Data S1

Dihydroalterperylenol (compound 1): ^{1}H NMR (500 MHz; DMSO-d6) δ 12.72 (1H; s; 3-OH), 12.32 (1H; s; 10-OH), 8.05 (1H; d; J=8.8 Hz; H-1), 7.99 (1H; d; J=8.8 Hz; H-12), 7.03 (1H; d; J=8.7 Hz; H-2), 6.94 (1H; d; J=8.7 Hz; H-11), 5.37 (1H; d; J=5.9 Hz; 7-OH), 5.28 (1H; s; 6a-OH), 4.52 (1H; m; H-7), 3.07 (1H; ddd; J=17.4; 14.4; 4.8 Hz; H-6b), 3.02 (1H; m; H-5β), 2.96 (1H; m; H-5α), 2.96 (1H; dd; J=16.0; 15.9 Hz; H-8β), 2.85 (1H; dd; J=15.8; 4.6 Hz; H-8α), 2.57 (1H; dt; J=17.1; 3.1 Hz; H-6β), 2.30 (1H; td; J=14.3; 3.8 Hz; H-6α); ^{13}C NMR (125 MHz; DMSO-d6) δ 206.1, 204.2, 161.0, 160.4, 140.7, 138.4, 132.9, 132.5, 124.8, 123.5, 117.9, 116.6, 115.6, 113.8, 68.0 , 64.7, 51.4, 47.5, 34.8, 33.5. ^{1}H and ^{13}C NMR spectra of compound 1 were shown in Figs. S2A and B.

Fonsecinone A (compound 2; Figs. S1 and 2): ^{1}H-NMR (500 MHz; CDCl3) *δ* 7.03 (1H; s; H-6), 6.95 (1H; s; H-7), 6.40 (1H; d; J=2.0 Hz; H-7'), 6.31 (1H; s; H-3), 6.15 (1H; d; J=2.0 Hz; H-9'), 5.98 (1H; s; H-3'), 3.99 (3H; s; 6'-OCH3), 3.75 (3H; s; 8-OCH3), 3.58 (3H; s; 8'-OCH3), 3.40 (3H; s; 10-OCH3), 2.46 (3H; s; 2-CH3), 2.10 (3H; s; 2'-CH3); ^{13}C-NMR (126 MHz; CDCl3) *δ* 20.6 (2-CH3), 20.7 (2'-CH3), 55.3 (8'-OCH3), 56.1 (8-OCH3), 56.3 (6'-OCH3), 61.3 (10-OCH3), 96.3 (C-9'), 97.2 (C-7'), 101.7 (C-7), 104.3 (C-4'a), 105.3 (C-10'), 106.1 (C-6), 107.4 (C-3'), 108.1 (C-10a), 108.5 (C-5'a), 109.4 (C-4a), 110.7 (C-3), 117.3 (C-9), 140.7 (C-9'a), 140.9 (C-6a), 150.9 (C-10'a), 155.2 (C-10b), 156.3 (C-5), 156.9 (C-10), 160.1 (C-8), 161.1 (C-6'), 161.7 (C-8'), 162.3 (C-5'), 167.2 (C-2'), 167.8 (C-2), 183.0 (C-4), 184.7 (C-4'). ^{1}H and ^{13}C NMR spectra of compound 2 were shown in Figs. S3A and B.

Aurasperone A (compound 3; Figs. S1-3): ^{1}H-NMR (500 MHz; CDCl3) *δ* 15.25 (1H; s; 5'-OH), 14.83 (1H; s; 5-OH), 7.15 (1H; s; H-10), 6.97 (1H; s; H-9), 6.41 (1H; d; J=2.2 Hz; H-7'), 6.21 (1H; d; J=2.2 Hz; H-9'), 6.06 (1H; s; H-3), 5.98 (1H; s; H-3'), 4.03 (3H; s; 6'-OCH3), 3.79 (3H; s; 8-OCH3), 3.62 (3H; s; 8'-OCH3), 3.46 (3H; s; 6-OCH3), 2.42 (3H; s; 2-CH3), 2.12 (3H; s; 2'-CH3)□^{13}C-NMR (125 MHz; CDCl3) *δ* 20.9 (2'-CH3), 20.9 (2-CH3), 55.3 (8'-OCH3), 56.1 (8-OCH3), 56.4 (6'-OCH3), 62.2 (6-OCH3), 96.6 (C-9'), 97.0 (C-7'), 101.4 (C-10), 101.5 (C-9), 104.4 (C-4'a), 104.9 (C-4a), 105.3 (C-10'), 107.4 (C-3'), 107.6 (C-3), 108.7 (C-5'a), 111.6 (C-5a), 117.8 (C-7), 140.7 (C-9'a), 140.8 (C-9a), 151.0 (C-10'a), 153.5 (C-10a), 158.7 (C-6), 160.3 (C-8), 161.2 (C-6'), 161.5 (C-8'), 162.1 (C-5), 162.8 (C-5'), 167.7 (C-2'), 167.8 (C-2), 184.6 (C-4), 184.7 (C-4'). ^{1}H and ^{13}C NMR spectra of compound 3 were shown in Figs. S4A and B.

3β,5α,9α-trihydroxy-(22E;24R)-ergosta-7,22-diene-6-one (compound 4; Figs. S1-4): ^{1}H NMR (500 MHz; MeOD) *δ* 5.61 (d; J=2.0 Hz; 1H), 5.23 (qd; J=15.3; 7.8 Hz; 2H), 3.96 (tt; J=11.6; 4.8 Hz; 1H), 2.76 (ddd; J=12.0; 6.7; 2.1 Hz; 1H), 2.30 (m; 2H), 1.05 (d; J=6.6 Hz; 3H), 1.01 (s; 3H), 0.94 (d; J=6.8 Hz; 3H), 0.86 (d; J=6.7 Hz; 3H), 0.84 (d; J=6.8 Hz; 3H), 0.66 (s; 3H); *δ* ^{13}C NMR (125 MHz; MeOD) *δ* 199.0, 163.9, 135.1, 132.3, 119.6, 78.8, 74.8, 66.4, 56.0, 51.5, 44.9, 42.8, 41.4, 40.2, 35.7, 34.8, 32.9, 29.6, 28.0, 27.7, 25.3, 22.2, 20.5, 19.5, 19.4, 19.0, 17.1, 11.7. ^{1}H and ^{13}C NMR spectra of compound 4 were shown in Figs. S5A and B.

