

Supplementary Materials

Phytochemical Constituents Identified from the Aerial Parts of *Lespedeza Cuneata* and Their Effects on Lipid Metabolism during Adipocyte Maturation

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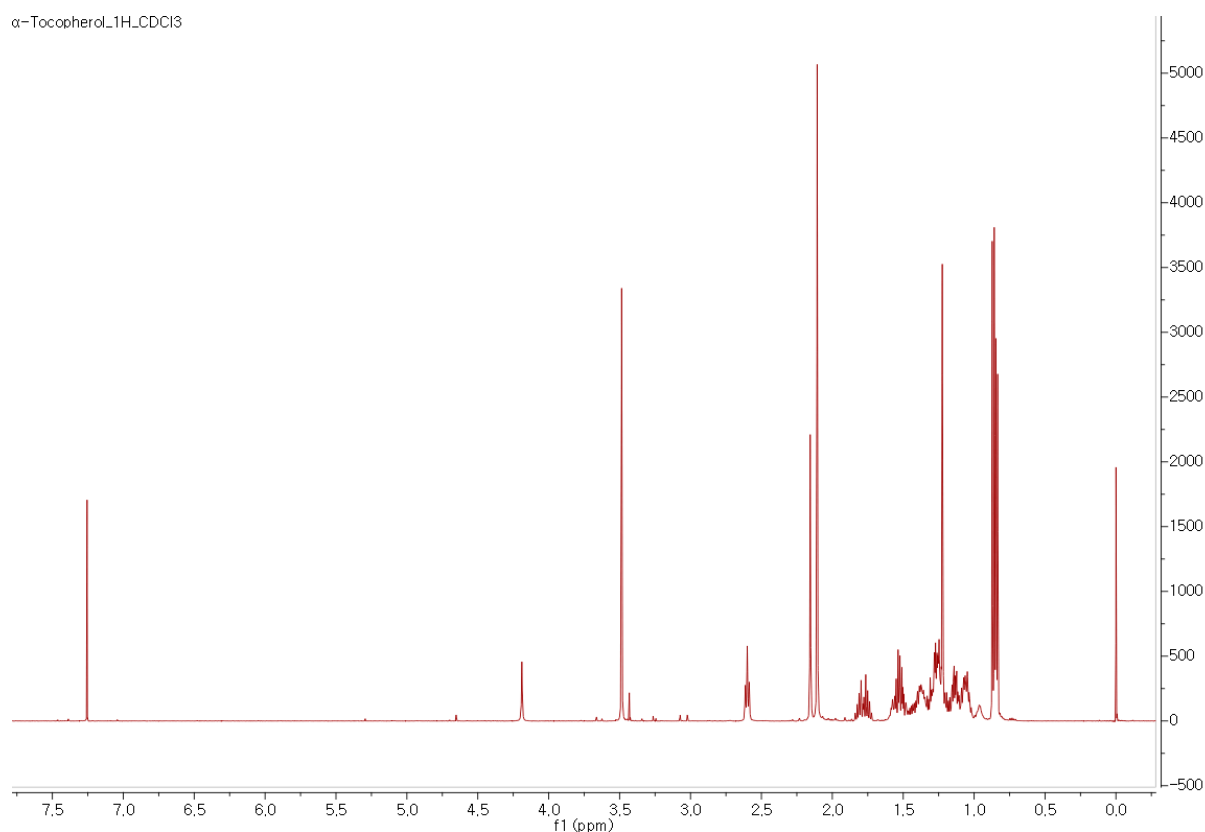


Figure S1. ¹H-NMR spectrum of compound 1 (in CDCl₃).

