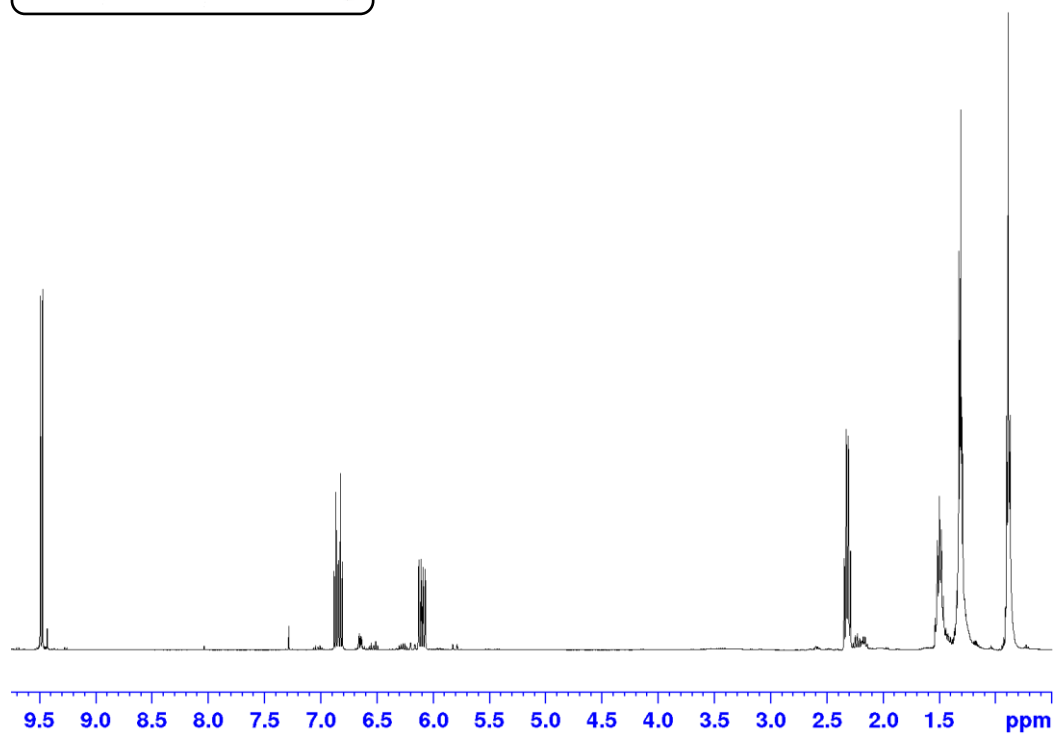
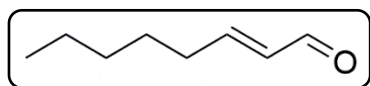


Figure S1. ^1H NMR of (E)-2-octenal (**2a**).

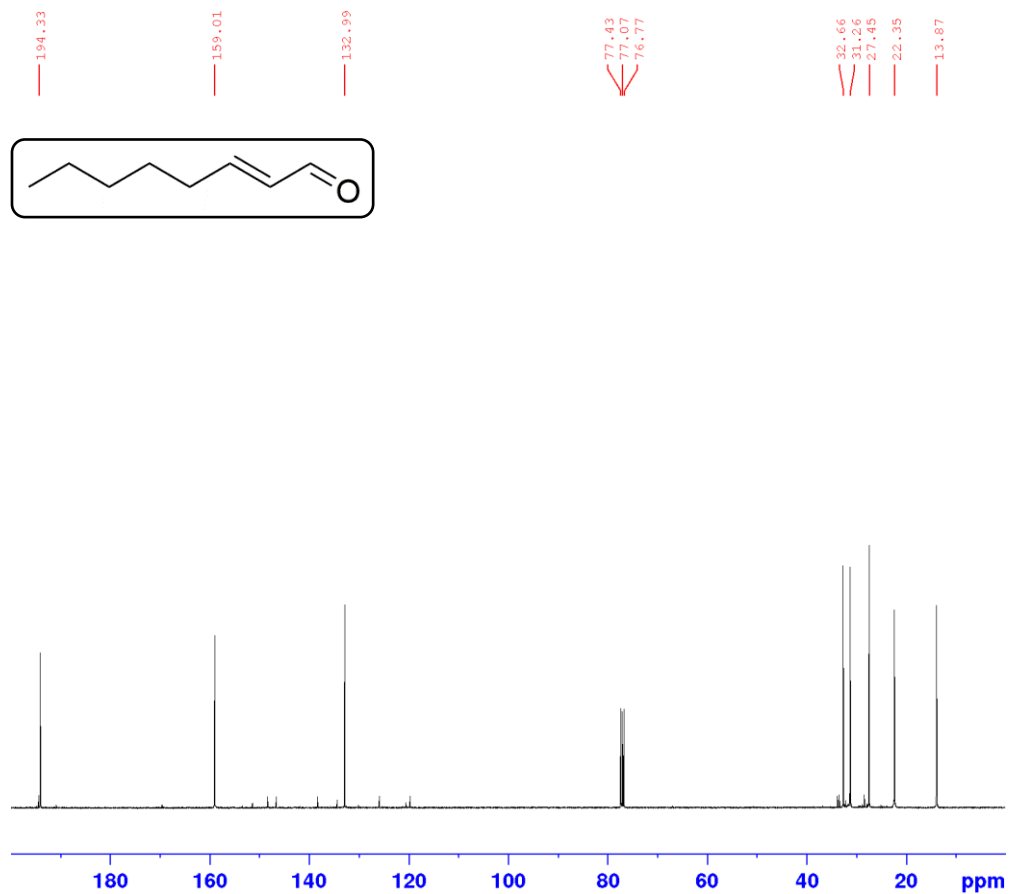


Figure S2. ^{13}C NMR of (E)-2-octenal (**2a**).