Gargalol B (compound 5; Figs. S1-5): ^{1}H NMR (500 MHz; MeOD) *δ* 5.23 (m; 1H), 5.16 (m; 1H), 5.03 (t; J=2.0 Hz; 1H), 3.91 (m; 1H) , 3.88 (m; 1H), 1.02 (m; 6H), 0.90 (d; J=6.8 Hz; 3H), 0.81 (dd; J=9.0; 6.8 Hz; 6H), 0.57 (s; 3H); ^{13}C NMR (125 MHz; MeOD) *δ* 142.3, 135.5, 131.9, 120.2, 74.4, 69.8, 66.5, 55.8, 50.2, 43.5, 42.8, 40.8, 40.4, 39.4, 35.0, 33.0, 29.8, 29.5, 28.0, 27.0, 26.5, 22.5, 20.6, 19.8, 19.5, 19.1, 17.2, 11.2. ^{1}H and ^{13}C NMR spectra of compound 5 were shown in Figs. S6A and B.

(22E;24R)-ergosta-7,22-dien-3β,5α,6β,9α-tetraol (compound 6; Figs. S1-6): ^{1}H NMR (500 MHz; MeOD) *δ* 5.31 (dt; J=5.0; 2.3 Hz; 1H), 5.26-5.13 (m; 2H), 4.18 (s; 2H), 4.03-3.93 (m; 1H), 3.57 (dt; J=5.3; 2.0 Hz; 1H), 2.12-1.91 (m; 2H), 1.84 (td; J=13.1; 12.1; 5.6 Hz; 1H), 1.70-1.62 (m; 1H), 1.62-1.38 (m; 4H), 1.38-1.24 (m; 2H), 1.06 (s; 3H), 1.03 (d; J=6.6 Hz; 3H), 0.92 (d; J=6.8 Hz; 3H), 0.84 (dd; J=8.0; 6.7 Hz; 6H); ^{13}C NMR (125 MHz; Methanol-d4) *δ* 143.2, 135.4, 132.0, 117.4, 77.4, 77.2, 76.9, 75.8, 73.0, 67.2, 55.9, 54.6, 43.5, 43.0, 42.7, 40.4, 39.2, 38.8, 36.9, 33.0, 32.7, 30.3, 27.9, 22.8, 21.9, 20.9, 19.7, 19.4, 18.1, 17.4, 12.1. ^{1}H and ^{13}C NMR spectra of compound 6 were shown in Figs. S7A and B.

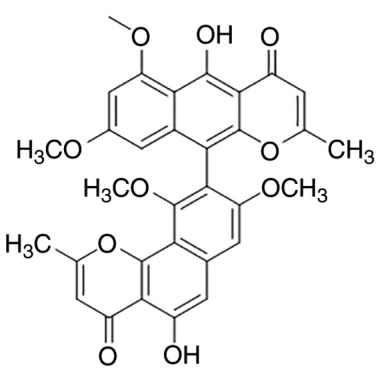
11-[(6-Deoxy-α-L-mannopyranosyl)oxy]-3-hydroxyhexadecanoic acid (compound 7; Figs. S1-7): ^{1}H-NMR (500 MHz; MeOD) *δ* 4.79 (1H; d; J=1.1 Hz; H-1), 3.75 (1H; d; J=1.1 Hz; H-2), 3.66 (2H; m; H-5; H-3), 3.36 (1H; t; J=9.6 Hz; H-4), 2.59 (1H; dd; J=7.0; 15.1 Hz; CH2CO2H), 2.49 (1H; dd; J=5.6; 15.1 Hz; CH2CO2H), 1.59 (4H; m; 2xCH2), 1.27~1.35 (18H; m; 8xCH2), 1.25 (3H; d; J=6.2 Hz; H-6), 0.9 (3H; t; J=6.8 Hz; CH3); ^{13}C-NMR (126 MHz; MeOD) *δ* 14.5, 17.9, 23.7, 25.9, 26.3, 30.3, 30.4 , 30.4, 30.7, 32.9, 33.0, 34.2, 35.1, 41.3, 70.1, 72.2, 72.6, 72.6, 74.0, 75.4, 100.4, 172.6. ^{1}H and ^{13}C NMR spectra of compound 7 were shown in Figs. S8A and B.

Penisochroman A (compound 8; Figs. S1-8): ^{1}H-NMR (500 MHz; MeOD) δ 6.02 (1H; s; H-5), 5.50 (1H; s; H-1), 4.05 (1H; m; H-3), 3.35 (3H; s; H-14), 2.56 (1H; dd; J=3.3; 16.8 Hz; H-4a), 2.47 (1H; dd; J=11.5; 16.9 Hz; H-4b), 1.55~1.62 (4H; m; H-9; H-10), 1.34~1.39 (4H; m; H-11; H-12), 0.94 (3H; t; J=6.9 Hz; H-13); ^{13}C-NMR (125 MHz; MeOD) δ: 14.4 (C-13), 23.7 (C-12), 26.5 (C-10), 33.0 (C-11), 35.4 (C-4), 36.7 (C-9), 49.9 (C-14), 67.6 (C-3), 97.1 (C-1), 103.2 (C-7), 105.7 (C-5), 112.6 (C-8a), 141.1 (C-4a), 161.0 (C-8), 162.8 (C-6), 177.9 (C-15). ^{1}H and ^{13}C NMR spectra of 8 were shown in Figs. S9A and B.

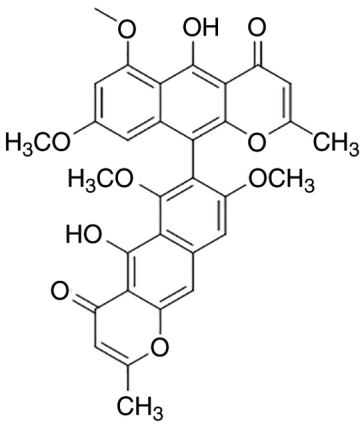
β-adenosine (compound 9; Figs. S1-9): ^{1}H NMR (600 MHz; MeOD) *δ* 7.99 (dd; J=8.1; 1.9 Hz; 1H), 5.90 (d; J=4.7 Hz; 1H), 5.78 (d; J=8.1 Hz; 1H), 4.22 (t; J=5.0 Hz; 1H), 4.17 (t; J=5.0 Hz; 1H), 4.05 (dt; J=4.9; 3.0 Hz; 1H), 3.86 (dd; J=12.4; 3.0 Hz; 1H), 3.76 (dd; J=12.4; 3.0 Hz; 1H); 13C NMR (150 MHz; MeOD) δ 166.2, 152.3, 142.6, 102.7, 90.4, 85.9, 75.3, 70.9, 61.9. ^{1}H and ^{13}C NMR spectra of compound 9 were show in Figs. S10A and B.