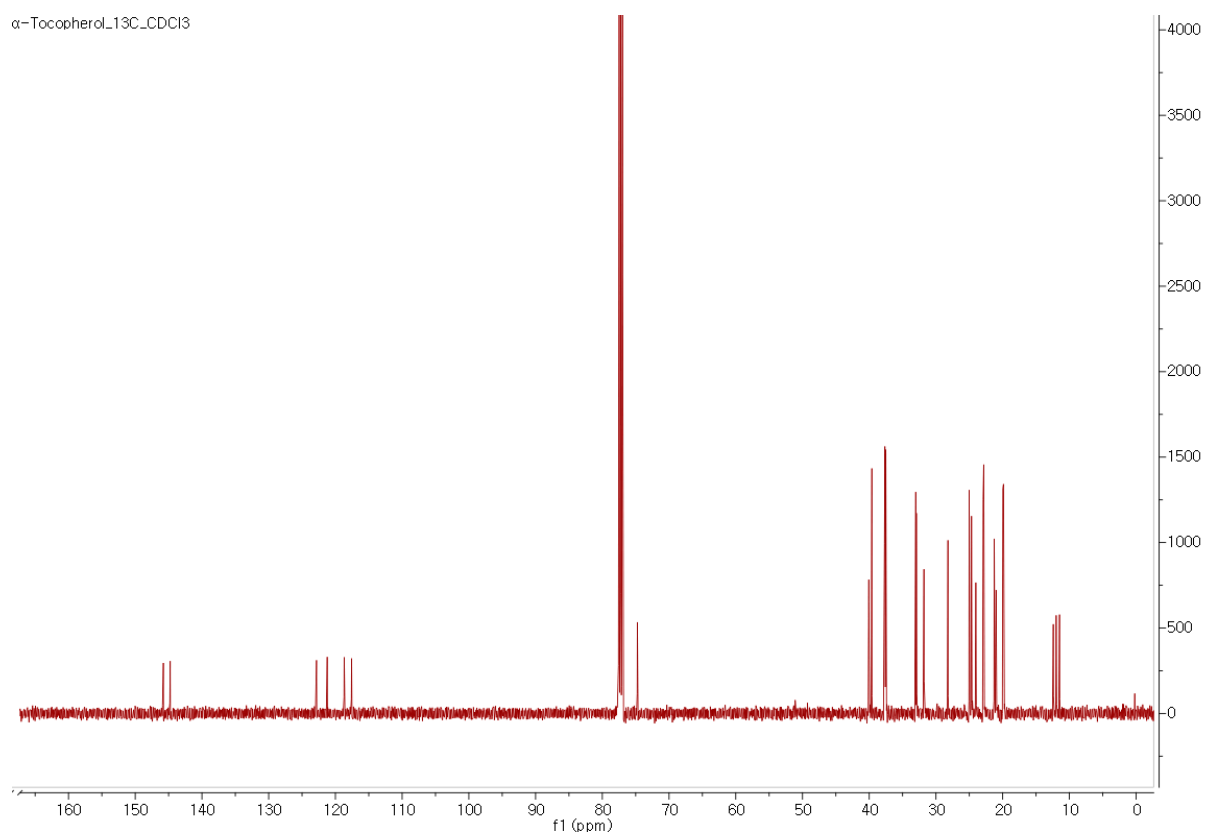


Figure S2. ^{13}C -NMR spectrum of compound **1** (in CDCl_3).

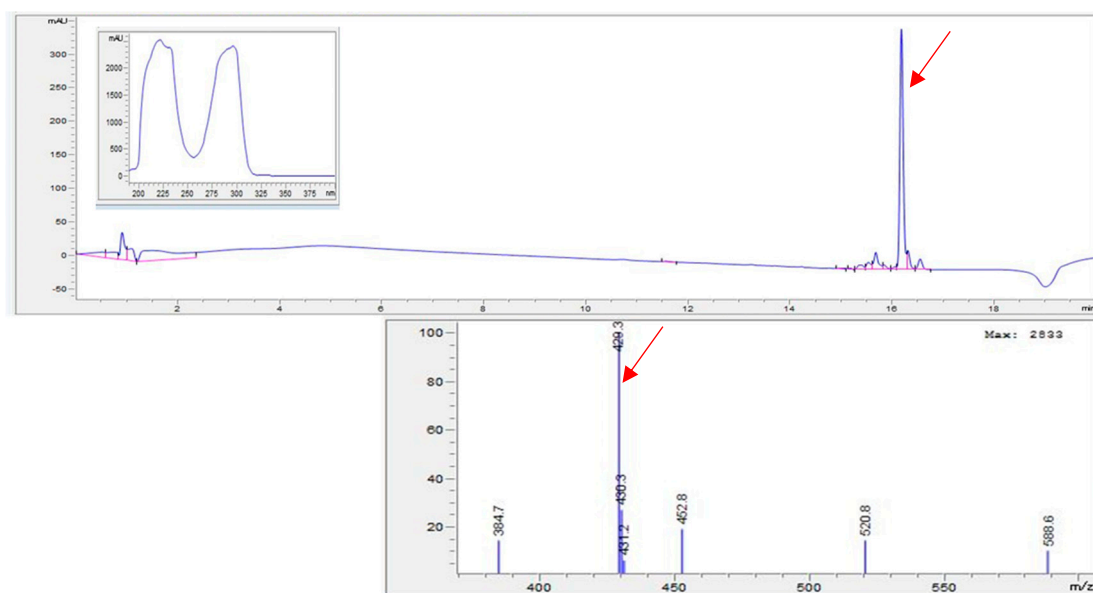


Figure S3. LC/MS data (detection wavelength was set as 254 nm) of compound **1**.