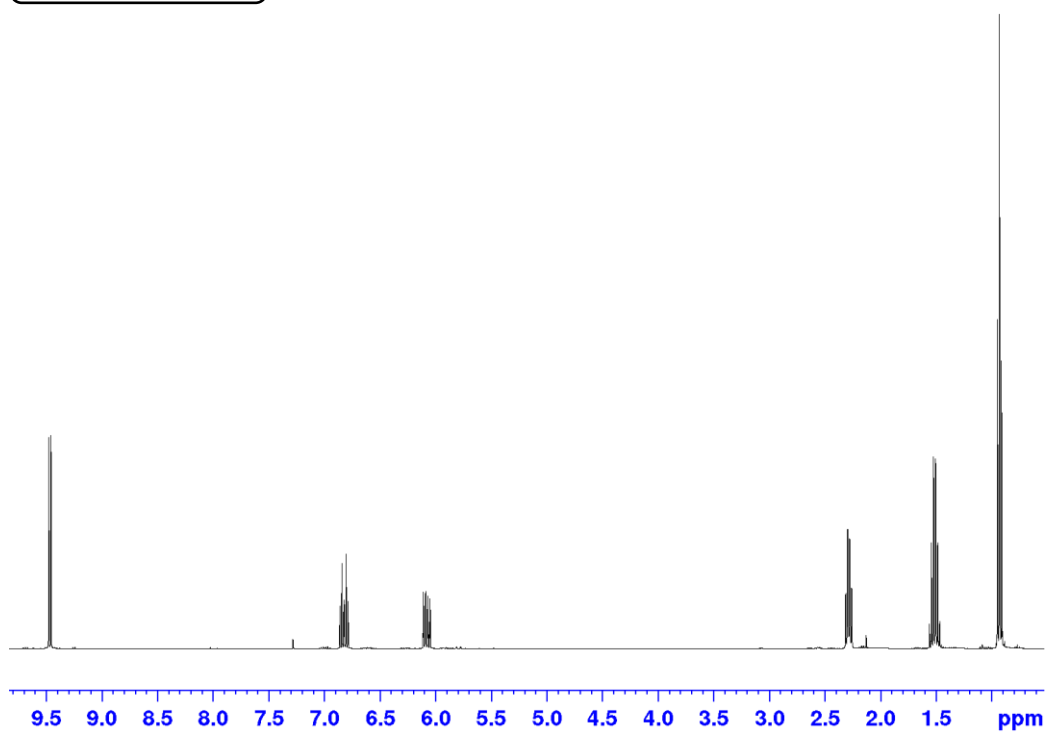
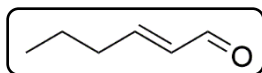


Figure S3. ^1H NMR of (*E*)-2-hexenal (**2d**).