Uridine (compound 10; Figs. S1-10): ^{1}H NMR (600 MHz; MeOD) δ 8.34 (s; 1H), 8.21 (s; 1H), 6.00 (d; J=6.5 Hz; 1H), 4.75 (dd; J=6.5; 5.1 Hz; 1H), 4.36 (dd; J=5.1; 2.6 Hz; 1H), 4.23 (q; J=2.7 Hz; 1H), 3.90 (dd; J=12.7; 2.5 Hz; 1H), 3.79 (dd; J=12.7; 2.8 Hz; 1H); ^{13}C NMR (150 MHz; MeOD) *δ* 157.3, 153.5, 149.8, 142.0, 120.7, 90.8, 87.9, 75.3, 72.4, 63.2. ^{1}H and ^{13}C NMR spectra of compound 10 were shown in Figs. S11A and B.

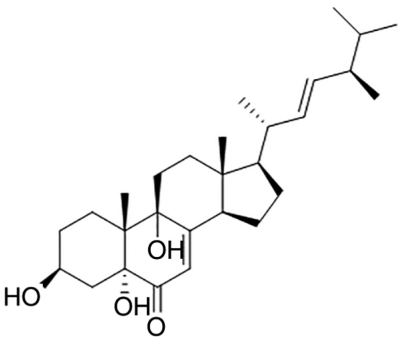
Figure S1. Chemical structures of compounds 2-10.



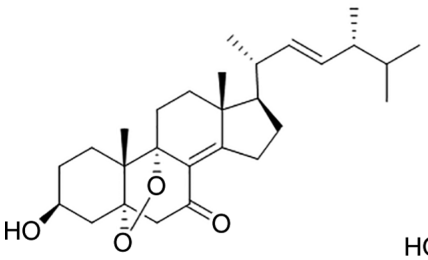
2



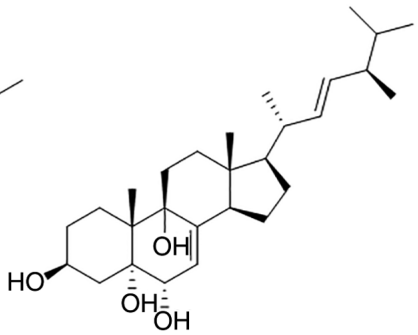
3



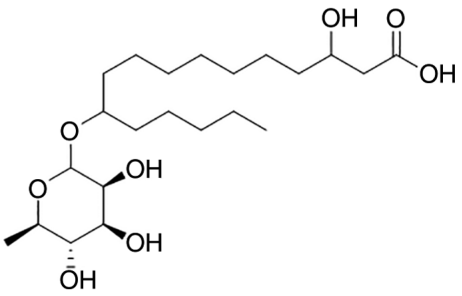
4



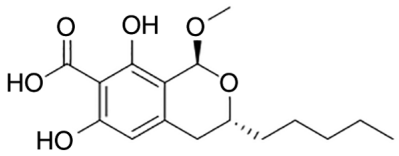
5



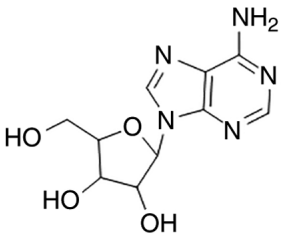
6



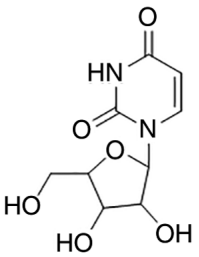
7



8



9



10

Figure S2. Two-dimensional nuclear magnetic resonance spectrum of compound 1. (A) Compound 1 1H-NMR spectrum in DMSO-d6 (500 MHz). (B) Compound 1 13C-NMR spectrum in DMSO-d6 (125 MHz).

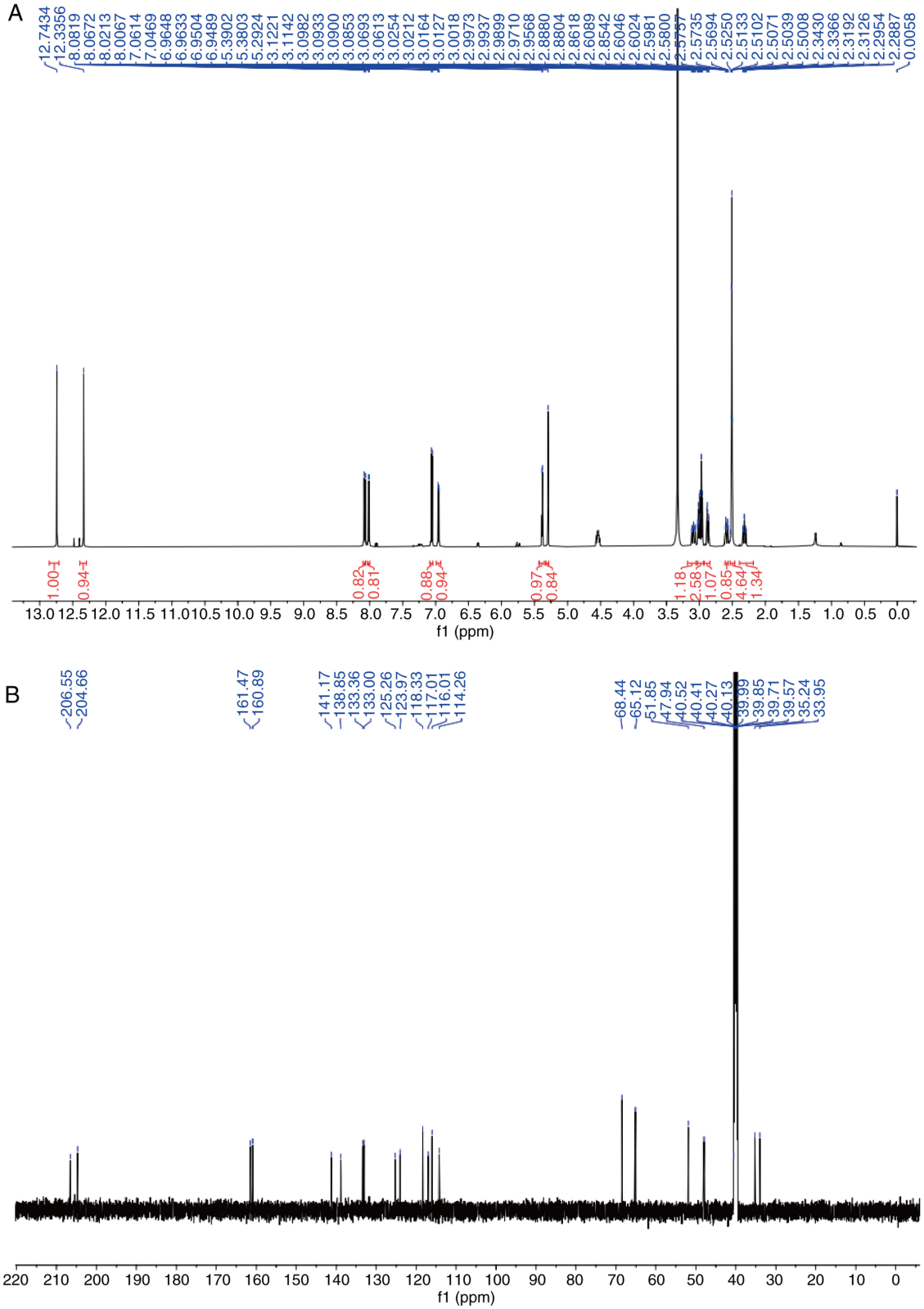


Figure S3. Two-d imensional nuclear magnetic resonance spectrum of compound 2. (A) Compound 2 1H-NMR spectrum in CDCl3 (500 MHz). (B) Compound 2 13C-NMR spectrum in CDCl3 (125 MHz).