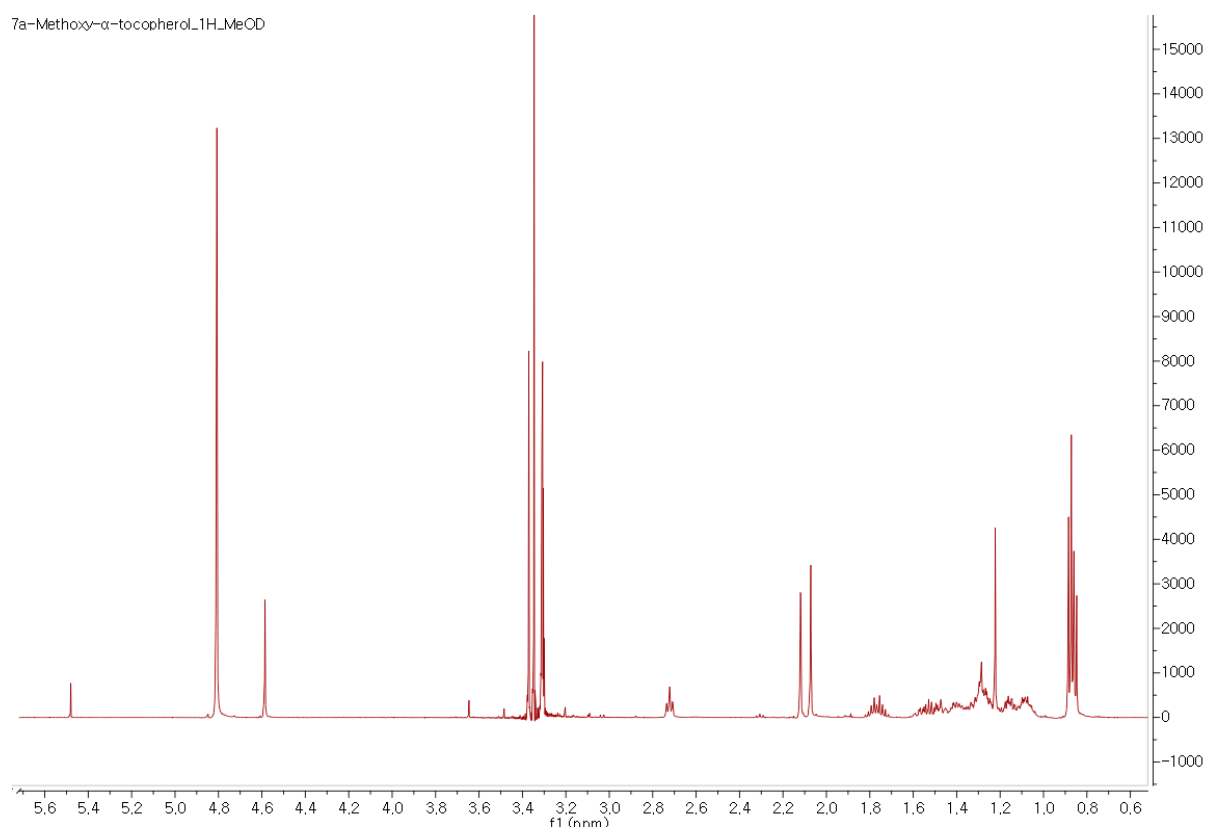


Figure S4. ^1H -NMR spectrum of compound 2 (in CD_3OD).

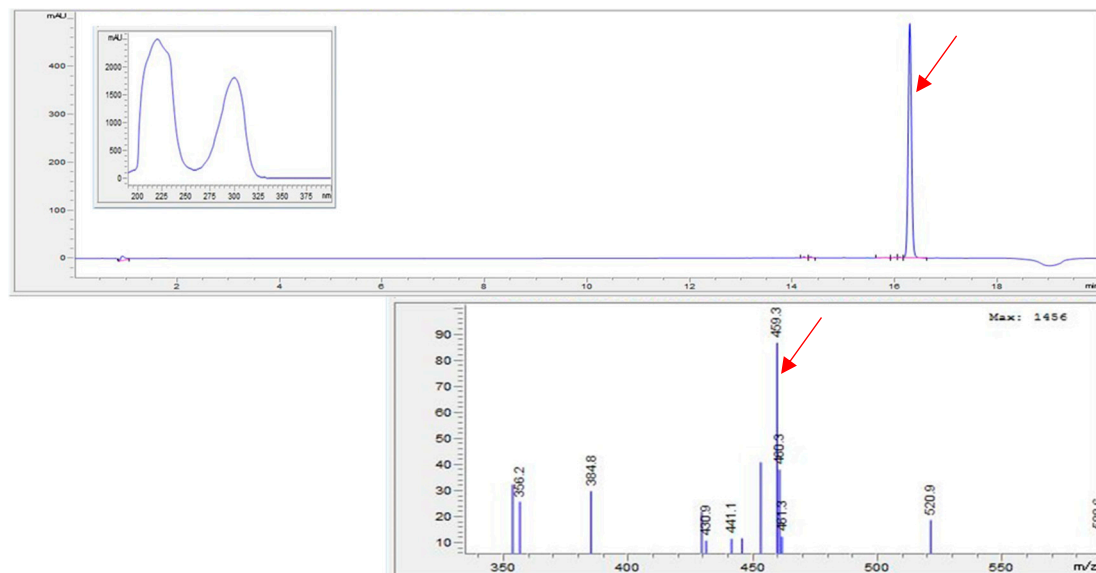


Figure S5. LC/MS data (detection wavelength was set as 315 nm) of compound 2.

