Electronic Supporting Information

Biomimetic Total Synthesis of Homodimericin A

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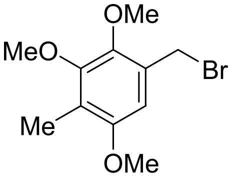
I Experimental Procedures and Spectroscopic Data of Compounds

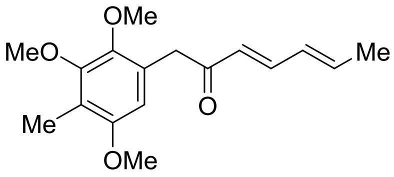
General Procedures. All reactions were carried out under a nitrogen atmosphere with dry solvents under anhydrous conditions, unless otherwise noted. Tetrahydrofuran (THF), diethyl ether (Et_2O), and toluene were distilled immediately before use from sodium-benzophenoneketyl. Methylene chloride (CH_2Cl_2) and 1, 2-Dichlorobenzene (1, 2-DCB) were distilled from calcium hydride and stored under an argon atmosphere. Reagents were purchased at the highest commercial quality and used without further purification, unless otherwise stated. Solvents for chromatography were used as supplied by Titan chemical. Reactions were monitored by thin layer chromatography (TLC) carried out on 0.2 mm Huanghai gel plates (60F-254) using UV light as visualizing agent and aqueous ammonium cerium nitrate/ammonium molybdate or basic aqueous potassium permanganate as developing agent. Huanghai silica gel (60, particle size 0.040–0.063 mm) was used for flash column chromatography.

NMR spectra were recorded on Bruker AV III 400 or 600, and calibrated by using residual undeuterated chloroform (δ_H = 7.26 ppm) and $CDCl_3$ (δ_C = 77.16 ppm), or undeuterated Dimethyl sulfoxide (δ_H = 2.50 ppm) and $(CD_3)_2SO$ (δ_C = 39.52 ppm) as internal references. The following abbreviations are used to designate multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, quint = quintet, br = broad. IR spectra were recorded on a Bruker Tensor-27 FT-IR spectrometer. High-resolution mass spectra (HRMS) were recorded on Waters AutoSpec Premier P776 mass spectrometer. Semi-prep-HPLC was carried out on an Agilent 1260 Series system using a Agilent ZORBAX SB-C18 5μ column (9.4×250 mm).



8

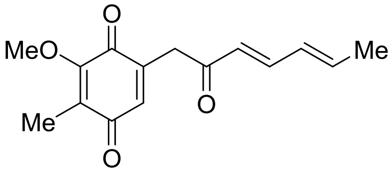
To a stirred suspension of **6**[1] (6.0 g, 28.27 mmol) in CH_2Cl_2 (140 mL) were sequentially added PBr_3 (13.77 mg, 4.78 mL, 50.88 mmol) at 0 °C. The reaction mixture was allowed to stir at 0 °C for 15 min before it was quenched with saturated aq. $NaHCO_3$ (100 mL). The resultant mixture was extracted with DCM (3 × 150 mL). The combined organic phases were washed with brine (100 mL), dried over anhydrous Na_2SO_4, and filtered. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography with petroleum ether/EtOAc (40: 1) to give **8** (6.61 g, 85%) as a white solid. **8**: R_f = 0.36 (silica, petroleum ether: EtOAc 20 : 1); IR (film): ν_{max} = 2937, 1588, 1485, 1464, 1405, 1335, 1246, 1132, 1088, 1032 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 6.58 (s, 1H), 4.56 (s, 2H), 3.92 (s, 3H), 3.82 (s, 3H), 3.80 (s, 3H), 2.12 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 154.14, 151.98, 145.43, 128.44, 122.27, 106.86, 60.88, 60.23, 55.80, 28.84, 9.04 ppm; HRMS (m/z): $[M]^+$ calcd for $C_{11}H_{15}BrO_3^+$ 274.0205, found 274.0206.



5

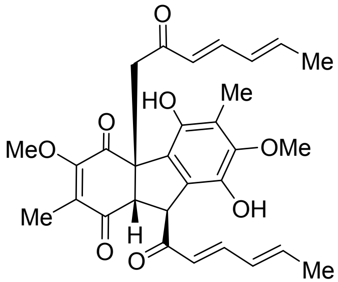
To a stirred solution of **A**[2] (6.39 g, 32.71 mmol) in THF (180 mL) were sequentially added KHMDS (27.26 mL, 1.0 M in THF, 27.26 mmol) and **8** (5.0 g, 18.17 mmol) at −78 °C. The reaction mixture was allowed to stir at −78 °C for 1 h, then were sequentially added TBAF (18.17 mL, 1.0 M in THF, 18.17 mmol), The reaction mixture was allowed to stir at 0 °C for 10 min before it was quenched with saturated aq. NH_4Cl (100 mL). The resultant mixture was extracted with EtOAc (3 × 100 mL). The combined organic phases were washed with brine (100 mL), dried over anhydrous Na_2SO_4, and filtered. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography with petroleum ether/EtOAc (20: 1) to give **5** (4.75 g, 90%) as a pale yellow oil. **5**: R_f =

0.25 (silica, Petroleum ether: EtOAc 10 : 1); IR (film): ν_{max} = 2935, 1637, 1594, 1464, 1405, 1241, 1129, 1087, 1033, 1001 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.32 – 7.21 (m, 1H), 6.41 (s, 1H), 6.22 – 6.17 (m, 1H), 6.15 (d, *J* = 15.4 Hz, 1H), 3.83 (s, 2H), 3.82 (s, 3H), 3.78 (s, 3H), 3.77 (s, 3H), 2.12 (s, 3H), 1.87 (d, *J* = 4.9 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 198.19, 154.04, 151.90, 145.15, 143.57, 140.58, 130.38, 126.72, 125.60, 119.91, 107.36, 60.63, 60.19, 55.77, 42.36, 18.80, 8.86 ppm; HRMS (m/z): [M]$^+$ calcd for $C_{17}H_{22}O_4^+$ 290.1518, found 290.1526.



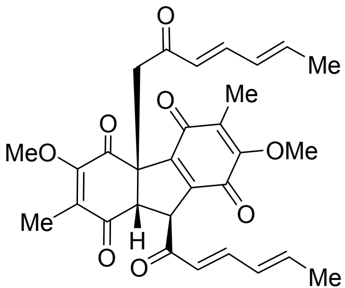
4

To a stirred suspension of **5** (1.4 g, 4.82 mmol) in CH_3CN (48 mL) were sequentially added $(NH_4)_6Ce(NO_3)_2$ (5.81 g, 10.61 mmol) in H_2O (26.5 mL) at 0 °C. The reaction mixture was allowed to stir at 0 °C for 10 min before it was quenched with saturated aq. NaCl (100 mL). The resultant mixture was extracted with Et_2O (3 × 80 mL). The combined organic phases were washed with brine (50 mL), dried over anhydrous Na_2SO_4, and filtered. The solvent was evaporated under vacuum to give **4** as a yellow oil and used in next step without further purification. **4**: R_f = 0.47 (silica, petroleum ether: EtOAc 3: 1); IR (film): ν_{max} = 3441, 2933, 2854, 2426, 1651, 1634, 1455, 1383, 1113, 992 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.25 – 7.16 (m, 1H), 6.55 (s, 1H), 6.29 – 6.17 (m, 2H), 6.12 (d, *J* = 15.5 Hz, 1H), 3.98 (s, 3H), 3.67 (s, 2H), 1.94 (s, 3H), 1.89 (d, *J* = 5.2 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 195.14, 187.82, 182.62, 155.98, 144.60, 141.77, 141.26, 135.01, 130.09, 129.03, 126.59, 60.79, 40.40, 18.90, 8.60 ppm; HRMS (m/z): [M]$^+$ calcd for $C_{15}H_{16}O_4^+$ 260.1049, found 260.1044.