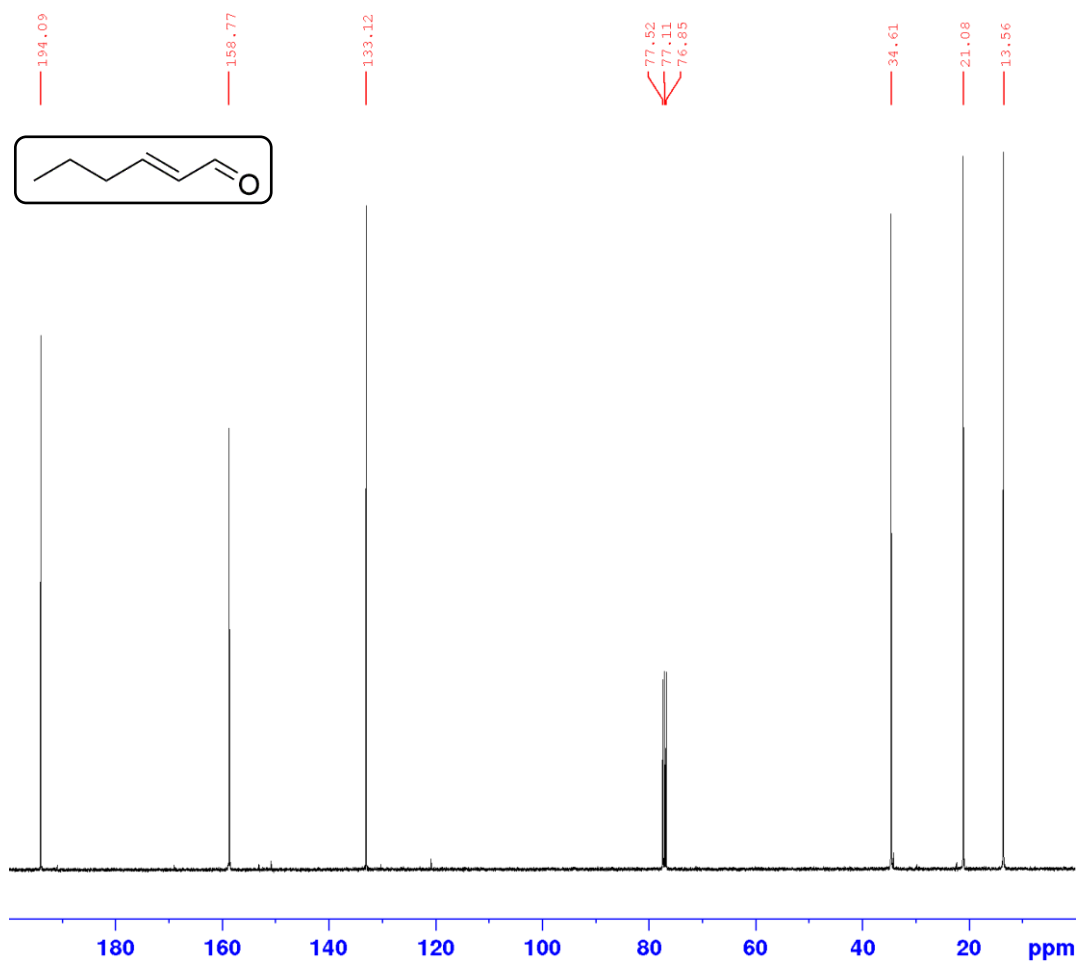


Figure S4. ^{13}C NMR of (*E*)-2-hexenal (**2d**).

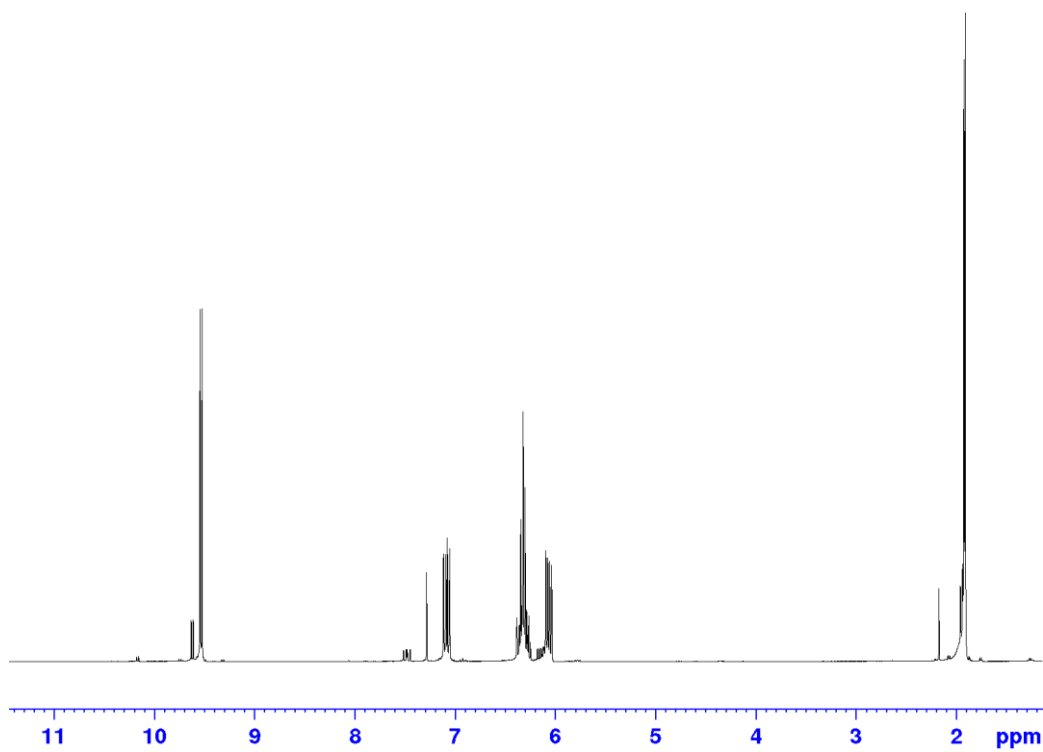
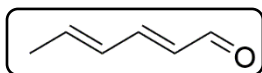


Figure S5. ^1H NMR of (*E,E*)-2,4-hexadienal (**2e**).