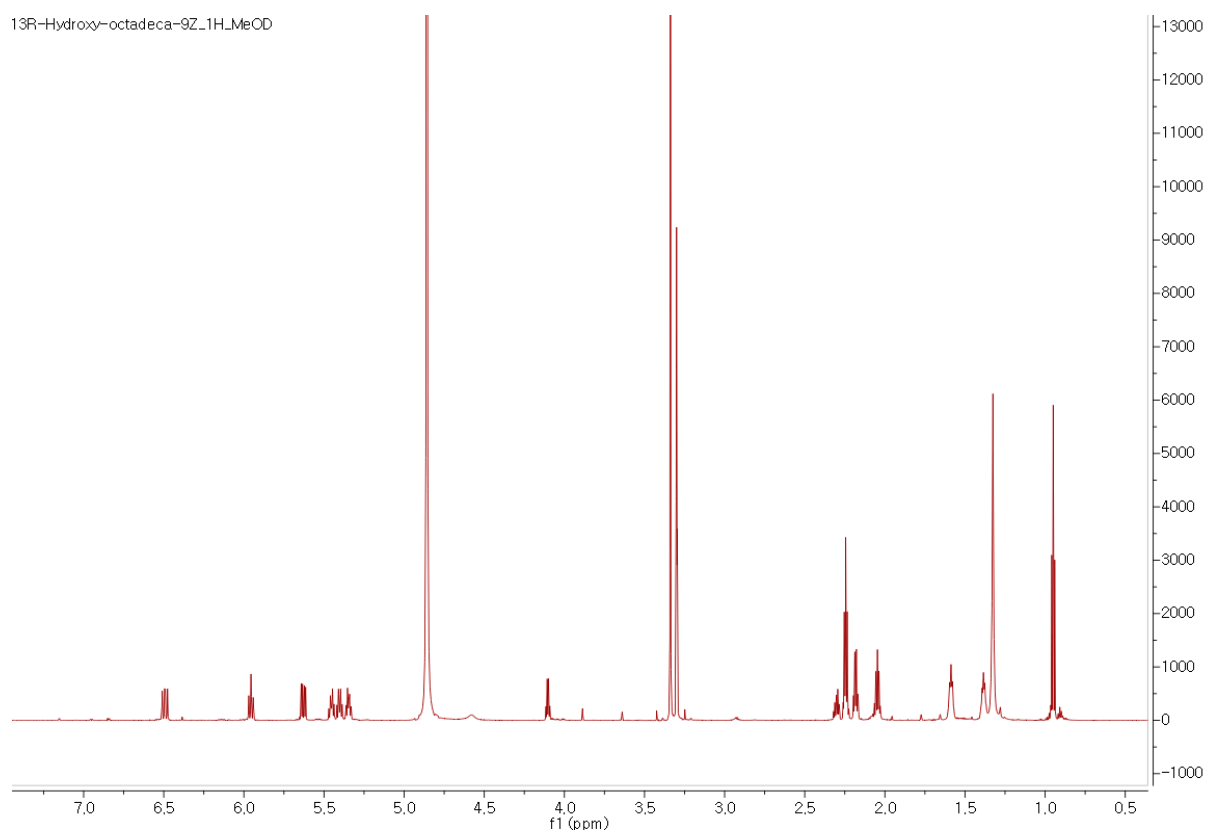


Figure S6. ^1H -NMR spectrum of compound **3** (in CD_3OD).

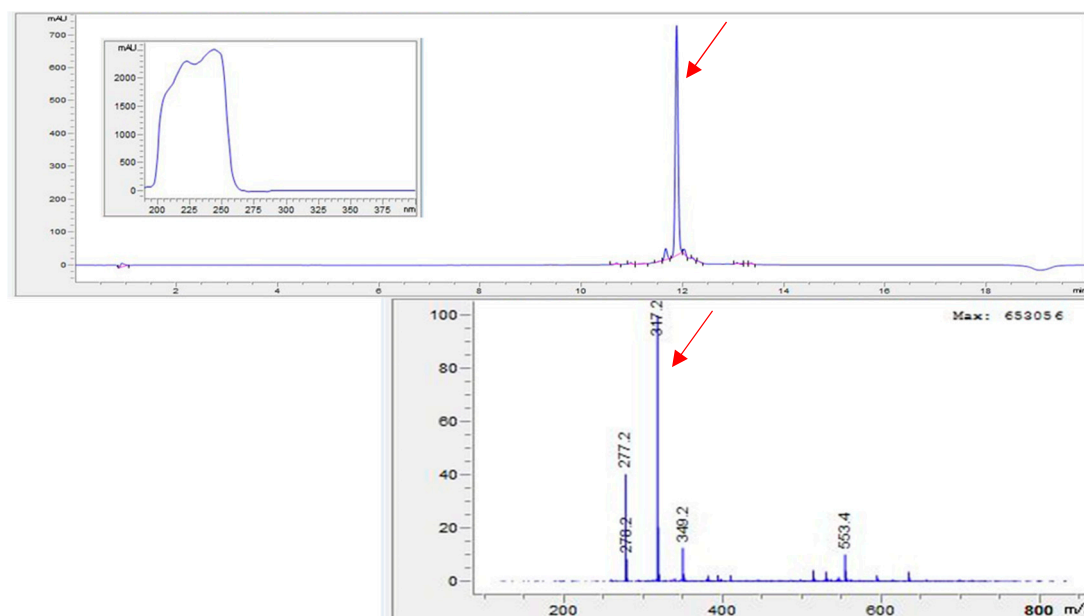


Figure S7. LC/MS data (detection wavelength was set as 254 nm) of compound **3**.