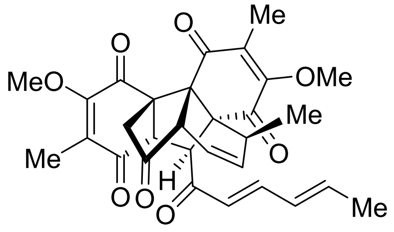
3

To a stirred solution of **4** (1.17 g, 4.5 mmol) in CH_3CN (45 mL) was added saturated aq. $NaHCO_3$ (12 mL) at 25 °C. The reaction mixture stirred at that temperature for 10 min before it was quenched with saturated aq. NH_4Cl (100 mL). The resultant mixture was extracted with EtOAc (3 × 100 mL). The combined organic phases were washed with saturated aq. NH_4Cl (3 × 50 mL) and brine (50 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was passed through a short plug of silica gel using EtOAc/petroleum ether (5: 1) as eluent to give **3** as a pale yellow solid (585 mg, 50%). **3**: $R_f = 0.35$ (silica, petroleum ether: EtOAc 3 : 1); IR (film): ν_{max} = 3427, 2937, 1653, 1633, 1593, 1465, 1336, 1193, 1123, 1001 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.65 (s, 1H), 7.41 (dd, *J* = 15.3, 9.8 Hz, 1H), 7.10 (dd, *J* = 15.6, 9.6 Hz, 1H), 6.44 (d, *J* = 15.3 Hz, 1H), 6.29 – 6.12 (m, 4H), 5.96 (d, *J* = 15.7 Hz, 1H), 5.50 (s, 1H), 5.09 (d, *J* = 1.6 Hz, 1H), 4.01 (s, 3H), 3.94 (d, *J* = 18.5 Hz, 1H), 3.70 (s, 3H), 3.46 (d, *J* = 18.5 Hz, 1H), 3.38 (d, *J* = 2.1 Hz, 1H), 2.13 (s, 3H), 1.98 (s, 3H), 1.86 – 1.84 (m, 6H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 199.62, 198.79, 197.20, 196.78, 159.92, 146.71, 145.87, 145.53, 145.18, 142.21, 141.65, 138.77, 133.68, 130.57, 130.19, 126.55, 126.25, 123.70, 120.55, 119.90, 60.81, 60.27, 59.41, 58.12, 54.72, 50.61, 18.92, 108.88, 10.10, 9.61 ppm; HRMS (m/z): $[M]^+$ calcd for $C_{30}H_{32}O_8^+$ 520.2097, found 520.2096.

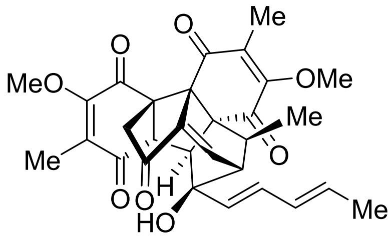


9

To a stirred suspension of **3** (250 mg, 0.480 mmol) in CH_3CN (3.5 mL) were sequentially added $(NH_4)_6Ce(NO_3)_2$ (526 mg, 0.960 mmol) in H_2O (1.6 mL) at 0 °C. The reaction mixture was allowed to stir at 0 °C for 5 min before it was quenched with saturated aq. NaCl (20 mL). The resultant mixture was extracted with EtOAc (3 × 30 mL). The combined organic phases were washed with brine (20 mL), dried over anhydrous Na_2SO_4, and filtered. The solvent was evaporated under vacuum to give **9** (232 mg, 93%) as a yellow solid and used in next step without further purification. **9**: $R_f = 0.43$ (silica, petroleum ether: EtOAc 3 : 1); IR (film): ν_{max} = 3429, 2930, 1658, 1636, 1595, 1448, 1331, 1193, 1115, 1002 cm^{-1}; ^{1}H NMR (400 MHz, CDCl$_3$): δ =7.59 (dd, *J* = 15.5, 10.5 Hz, 1H), 7.05 (dd, *J* = 15.5, 9.7 Hz, 1H), 6.37 – 6.28 (m, 1H), 6.26 – 6.09 (m, 4H), 5.97 (d, *J* = 15.5 Hz, 1H), 4.71 (d, *J* = 2.1 Hz, 1H), 3.99 (s, 3H), 3.94 (s, 3H), 3.76 (d, *J* = 17.8 Hz, 1H), 3.75 (d, *J* = 2.0 Hz, 1H), 2.70 (d, *J* = 17.9 Hz, 1H), 1.88 – 1.85 (m, 9H), 1.83 (d, *J* = 4.8 Hz, 3H) ppm; ^{13}C NMR (101 MHz, CDCl$_3$): δ = 197.56, 196.84, 196.08, 188.42, 184.93, 180.15, 160.59, 156.07, 147.74, 147.51, 146.81, 144.08, 143.02, 141.34, 130.40, 130.12, 129.16, 126.88, 125.55, 61.08, 60.94, 59.82, 57.69, 57.58, 43.72, 18.95, 18.85, 9.52, 8.77 ppm; HRMS (m/z): [M]$^+$ calcd. for $C_{30}H_{30}O_8^+$ 518.1941, found 518.1943.



2

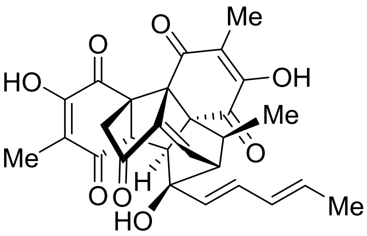


10

A solution of quinine **9** (200 mg, 0.385 mmol) in dry 1, 2-dichlorobenzene (40 mL). The resulting mixture was rigorously degassed three times by the freeze-pump-thaw process (–78 °C to 25 °C, argon). The reaction mixture was heated at 170 °C for 3 h in the dark. After cooling to RT and purification of the crude residue via silica gel flash column chromatography with petroleum ether → acetone/CH$_2$Cl$_2$ (1: 50 → 1: 25) to give **2** (50 mg, 25%) as a pale yellow solid **2**: R_f = 0.5 (silica, Acetone: DCM 1: 25); IR (film): ν_{max} = 3436, 2947, 1667, 1592, 1452, 1303, 1194, 1118, 1009, 867 cm^{-1}; ^{1}H NMR (400 MHz, CDCl$_3$): δ = 7.37 (dd, *J* = 15.2, 9.8 Hz, 1H), 7.13 (dd, *J* = 7.3, 3.4 Hz, 1H), 6.61 (d, *J* = 15.3 Hz, 1H), 6.39 – 6.18 (m, 2H), 4.06 (s, 3H), 3.85 (s, 3H), 3.82 (s, 1H), 3.49 (d, *J* = 12.6 Hz, 1H), 3.10 (d, *J* = 17.6 Hz, 1H), 2.53 (d, *J* = 17.6 Hz, 1H), 2.29 – 2.16 (m, 2H), 2.09 – 2.01 (m, 1H), 2.00 (s, 3H), 1.88 (d, *J* = 5.4 Hz, 3H), 1.81 (s, 3H), 0.75 (d, *J* = 7.0 Hz, 3H) ppm; ^{13}C NMR (101 MHz, CDCl$_3$): δ = 196.59, 196.07, 195.49, 195.34, 193.40, 193.24, 160.00, 159.93, 144.84, 142.79, 140.08, 137.67, 134.86, 130.37, 130.30, 127.49, 65.86, 63.73, 63.56, 59.61, 59.56, 57.97, 45.25, 35.25, 30.83, 29.67, 19.00, 18.98, 9.70, 9.22 ppm; HRMS (m/z): [M]$^+$ calcd for $C_{30}H_{30}O_8^+$ 518.1941, found 518.1949.