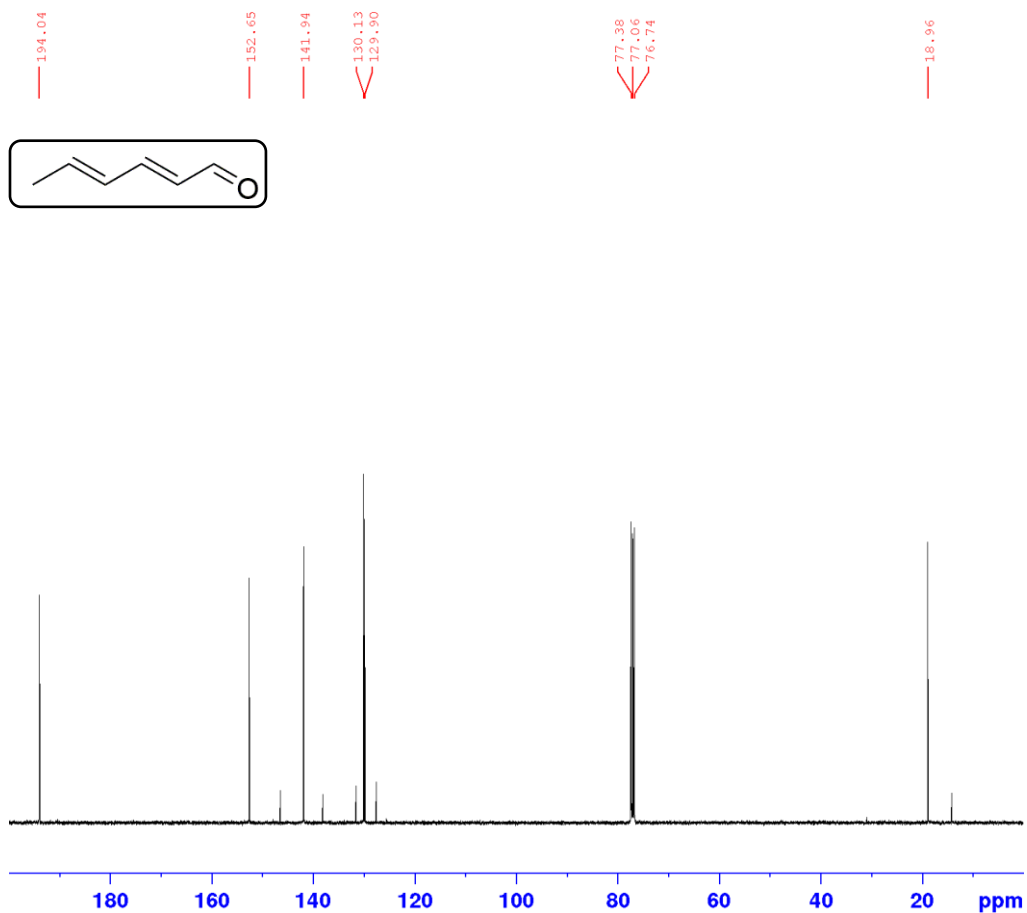


Figure S6. ^{13}C NMR of (*E,E*)-2,4-hexadienal (**2e**).

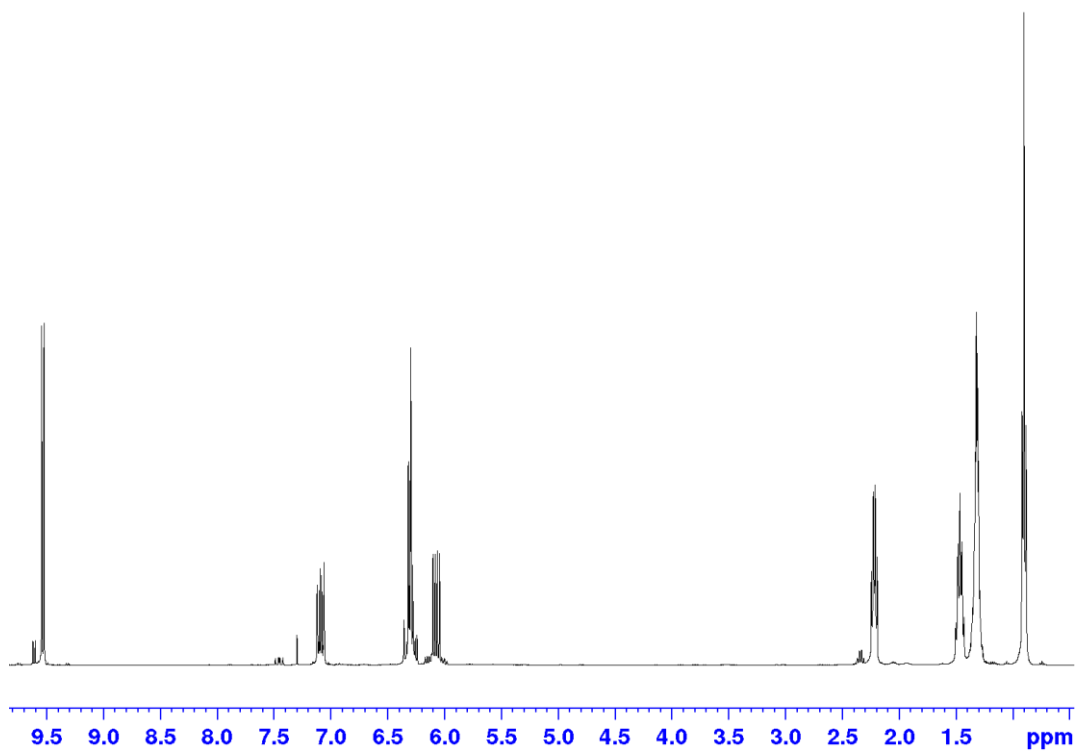
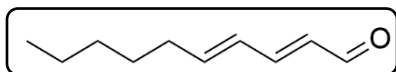


Figure S7. ^1H NMR of (*E,E*)-2,4-decadienal (**2f**).