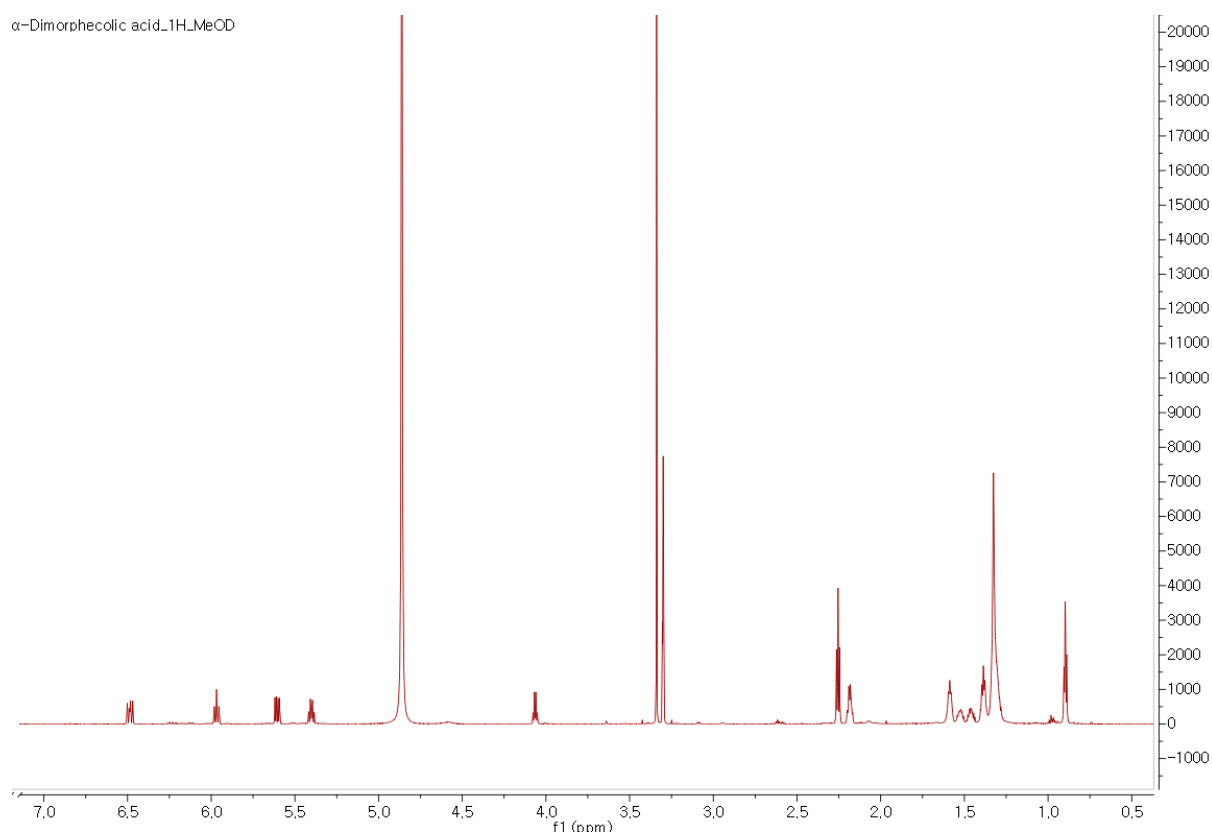


Figure S8. ^1H -NMR spectrum of compound **4** (in CD_3OD).

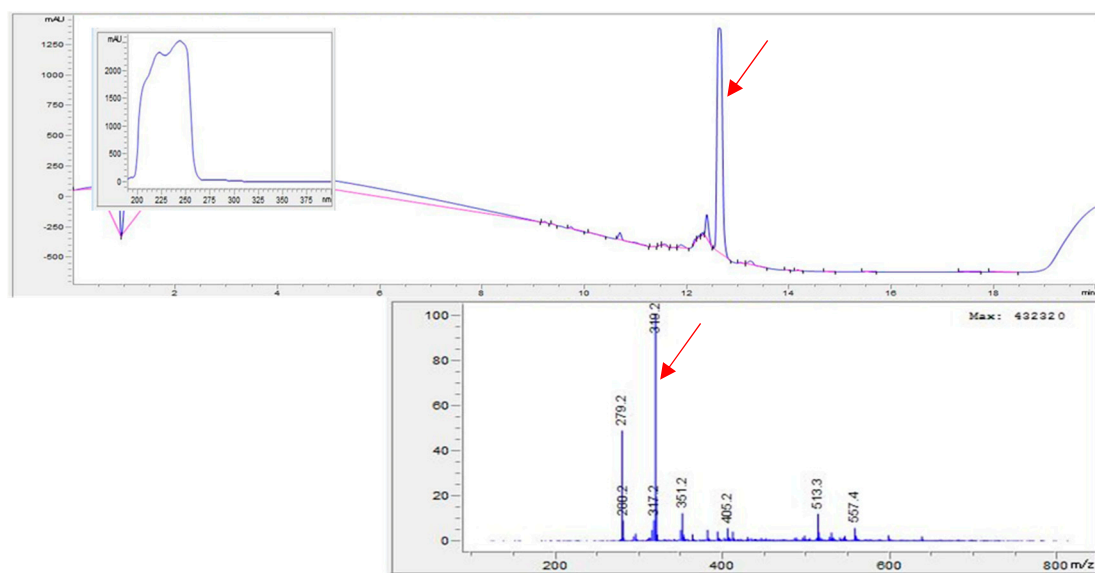


Figure S9. LC/MS data (detection wavelength was set as 210 nm) of compound **4**.