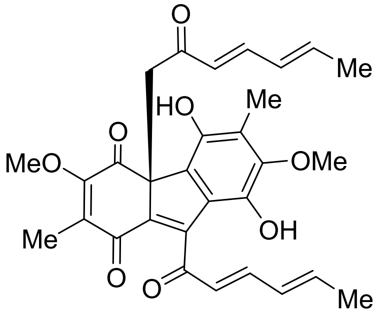
10 (30 mg, 15%) red solid. **10**: $R_f = 0.25$ (silica, Acetone: DCM 1: 25)

IR (film): ν_{max} = 3443, 2939, 1737, 1667, 1606, 1449, 1374, 1296, 1139, 994 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 6.69 (d, *J* = 5.6 Hz, 1H), 6.49 (dd, *J* = 15.4, 10.2 Hz, 1H), 6.11 – 5.94 (m, 1H), 5.90 – 5.84 (m, 2H), 3.91 (s, 3H), 3.82 (s, 3H), 3.73 (d, *J* = 5.5 Hz, 1H), 3.39 (d, *J* = 5.5 Hz, 1H), 2.88 (d, *J* = 17.7 Hz, 1H), 2.68 (dd, *J* = 5.6, 3.3 Hz, 1H), 2.40 (d, *J* = 17.7 Hz, 1H), 2.26 – 2.11 (m, 2H), 2.04 (s, 3H), 1.89 (s, 3H), 1.79 (d, *J* = 6.6 Hz, 3H), 0.88 (d, *J* = 6.9 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 198.08, 197.30, 195.19, 194.61, 192.06, 159.66, 158.81, 139.59, 137.63, 135.64, 135.33, 134.92, 132.56, 132.05, 130.37, 85.20, 66.10, 64.65, 64.31, 60.12, 59.99, 58.21, 55.92, 52.72, 46.73, 39.49, 18.24, 13.16, 9.90, 9.68 ppm; HRMS (m/z): $[M]^+$ $C_{30}H_{30}O_8^+$ 518.1941, found 518.1940.



Homodimericin **A (1)**

To a stirred solution of **10** (18 mg, 0.035 mmol) in toluene (1 mL) was added LiI (69 mg, 0.520 mmol) at 25 °C. The resultant mixture was allowed to stir at 70 °C for 15 h before it was quenched with 1M HCl (20 mL). The mixture so obtained was extracted with EtOAc (3 × 50 mL). The combined organic phases were washed with brine (50 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by semi-preparative HPLC to give **1** (13 mg, 76%) as a colorless solid. **1**: $R_f = 0.46$ (silica, DCM: MeOH 10: 1); IR (film): ν_{max} = 3426, 2930, 1727, 1654, 1386, 1354, 1171, 1118, 994, 896 cm^{-1}; ^1H NMR (600 MHz, *d*$_6$-DMSO): δ = 6.47 (d, *J* = 5.7 Hz, 1H), 6.35 (dd, *J* = 15.4, 10.4 Hz, 1H), 6.10 (dd, *J* = 14.4 Hz, 10.9 Hz, 1H), 5.84 (d, *J* = 15.5 Hz, 1H), 5.79 – 5.70 (m, 1H), 3.56 (d, *J* = 4.7 Hz, 1H), 3.08 (d, *J* = 4.8 Hz, 1H), 2.68 (dd, *J* = 5.3, 3.4 Hz, 1H), 2.63 (d, *J* = 18.1 Hz, 1H), 2.58 (d, *J* = 18.1 Hz, 1H), 2.12 – 2.06 (m, 1H), 1.83 (s, 3H), 1.75 (d, *J* = 6.5 Hz, 3H), 1.71 (s, 3H), 0.70 (d, *J* = 6.8 Hz, 3H) ppm; ^{13}C NMR (150 MHz, *d*$_6$-DMSO): δ = 199.44, 195.57, 194.81 (2C), 193.87, 158.02 (2C), 139.16, 137.43, 135.77, 131.10, 130.09, 128.98, 125.72, 124.40, 84.32, 64.74, 64.24, 62.85, 59.57, 55.07, 51.58, 47.56, 18.03, 12.43, 9.53, 9.23 ppm; HRMS (m/z): $[M]^+$ $C_{28}H_{26}O_8^+$ 490.1628, found 490.1622.



11

To a stirred suspension of **9** (40 mg, 0.077 mmol) in DCM (0.8 mL) were sequentially added BF_3•OEt_2 (19 μL, 0.154 mmol) at −78 °C. The reaction mixture was allowed to stir at 0 °C for 50 min before it was quenched with saturated aq. $NaHCO_3$ (20 mL). The resultant mixture was extracted with EtOAc (3 × 20 mL). The combined organic phases were washed with brine (20 mL), dried over anhydrous Na_2SO_4, and filtered. the solvent was evaporated under vacuum, and the residue was purified by flash column chromatography with petroleum ether/EtOAc (3: 1) to give **11** (20 mg, 50%) as a yellow oil. **11**: $R_f = 0.32$ (silica, petroleum ether: EtOAc 3 : 1); IR (film): ν_{max} = 3420, 2937, 1633, 1586, 1424, 1341, 1235, 1109, 997, 952 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$):δ = 7.94 (s, 1H), 7.12 (dd, J = 15.5, 10.0 Hz, 1H), 7.02 (dd, J = 15.4, 10.6 Hz, 1H), 6.36 (d, J = 15.5 Hz, 1H), 6.32 – 6.16 (m, 3H), 6.16 – 6.01 (m, 2H), 5.91 (d, J = 15.5 Hz, 1H), 4.09 (s, 3H), 3.75 (s, 3H), 3.47 (d, J = 14.9 Hz, 1H), 3.20 (s, 1H), 2.23 (s, 3H), 1.97 (s, 3H), 1.85 (d, J = 5.6 Hz, 6H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 197.57, 194.39, 193.60, 182.31, 161.15, 147.71, 147.43, 146.33, 145.31, 145.24, 143.36, 142.47, 140.59, 137.35, 135.77, 130.81, 130.15, 127.90, 126.89, 123.88, 123.75, 123.32, 65.97, 60.95, 60.24, 48.42, 19.13, 19.08, 10.20, 9.77 ppm; HRMS (m/z): $[M]^+$ $C_{30}H_{30}O_8^+$ 518.1941, found 518.1933.