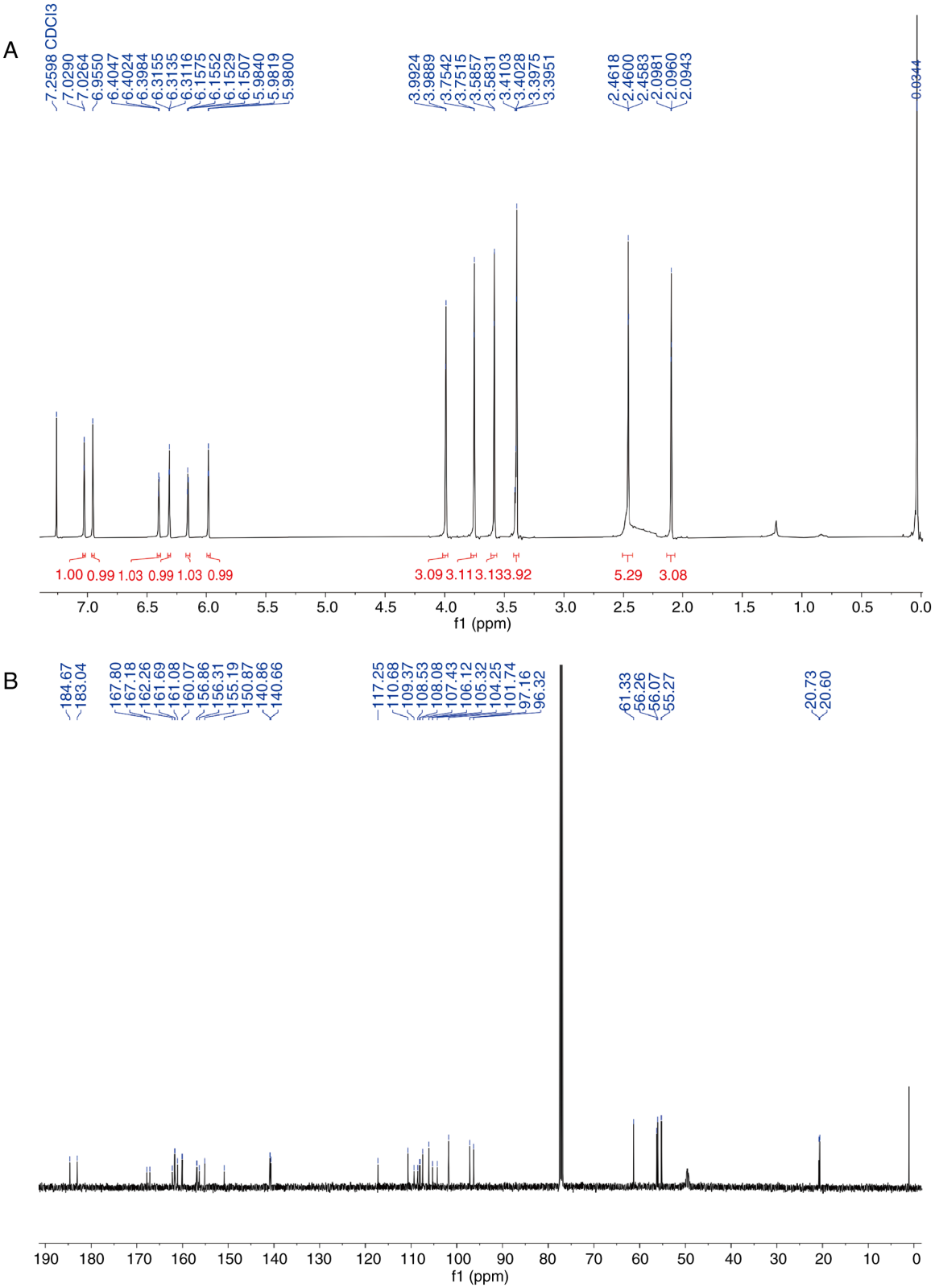


Figure S4. Two-dimensional nuclear magnetic resonance spectrum of compound 3. (A) Compound 3 1H-NMR spectrum in CDCl3 (500 MHz). (B) Compound 3 13C-NMR spectrum for 3 in CDCl3 (125 MHz).