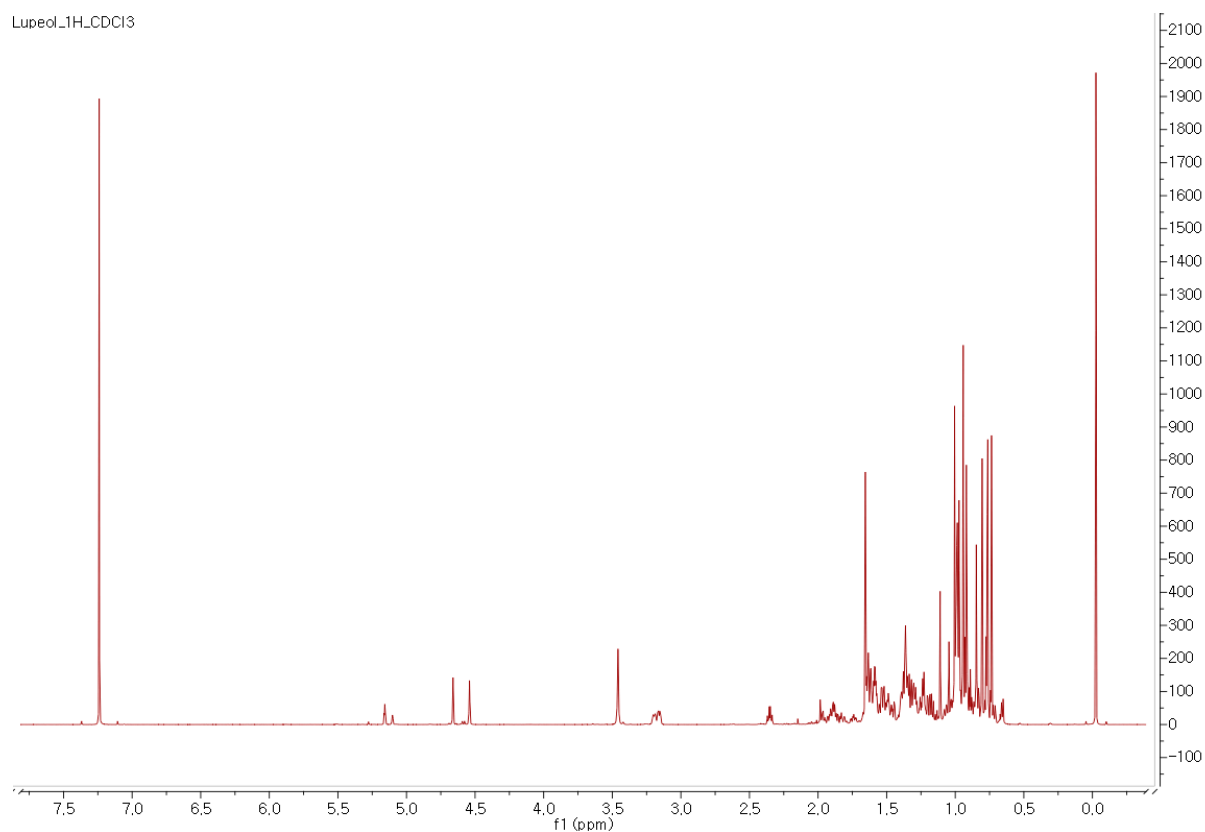


Figure S10. ^1H -NMR spectrum of compound **5** (in CDCl_3).

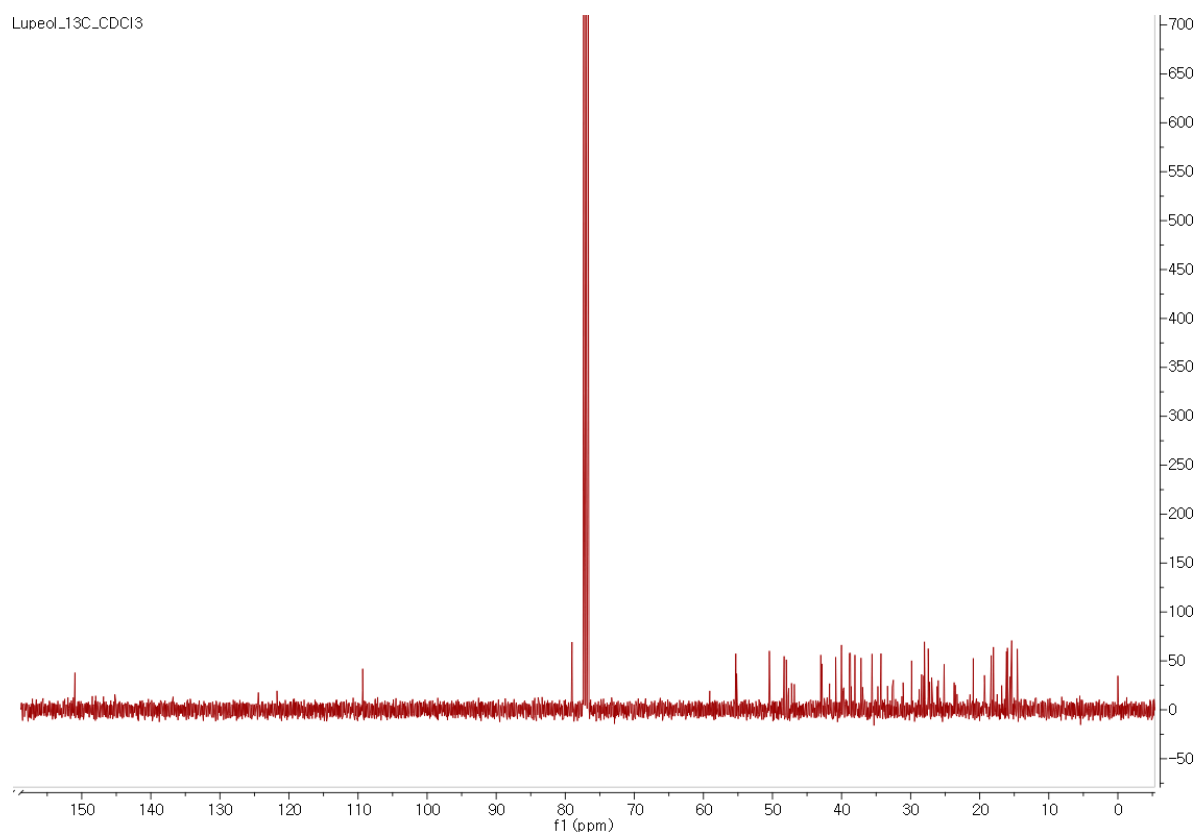


Figure S11. ^{13}C -NMR spectrum of compound **5** (in CDCl_3).