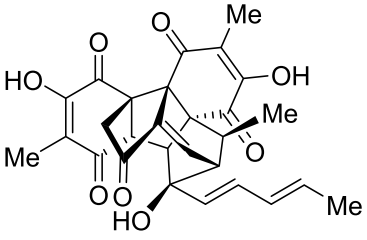
II References

(1) (a) Magnus, P.; Matthews, K. S.; Lynch, V. *Org. Lett.* **2003**, *5*, 2181. (b) Saito, T.; Morimoto, M.; Akiyama, C.; Matsumoto, T.; Suzuki, K. *J. Am. Chem. Soc.* **1995**, *117*, 10757.

(2) Kurono, N.; Yamaguchi, M.; Suzuki, K.; Ohkuma, T. *J. Org. Chem.* **2005**, *70*, 6530.

III Comparison of the Spectra and Data of Natural and Synthetic Homodimericin A

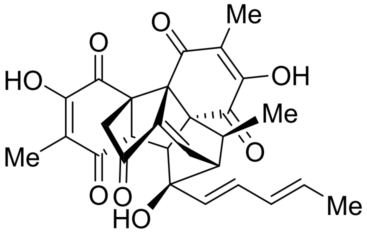
Table 1. Comparison of the ^{1}H NMR spectroscopic data (d_6-DMSO) of natural and synthetic homodimericin A



Homodimericin A

Natural δ_H [ppm, mult, J (Hz)] 600 MHz		**Synthetic** δ_H [ppm, mult, J (Hz)] 600 MHz		**Err** (Natural–Synthetic) $\Delta\delta_H$ (ppm)
6.50	1 H, d, 5.8	6.47	1 H, d, 5.7	−0.03
6.35	1 H, dd, 15.4, 10.7	6.35	1 H, dd, 15.4, 10.4	−
6.10	1 H, dd, 14.9, 10.7	6.10	1 H, dd, 14.4, 10.9	–
5.85	1 H, d, 15.4	5.84	1 H, d, 15.5	–0.01
5.74	1 H, dq 14.9, 6.7	5.75	1 H, m	–0.01
3.62	1 H, d, 5.0	3.56	1 H, d, 4.7	−0.06
3.08	1 H, d, 5.0	3.08	1 H, d, 4.8	−
2.71	1 H, dd, 3.5, 5.8	2.68	1 H, dd, 3.4, 5.3	−0.03
2.70	1 H, d, 18.0	2.63	1H, d, 18.1	−0.07
2.60	1H, d, 18.0	2.58	1H, d, 18.1	−0.02
2.11	1 H, qd, 3.5, 6.9	2.09	1H, m	–0.02
1.84	3 H, s	1.83	3H, s	–0.01
1.76	3 H, d, 6.7	1.75	3 H, d, 6.5	–0.01
1.74	3 H, s	1.71	3 H, s	–0.03
0.70	3 H, d, 6.9	0.70	3 H, d, 6.8	–

Table 2. Comparison of the ^{13}C NMR spectroscopic data (d_6-DMSO) of natural and synthetic homodimericin A