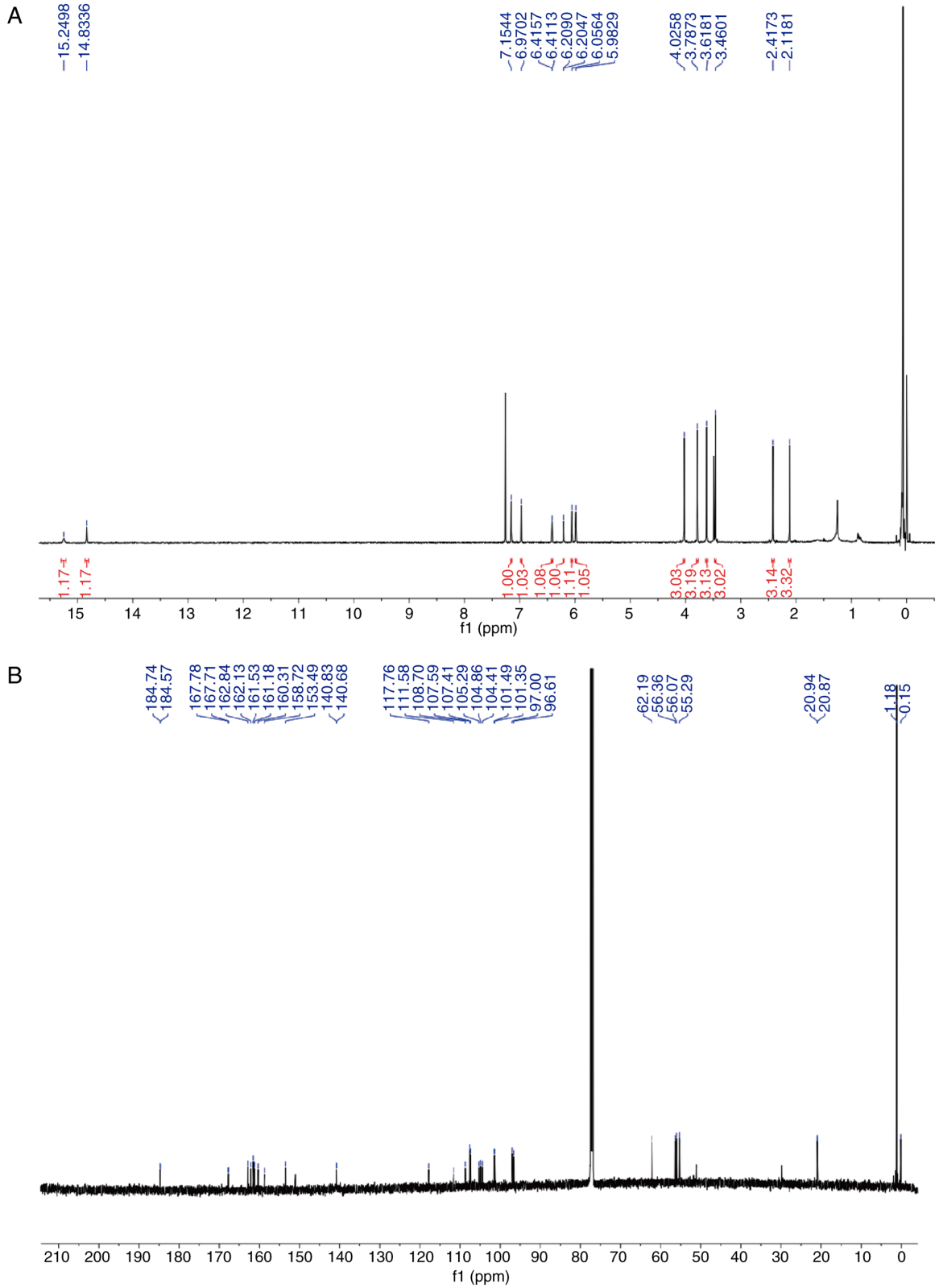


Figure S5. Two-dimensional nuclear magnetic resonance spectrum of compound 4. (A) Compound 4 1H-NMR spectrum in MeOD (500 MHz). (B) Compound 4 13C-NMR spectrum in MeOD (125 MHz).

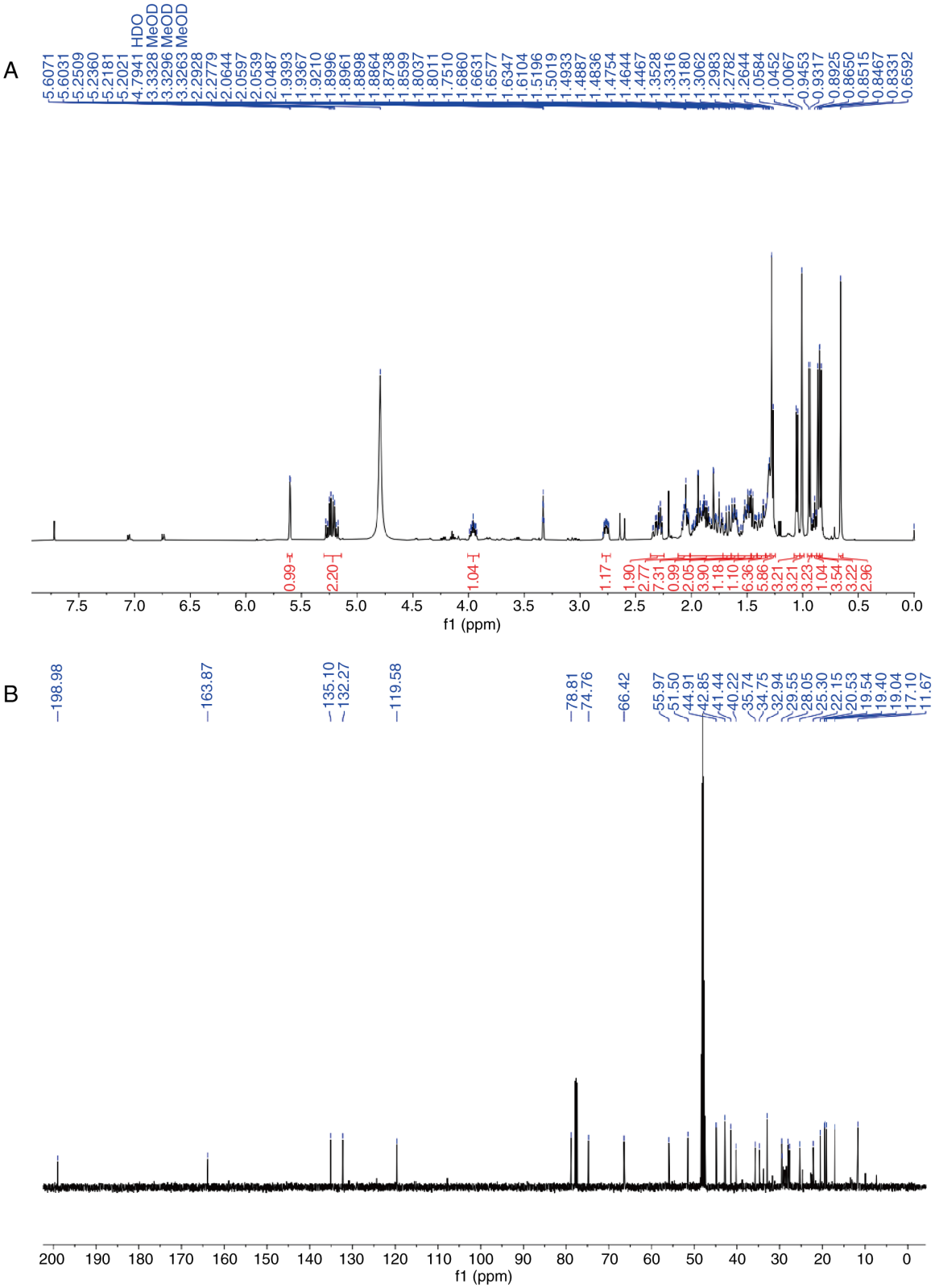


Figure S6. Two-dimensional nuclear magnetic resonance spectrum of compound 5. (A) Compound 5 1H-NMR spectrum in MeOD (500 MHz). (B) Compound 5 13C-NMR spectrum in MeOD (125 MHz).