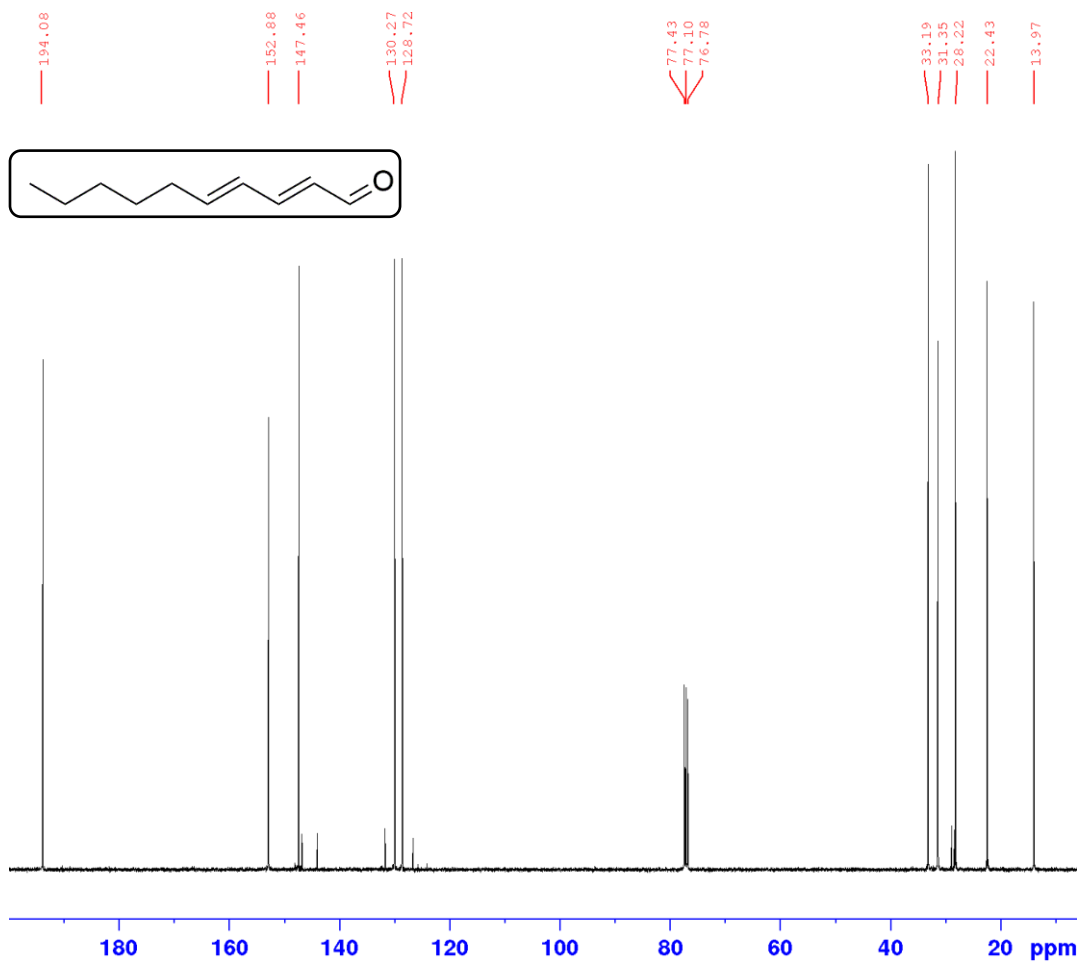


Figure S8. ^{13}C NMR of (*E,E*)-2,4-decadienal (**2f**).

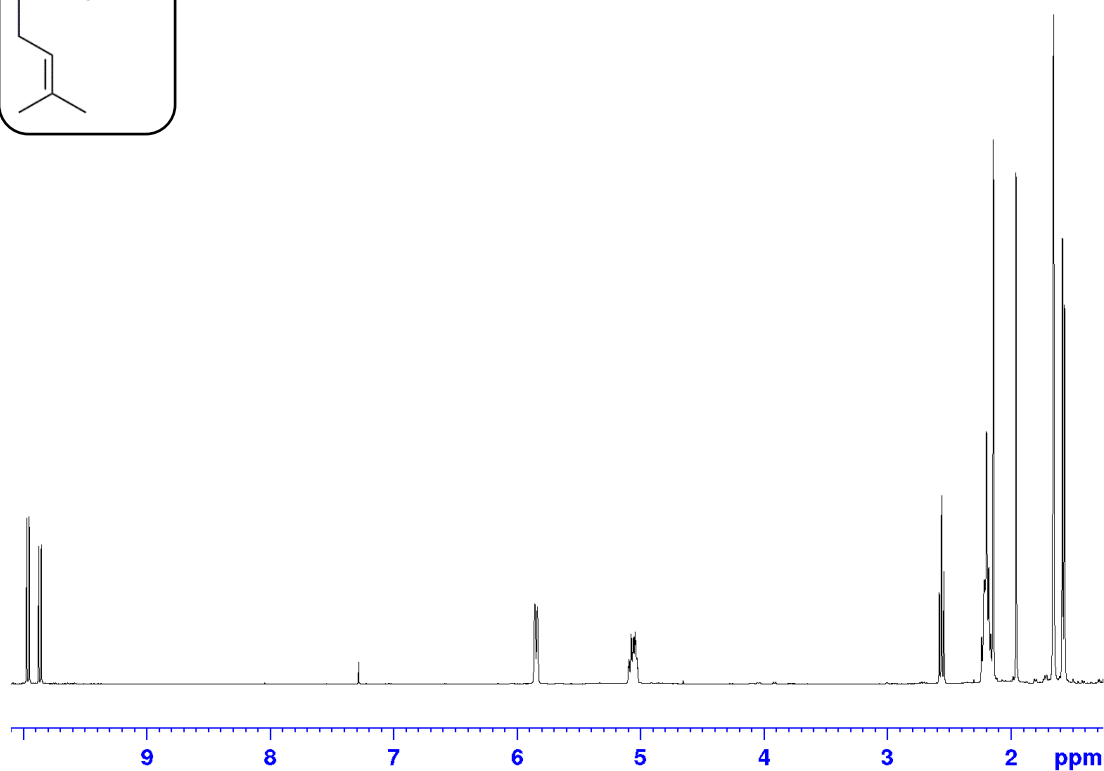
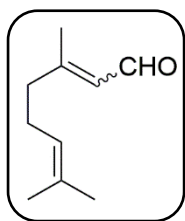


Figure S9. ¹H NMR of citral (2g).