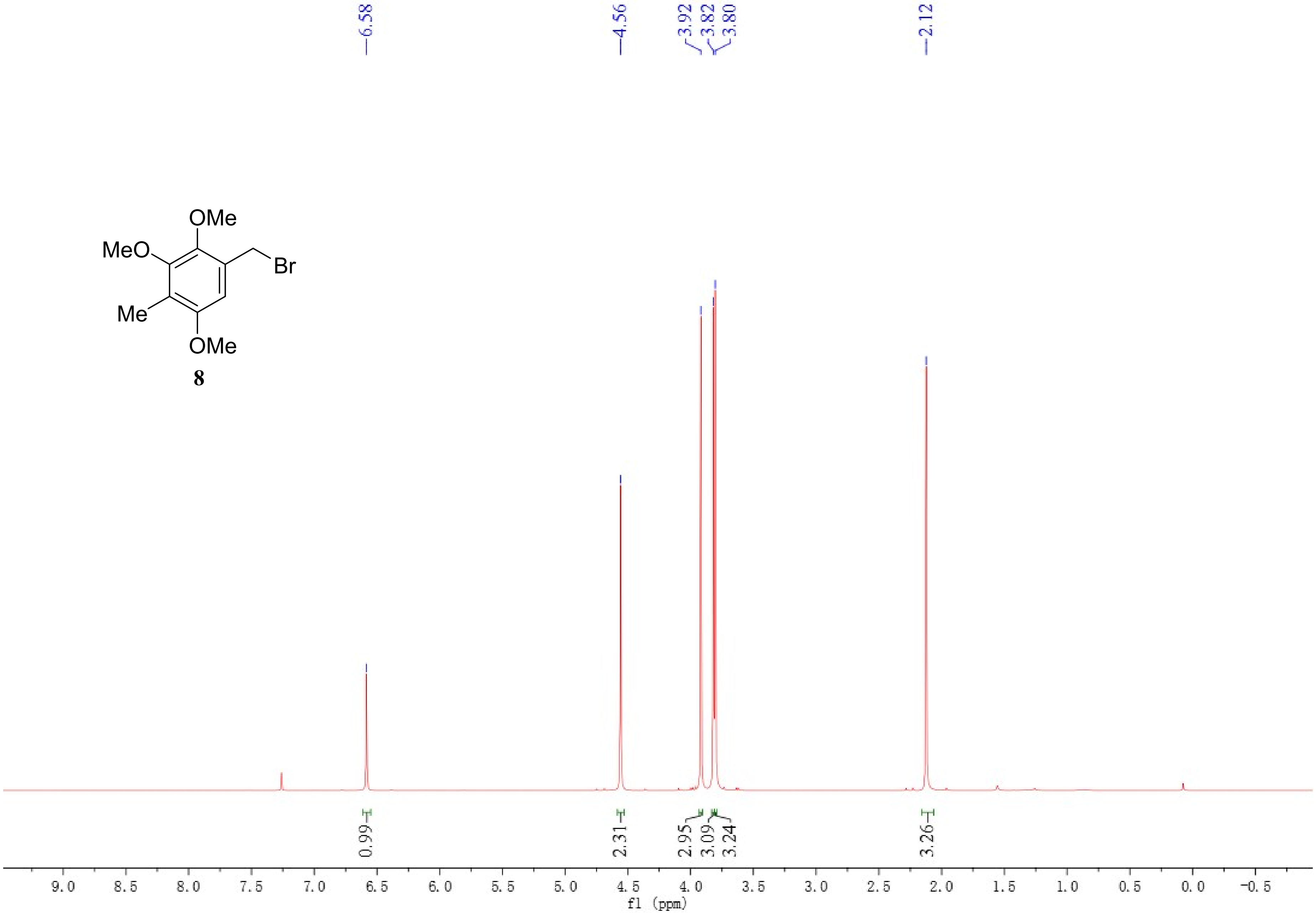


Homodimericin A

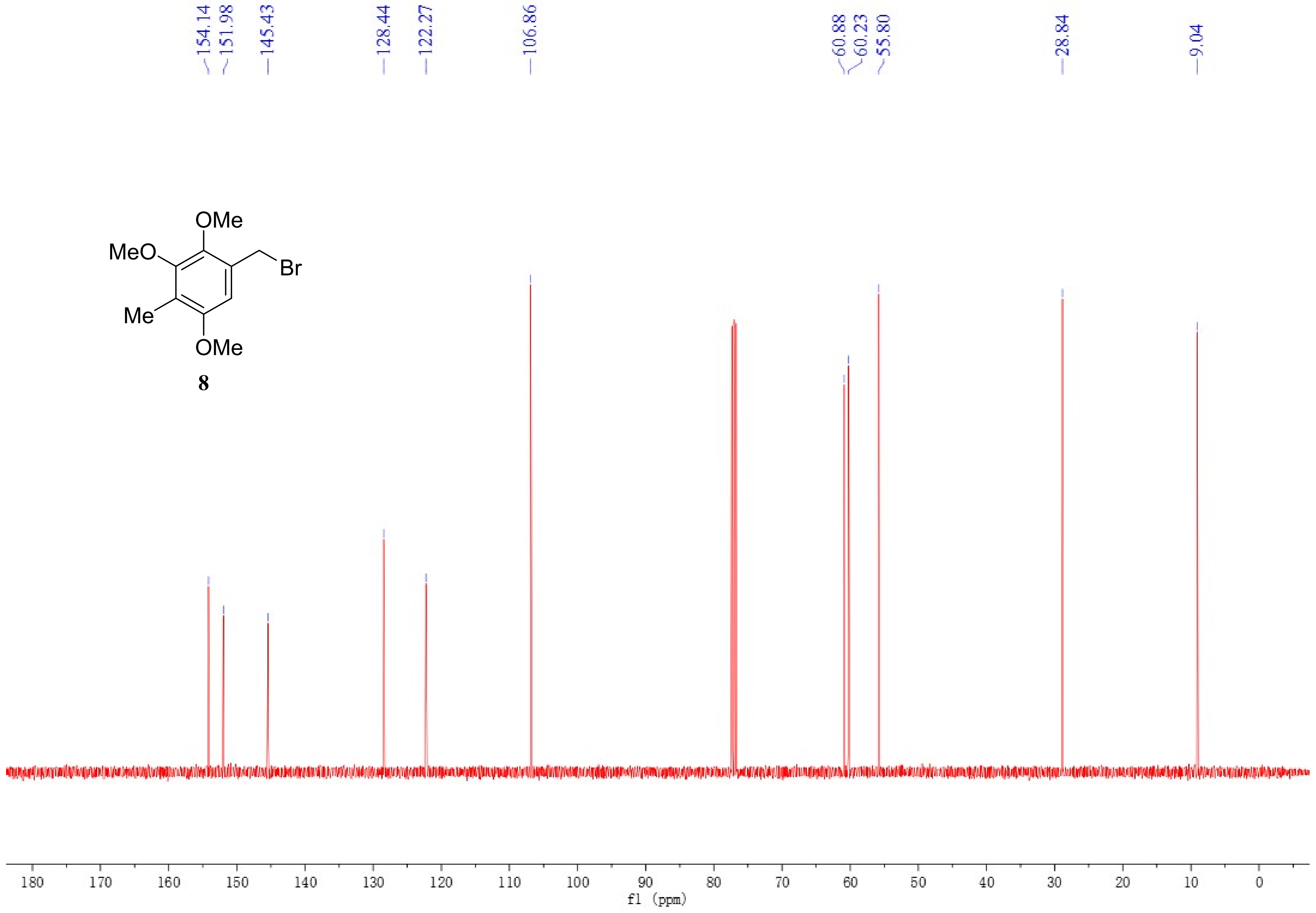
Natural δ_C (ppm) 125 MHz	**Synthetic** δ_C (ppm) 150 MHz	**Err** (Natural–Synthetic) $\Delta\delta_C$ (ppm)
199.2	199.4	+0.2
196.0	195.6	−0.4
195.1	194.8	−0.3
195.1	194.8	−0.3
193.0	193.8	−0.8
156.1	158.0	+1.9
156.1	158.0	+1.9
138.6	139.1	+0.5
137.2	137.4	+0.2
136.1	135.7	−0.4
131.0	131.1	+0.1
130.2	130.0	−0.2
129.0	128.9	−0.1
126.3	125.7	−0.6
125.6	124.4	−1.2
84.3	84.3	−
64.8	64.7	−0.1
64.4	64.2	−0.2
62.9	62.8	−0.1
59.6	59.5	−0.1
55.1	55.0	−0.1
51.6	51.5	−0.1

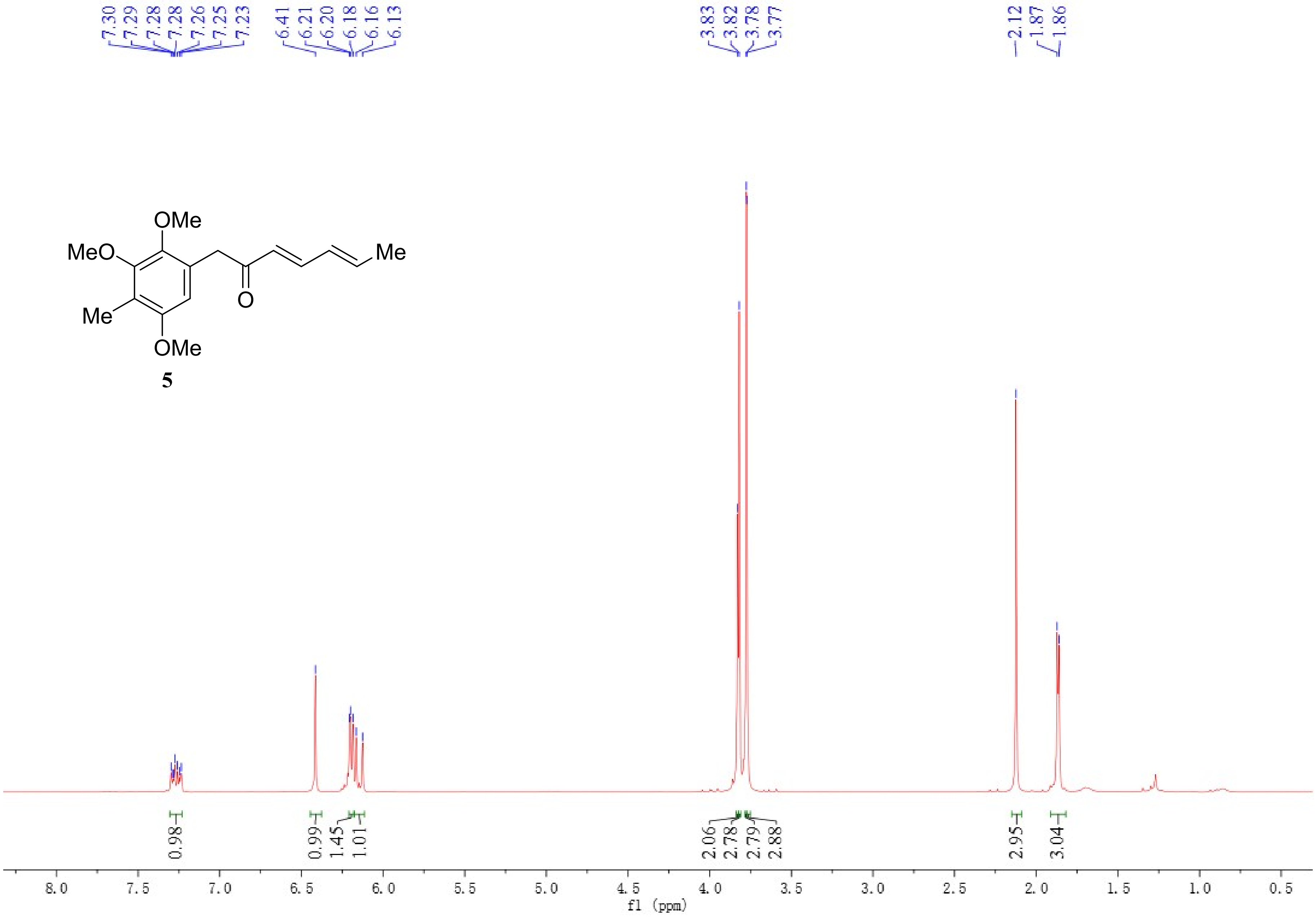
47.3	47.5	+0.2
18.0	18.0	−
12.3	12.4	−0.1
9.5	9.5	−
9.1	9.2	−0.1