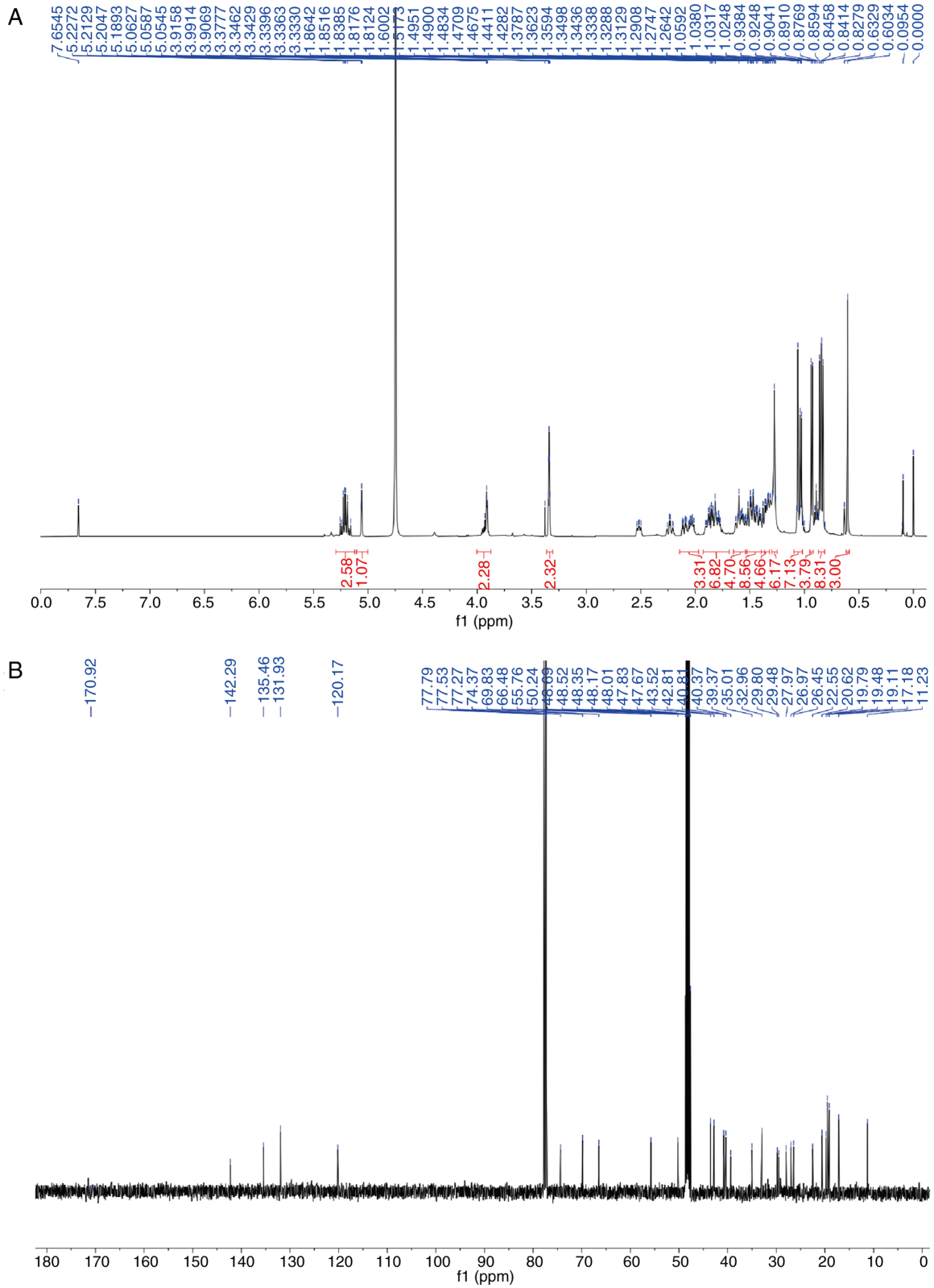


Figure S7. Two-dimensional nuclear magnetic resonance spectrum of compound 6. (A) Compound 6 1H-NMR spectrum in MeOD (500 MHz). (B) Compound 6 13C-NMR spectrum in MeOD (125 MHz).