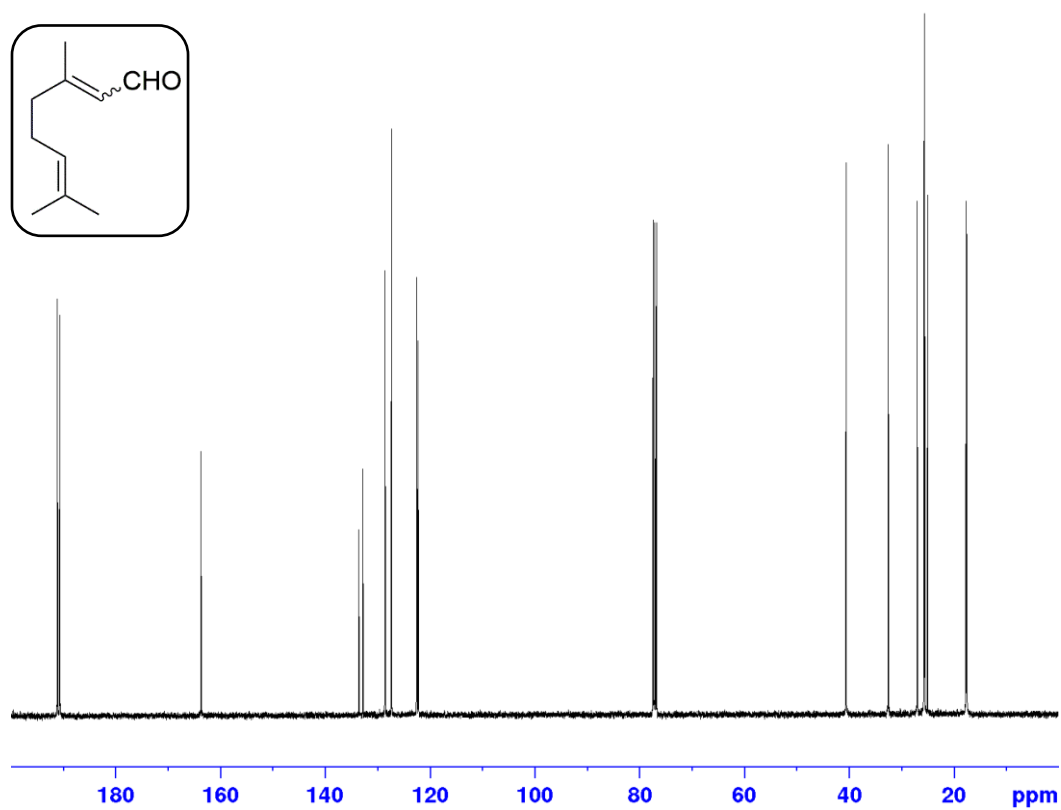
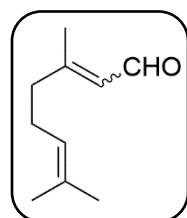


Figure S10. ¹³C NMR of citral (2g).

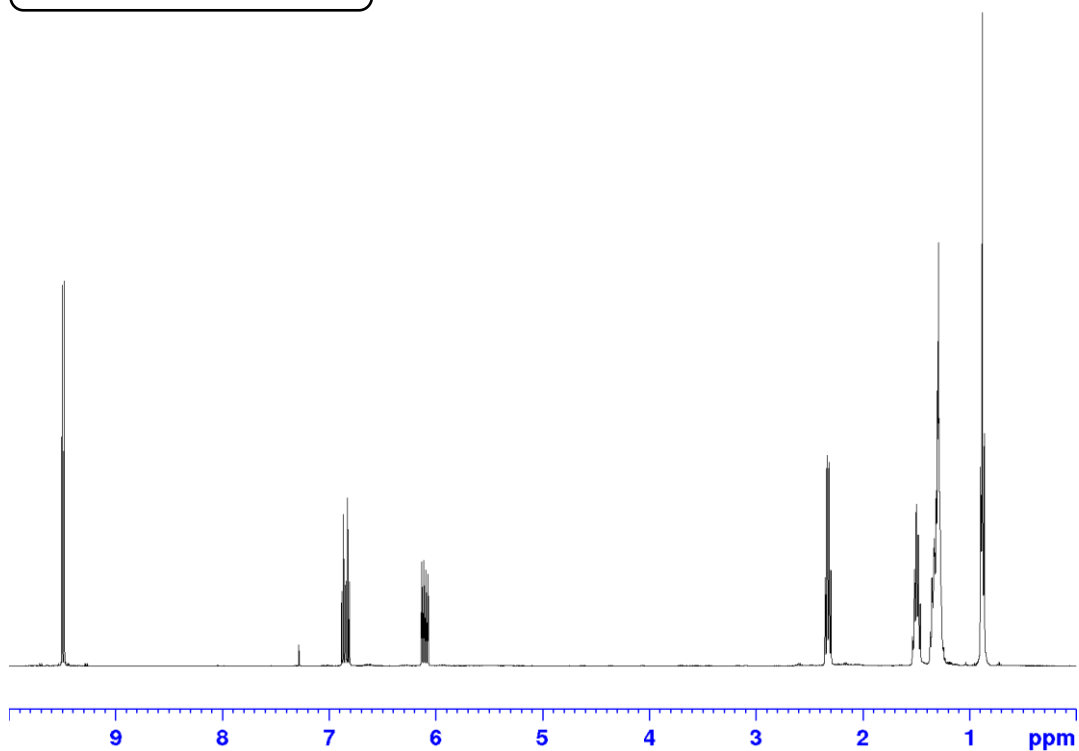
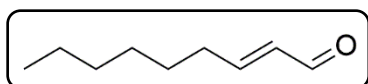