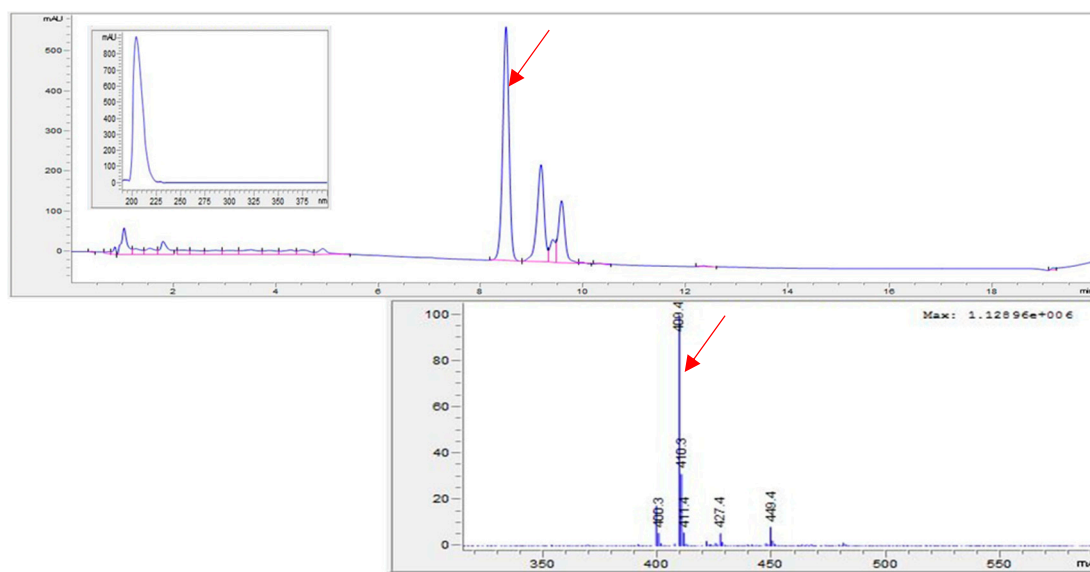


Figure S12. LC/MS data (detection wavelength was set as 210 nm) of compound 5.

General Experimental Procedures

Bruker IFS-66/S FT-IR spectrometer was applied for IR spectra and Agilent 8453 UV–visible spectrophotometer was used for UV spectra. Varian UNITY INOVA 500 NMR spectrometer was operated for NMR spectra at 500 MHz (^1H) and 125 MHz (^{13}C), with chemical shifts given in ppm (δ) for ^1H and ^{13}C NMR analyses. Semi-preparative high-performance liquid chromatography (HPLC) utilized a Waters 1525 binary HPLC pump equipped with a Waters 996 photodiode array detector (Waters Corporation, Milford, MA, USA) using a Phenomenex Luna phenyl-hexyl column (250 \times 10 mm, 10 μm) at flow rate of 2 mL/min (Phenomenex, Torrance, CA, USA). LC/MS analysis was carried out using an Agilent 1200 Series HPLC system equipped with a diode array detector and a 6130 Series ESI mass spectrometer. The column for LC/MS was an analytical Kinetex C₁₈ 100 Å column (100 \times 2.1 mm, 5 μm) at flow rate of 0.3 mL/min (Phenomenex). Generally, open-column chromatography was conducted on silica gel 60 column (Merck, 230–400 mesh) and reversed-phase (RP)-C₁₈ silica gel column (Merck, 230–400 mesh). Sephadex LH-20 column (Pharmacia, Uppsala, Sweden) was used for molecular sieve column chromatography and Diaion HP-20 (Mitsubishi Chemical, Tokyo, Japan) was also used for open-column chromatography. Merck precoated silica gel F₂₅₄ plates and RP-C₁₈ F_{254s} plates were employed for thin layer chromatography. The chromatographic spots were visualized under UV light (254 and 365 nm) or by heating after spraying with anisaldehyde-sulfuric acid.

NMR and physical data of the isolated compounds

1. α -. Tocopherol (1)

Light-yellow oil; IR (KBr) ν_{max} 3483, 1612, 1457, 1265, 1073 cm^{-1} ; (–)-ESIMS m/z : 429.3 [M – H] $^-$; ^1H NMR (500 MHz, CDCl_3): δ_{H} 0.87–0.91 (3H \times 4, m, H-4'a, H-8'a, H-12'a, and H-13'), 1.26 (3H, s, H-2a), 2.14, 2.14, 2.15 (3H \times 3, s, H-5a, H-7a, H-8b), 2.63 (2H, m, H-4), 4.21 (1H, brs, 6-OH); ^{13}C NMR (125 MHz; CDCl_3): δ_{C} 11.1 (C-5a), 11.6 (C-7a), 12.1 (C-8b), 19.6 (C-8'a), 19.6 (C-4'a), 20.7 (C-4), 20.9 (C-2'), 22.5 (C-13'), 22.6 (C-12'a), 23.7 (C-2a), 24.3 (C-6'), 24.7 (C-10'), 27.9 (C-12'), 31.5 (C-3), 32.6 (C-8'), 32.7 (C-4'), 37.2 (C-9'), 37.3 (C-3'), 37.4 (C-5'), 37.4 (C-7'), 39.3 (C-11'), 39.7 (C-1'), 74.4 (C-2), 117.2 (C-3'), 118.4 (C-4a), 121.0 (C-5), 122.5 (C-8), 144.4 (C-8a), 145.5 (C-6).