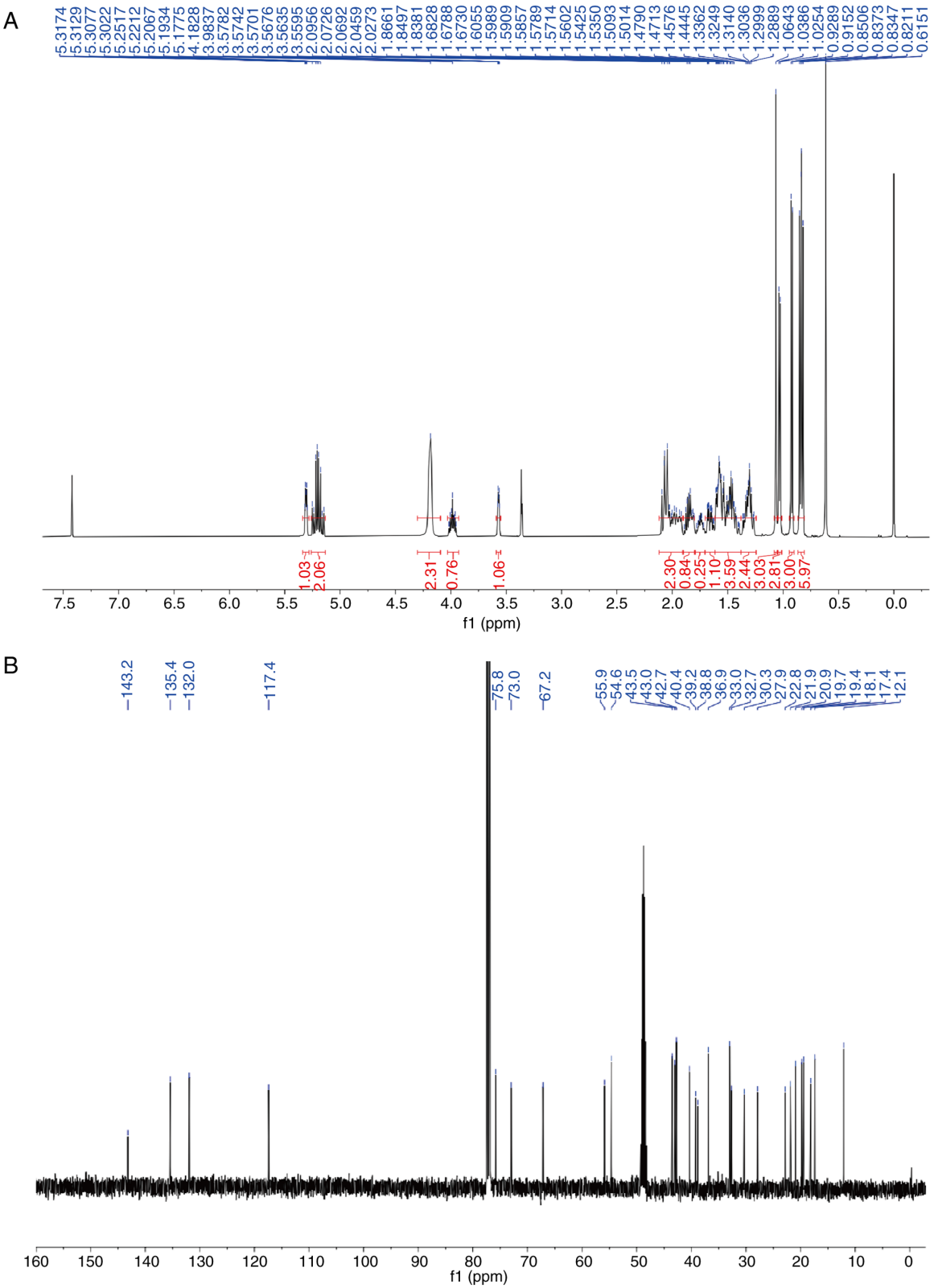


Figure S8. Two-dimensional nuclear magnetic resonance spectrum of compound 7. (A) Compound 7 1H-NMR spectrum in MeOD (500 MHz). (B) Compound 7 13C-NMR spectrum in MeOD (125 MHz).

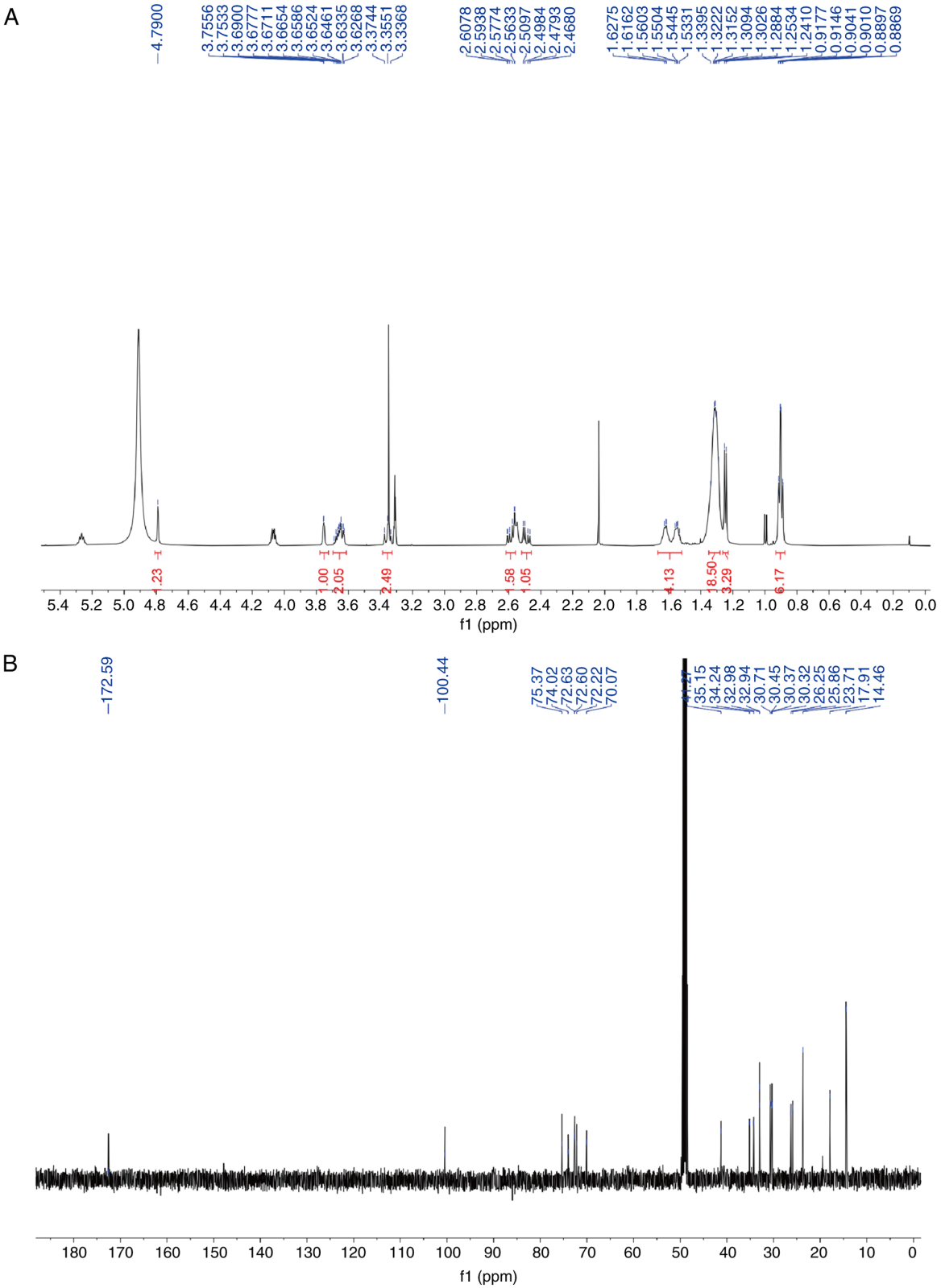


Figure S9. Two-dimensional nuclear magnetic resonance spectrum of compound 8. (A) Compound 8 1H-NMR spectrum in MeOD (500 MHz). (B) Compound 8 13C-NMR spectrum in MeOD (125 MHz).