Figure S11. ^1H NMR of (*E*)-2-nonenal (**2b**).

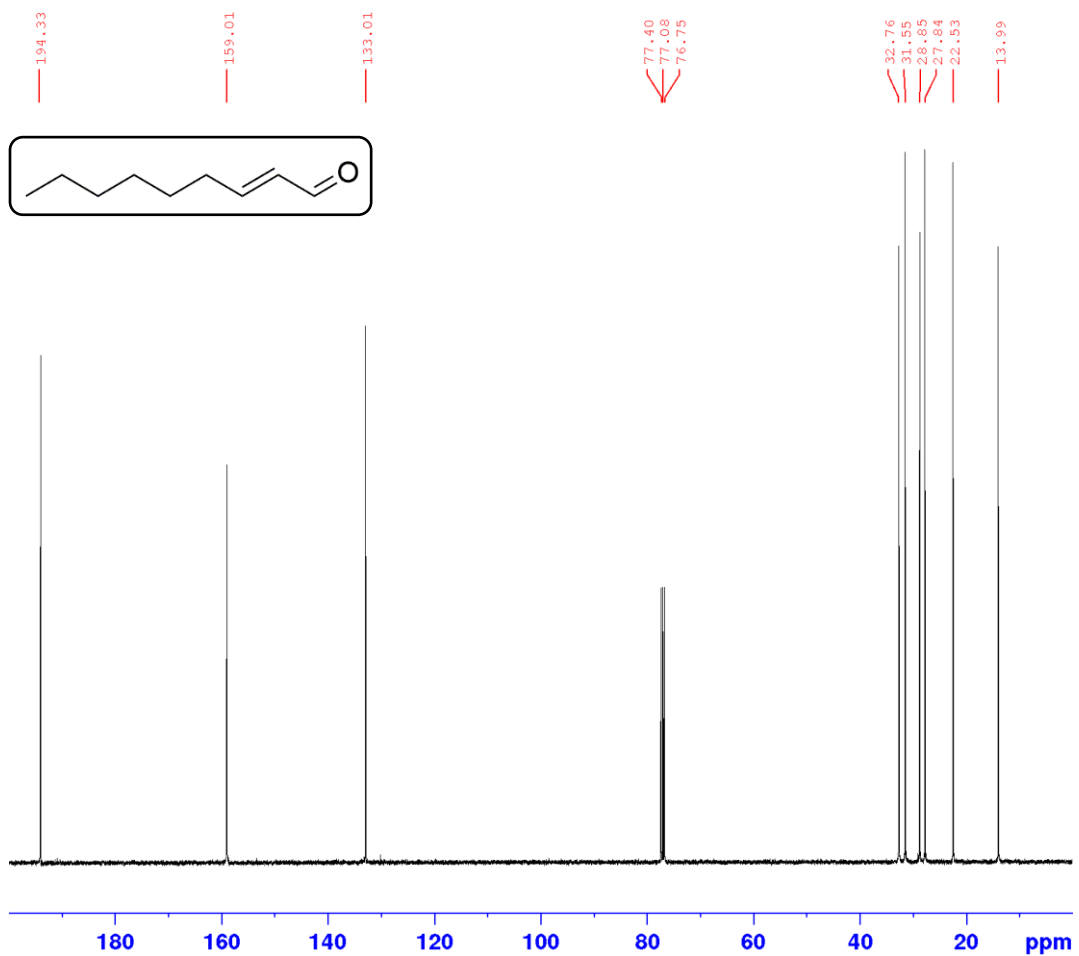


Figure S12. ^{13}C NMR of (*E*)-2-nonenal (**2b**).