2.7. *a*-Methoxy- α -tocopherol (2)

Colorless oil; IR (KBr) ν_{\max} 3394, 1610, 1460, 1264, 1073 cm^{-1} ; (-)-ESIMS m/z : 459.3 [M - H]⁻; ¹H NMR (500 MHz; CD₃OD): δ_{H} 0.85–0.89 (3H \times 4, m, H-4'a, H-8'a, H-12'a, and H-13'a), 1.24 (3H, s, H-2a), 1.79 (2H, m, H-3), 2.07 (3H, s, H-8b), 2.12 (3H, s, H-5a), 2.71 (2H, t, J = 6.5 Hz, H-4), 3.37 (3H, s, 7a-OMe), 4.59 (2H, s, H-7a); ¹³C NMR (125 MHz; CDCl₃): δ_{C} 10.9 (C-5a), 11.0 (C-8b), 19.7 (C-8a), 19.8 (C-4a), 20.9 (C-4), 21.1 (C-2), 22.7 (C-13), 22.8 (C-12a), 23.9 (C-2a), 24.5 (C-6), 24.9 (C-10), 28.1 (C-12), 31.5 (C-3), 32.8 (C-8), 32.9 (C-4), 37.4 (C-9), 37.5 (C-3, 5, 7), 39.4 (C-11), 39.8 (C-1), 58.1 (7a-OMe), 70.7 (C-7a), 74.7 (C-2), 118.8 (C-7), 120.4 (C-4a), 120.5 (C-5), 121.0 (C-8), 144.8 (C-8a), 147.1 (C-6).

3.13(. R)-Hydroxy-octadeca-(9Z,11E,15Z)-trien-oic acid (3)

Yellow oil; IR (KBr) ν_{\max} 3625, 3025, 2940, 1720, 1675, 1655, 984, 964 cm^{-1} ; ESIMS m/z : 317.2 [M + Na]⁺; ¹H NMR (500 MHz; CD₃OD): δ_{H} 0.94 (3H, t, J = 7.5, H-18), 1.38 (6H, m, H-4, H-5, and H-6), 1.39 (2H, m, H-7), 1.59 (2H, m, H-3), 2.06 (2H, qd, J = 7.5, 7.5 Hz, H-17), 2.20 (2H, m, H-23), 2.30 (4H, t, J = 7.5 Hz, H-2 and H-14), 4.11 (1H, dd, J = 6.5, 6.0 Hz, H-13), 5.34 (1H, m, H-15), 5.40 (1H, m, H-9), 5.46 (1H, m, H-16), 5.60 (1H, dd, J = 15.5, 6.5 Hz, H-12), 5.96 (1H, t, J = 10.5 Hz, H-10), 6.50 (1H, dd, J = 15.0, 10.5 Hz, H-11); ¹³C NMR (125 MHz; CDCl₃): δ_{C} 14.3 (C-18), 20.8 (C-17), 24.7 (C-3), 27.7 (C-8), 28.9 (C-4, C-5, and C-6), 29.4 (C-7), 33.8 (C-2), 35.3 (C-14), 72.2 (C-13), 123.8 (C-15), 126.0 (C-11), 127.9 (C-10), 133.0 (C-9), 135.0 (C-12), 135.4 (C-16), 178.4 (C-1).

4.α-. Dimorphecolic acid (4)

Yellow gum; IR (KBr) ν_{\max} 3600, 3025, 2935, 1715, 1675, 1655, 985, 950 cm^{-1} ; ESIMS m/z : 319.2 [M + Na]⁺; ¹H NMR (500 MHz, CD₃OD): δ_{H} 0.91 (3H, t, J = 6.5 Hz, H-18), 1.20–1.51 (16H, m), 1.53–1.60 (4H, m), 2.17 (2H, m, H-14), 2.26 (2H, t, J = 7.0 Hz, H-2), 4.07 (1H, q, J = 7.0 Hz, H-9), 5.38 (1H, dt, J = 11.0, 7.0 Hz, H-13), 5.60 (1H, dd, J = 15.0, 7.0 Hz, H-10), 5.95 (1H, dd, J = 11.0, 11.0 Hz, H-12), 6.49 (1H, dd, J = 15.0, 11.0 Hz, H-11); ¹³C NMR (125 MHz, CD₃OD): δ_{C} 14.7 (C-18), 23.8 (C-17), 26.4 (C-3), 26.8 (C-7), 28.9 (C-14), 30.5 (C-6), 30.7 (C-5), 30.7 (C-15), 30.8 (C-4), 32.8 (C-16), 35.4 (C-2), 38.7 (C-8), 73.6 (C-9), 126.8 (C-11), 129.6 (C-12), 133.2 (C-13), 137.5 (C-10), 178.1 (C-1).

5. Lupeol (5)

White powder; IR (KBr) ν_{\max} 3326, 2931, 1631, 1450, 1377, 1035, 874 cm^{-1} ; ESIMS m/z : 427.4 [M + H]⁺; ¹H NMR (500 MHz, CDCl₃): δ_{H} 0.78, 0.81, 0.85, 0.96, 0.98, 1.04, and 1.71 (each 3H, s, H-23, H-24, H-25, H-26, H-27, H-28, and H-30), 2.39 (1H, dt, J = 9.5, 4.0 Hz, H-19), 3.20 (1H, dd, J = 11.5, 5.0 Hz, H-3), 4.58 (1H, brs, H-29b), 4.69 (1H, brs, H-29a); ¹³C NMR (125 MHz, CDCl₃): δ_{C} 15.0 (C-27), 15.9 (C-24), 16.4 (C-26), 16.6 (C-25), 18.5 (C-28), 18.8 (C-6), 19.8 (C-30), 21.4 (C-11), 25.6 (C-12), 27.9 (C-15), 27.9 (C-2), 28.5 (C-23), 30.3 (C-21), 34.7 (C-7), 36.0 (C-16), 37.6 (C-10), 38.5 (C-13), 39.2 (C-1), 39.3 (C-4), 40.5 (C-22), 41.3 (C-8), 43.3 (C-14), 43.5 (C-17), 48.4 (C-18), 48.7 (C-19), 50.8 (C-9), 55.7 (C-5), 79.4 (C-3), 109.7 (C-29), 151.2 (C-20).