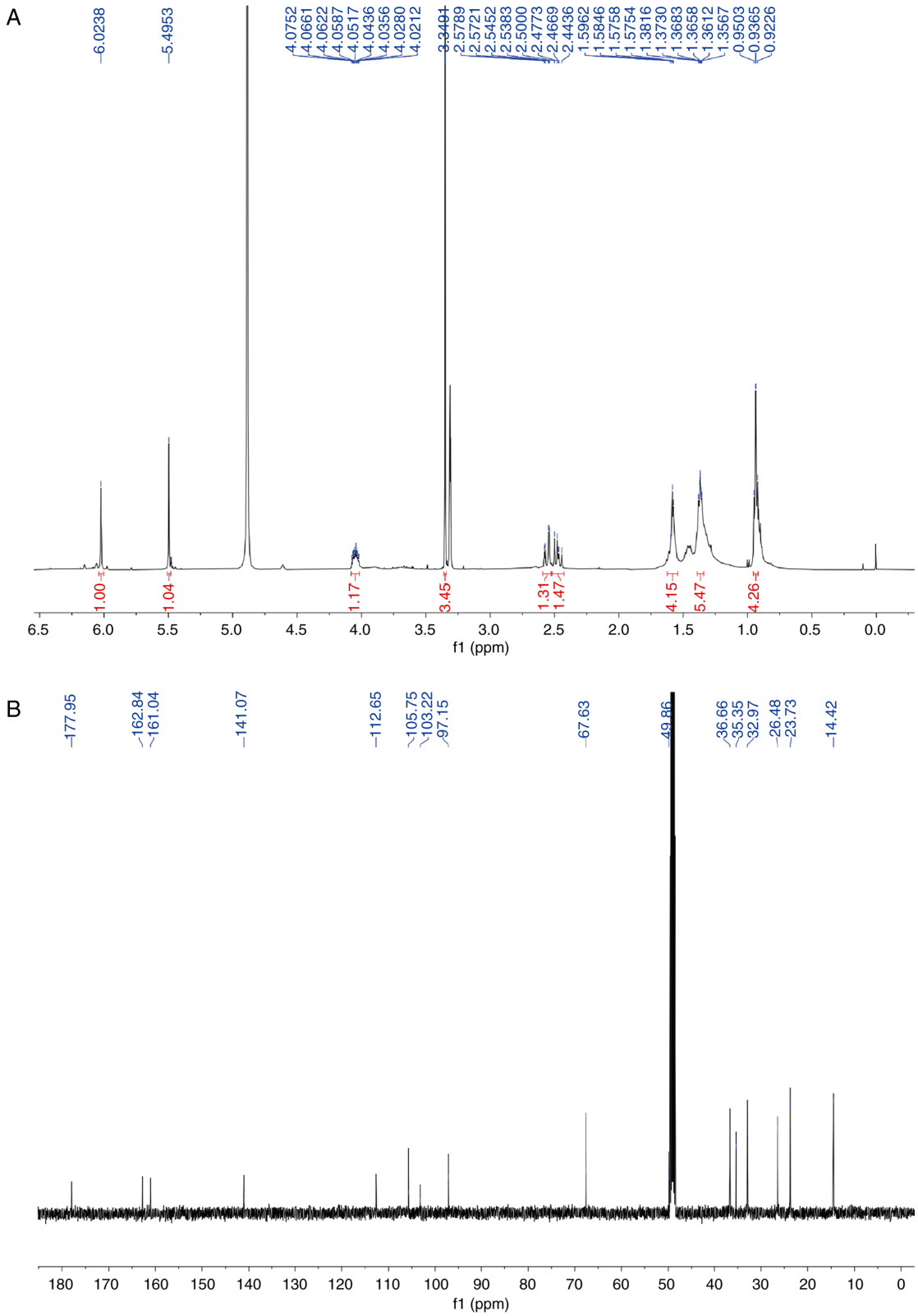


Figure S10. Two-dimensional nuclear magnetic resonance spectrum of compound 9. (A) Compound 9 1H-NMR spectrum in MeOD (600 HMz). (B) Compound 9 13C-NMR spectrum in MeOD (200 MHz).

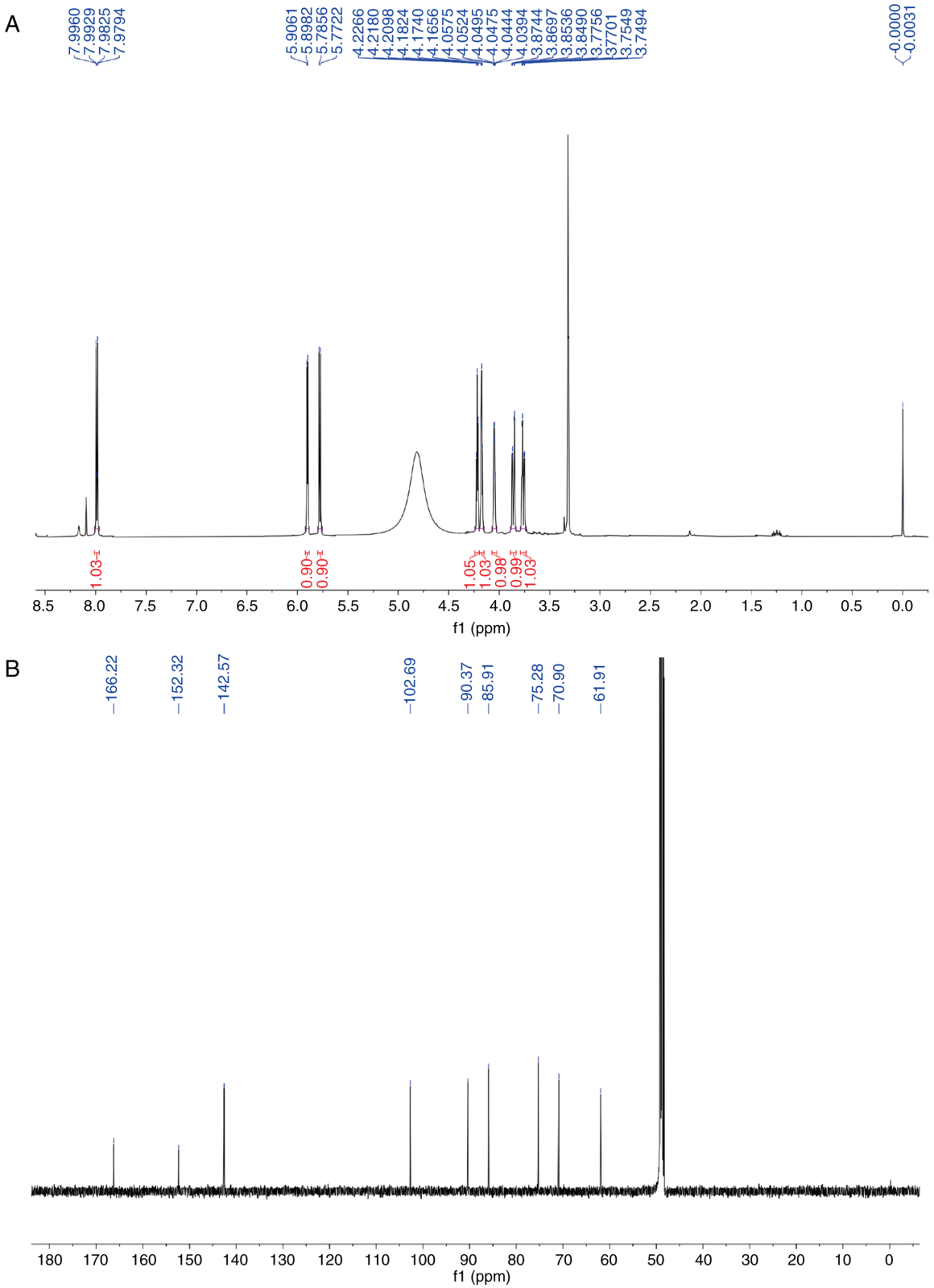


Figure S11. Two-dimensional nuclear magnetic resonance spectrum of compound 10. (A) Compound 10 1H-NMR spectrum in MeOD (600 HMz). (B) Compound 10 13C-NMR spectrum in MeOD (200 HMz).