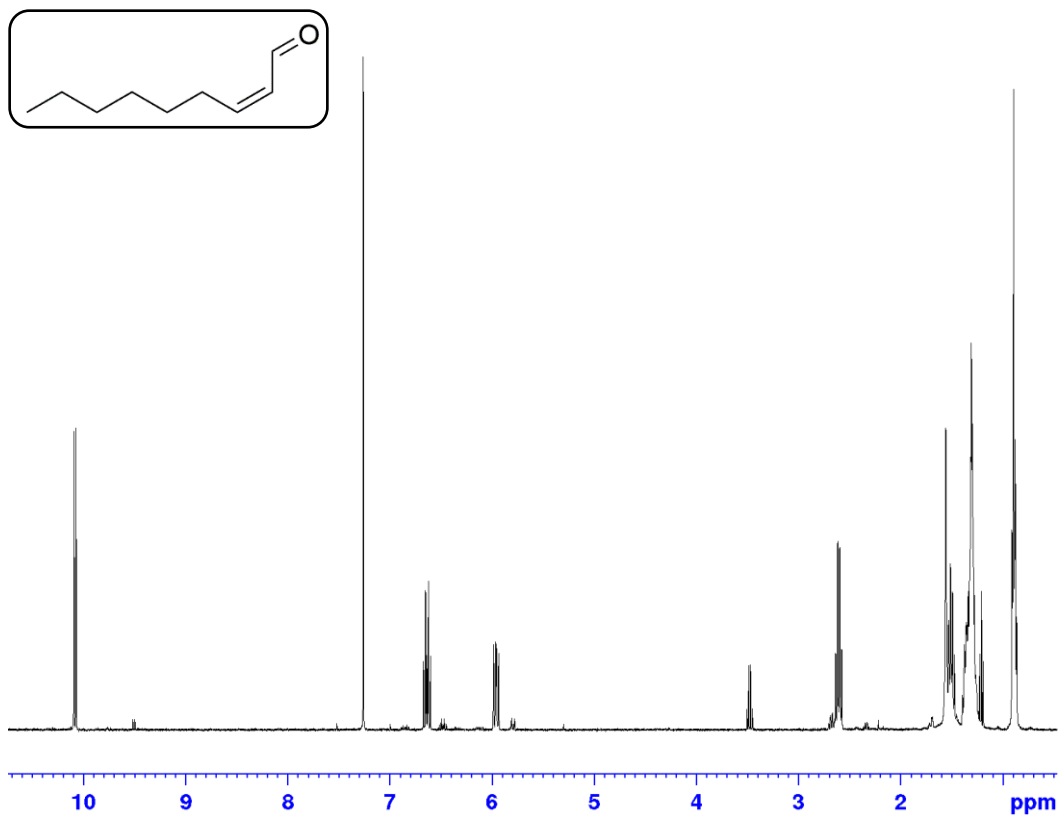


Figure S13. ¹H NMR of (Z)-2-nonenal (**1n**).

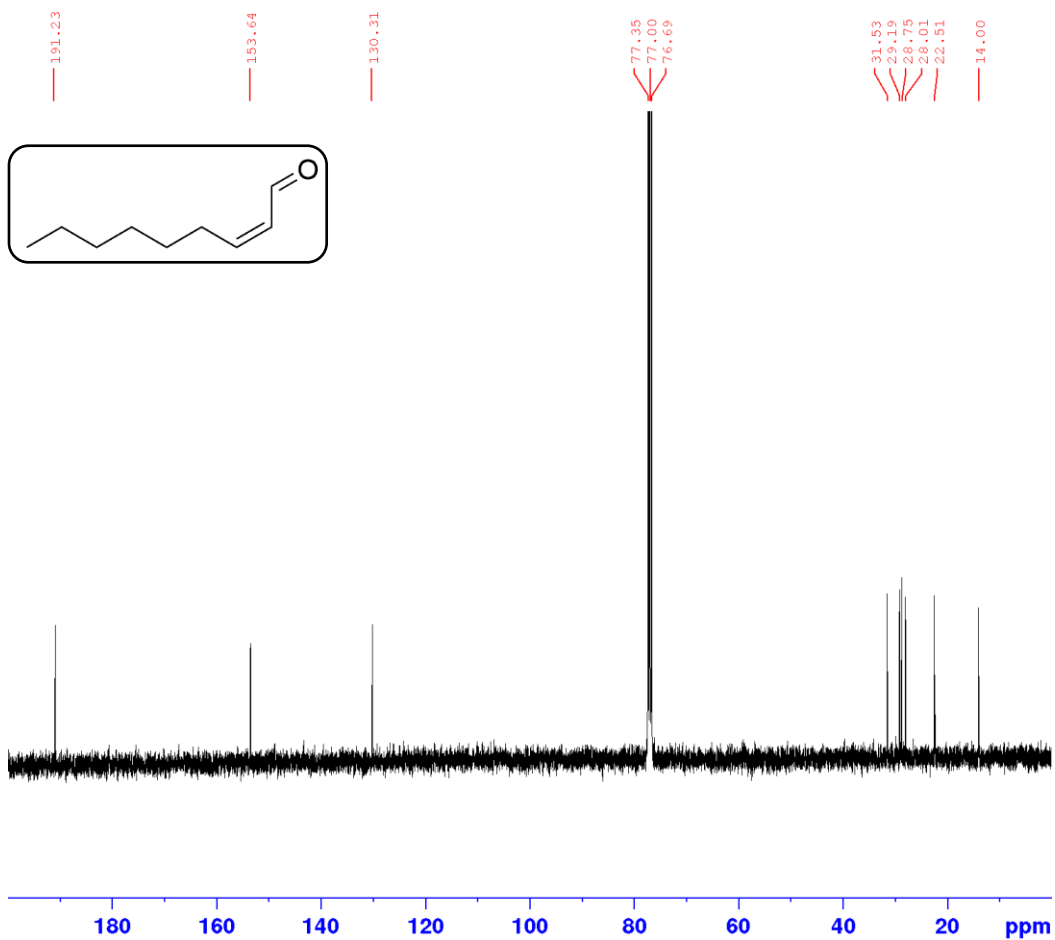


Figure S14. ¹³C NMR of (Z)-2-nonenal (**1n**).

References

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