IV ^{1}H and ^{13}C NMR Spectra of Compounds



8


154.14
151.98
145.43
128.44
122.27
106.86
60.88
60.23
55.80
28.84
9.04
OMe
MeO
Br
Me
OMe
8
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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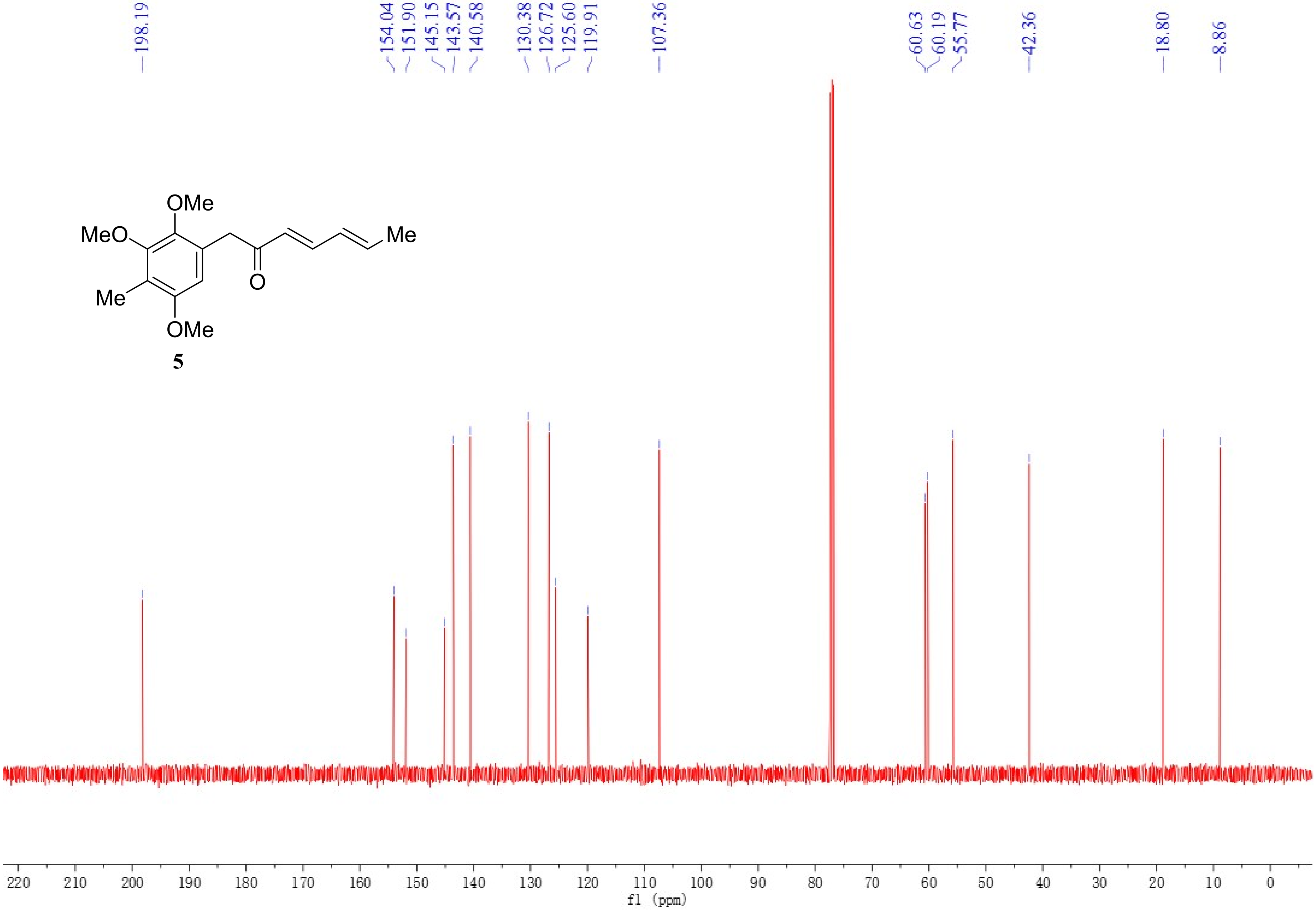
7.29
7.28
7.28
7.26
7.25
7.23
6.41
6.21
6.20
6.18
6.16
6.13
3.83
3.82
3.78
3.77
2.12
1.87
1.86
OMe
MeO
Me
OMe
O
Me
0.98
0.99
1.45
1.01
2.06
2.78
2.79
2.88
2.95
3.04
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

5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154.04
151.90
145.15
143.57
140.58
130.38
126.72
125.60
119.91
107.36
60.63
60.19
55.77
42.36
18.80
8.86
OMe
MeO
Me
OMe
O
Me
5
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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50
40
30
20
10
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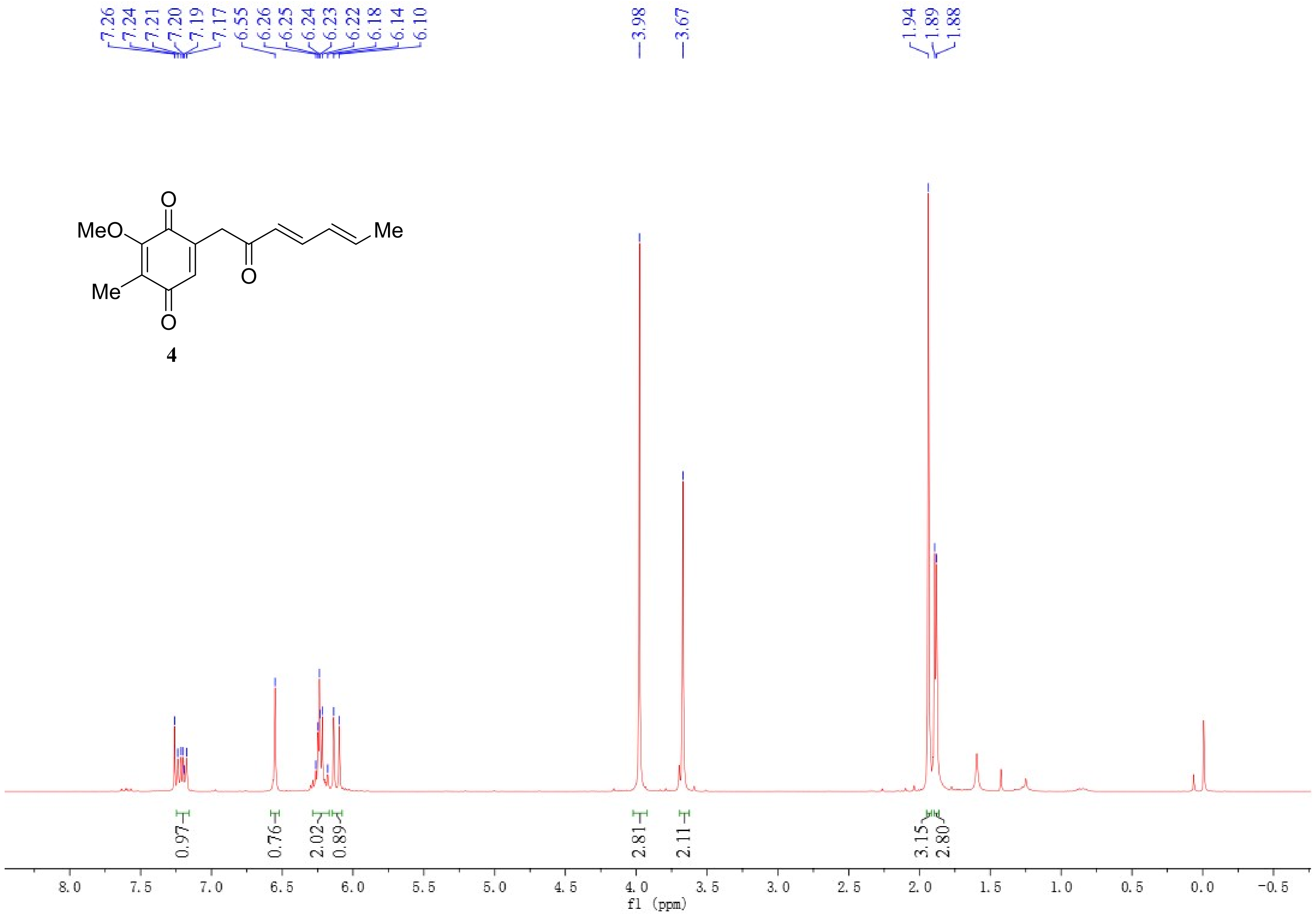
f1 (ppm)


4

7.26
7.24
7.21
7.20
7.19
7.17
6.55
6.26
6.25
6.24
6.23
6.22
6.18
6.14
6.10
3.98
3.67
1.94
1.89
1.88
MeO
Me
O
O
O
Me
0.97
0.76
2.02
0.89
2.81
2.11
3.15
2.80
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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0.5
0.0
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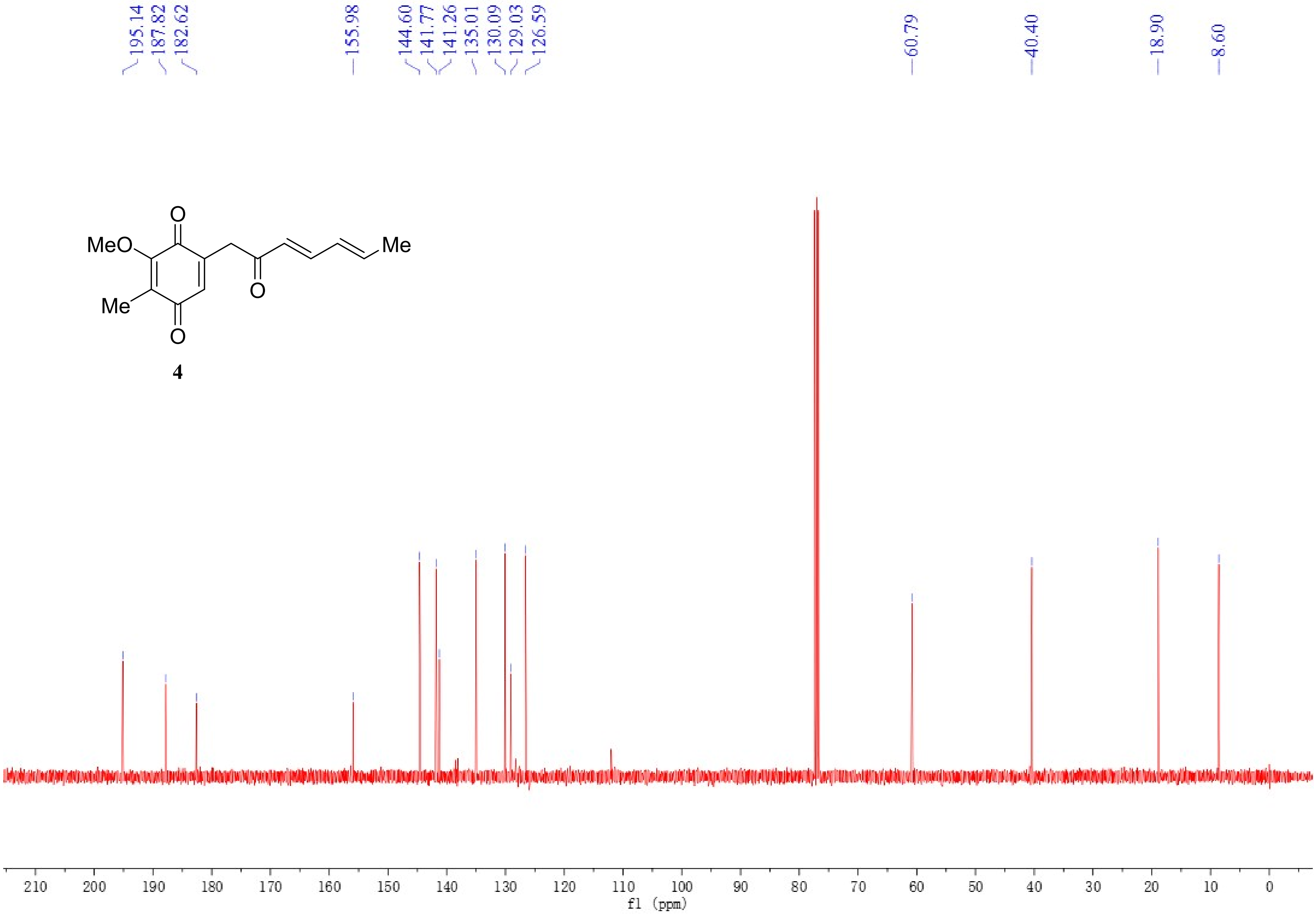
f1 (ppm)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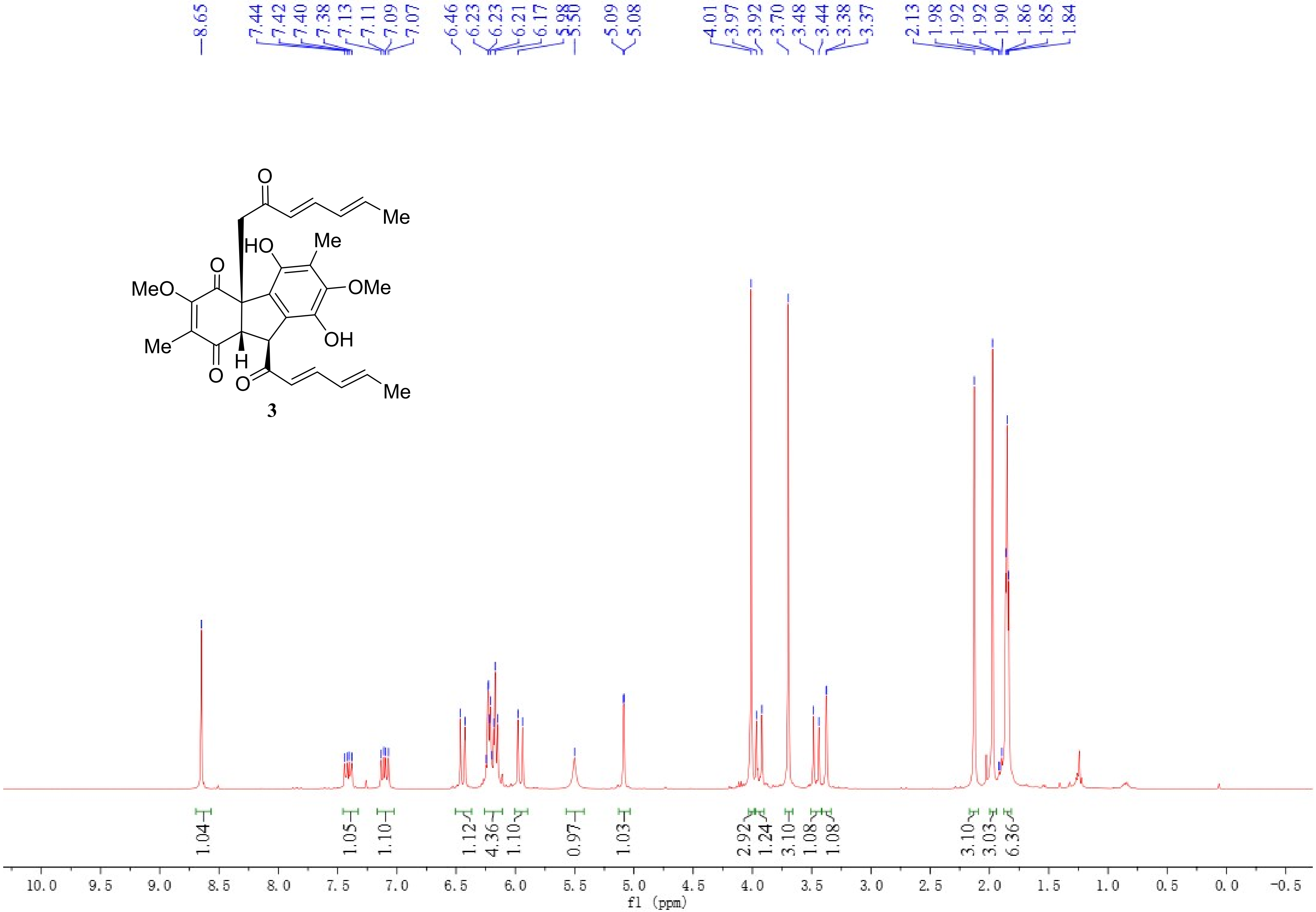
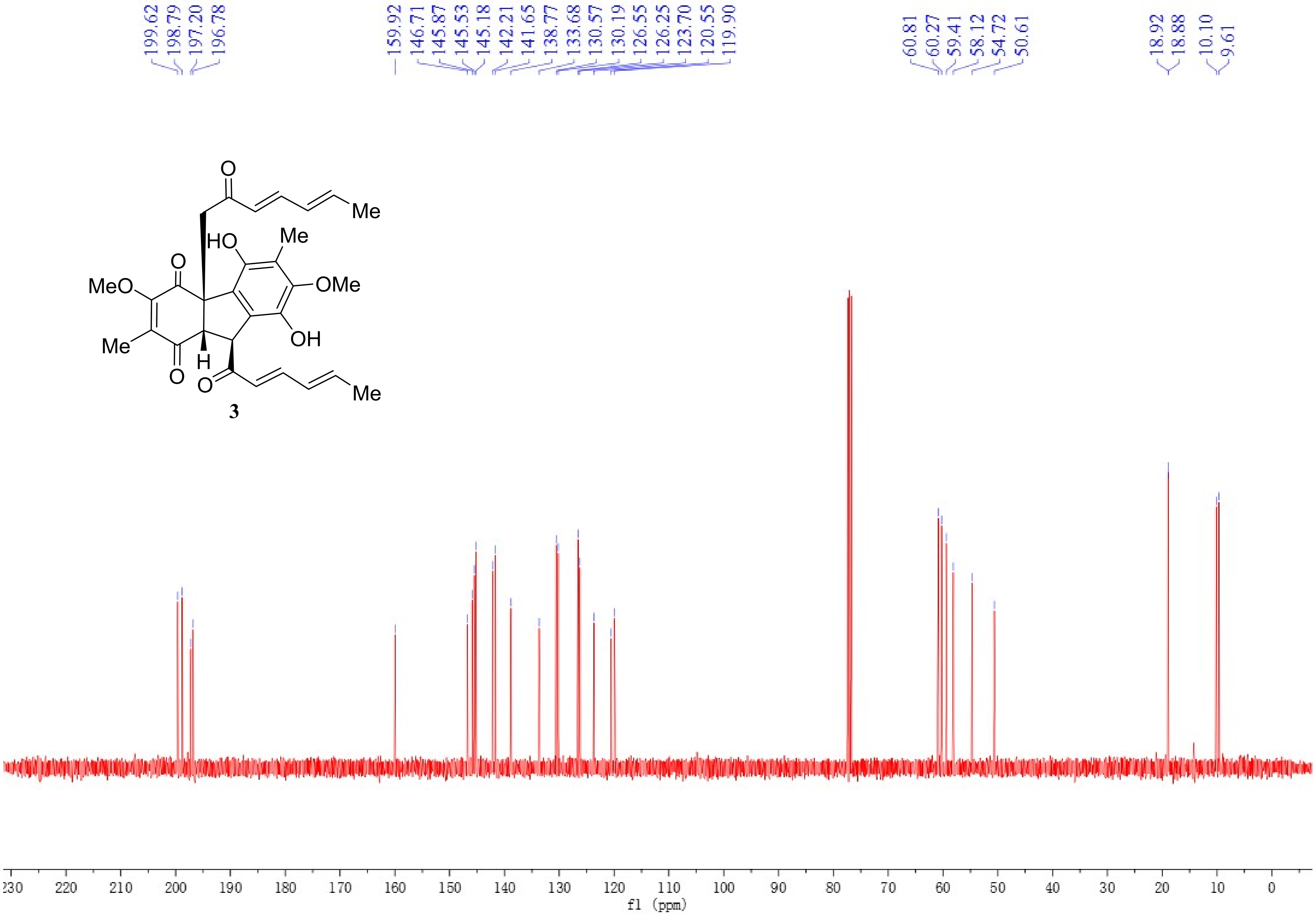
187.82
182.62
155.98
144.60
141.77
141.26
135.01
130.09
129.03
126.59
60.79
40.40
18.90
8.60
MeO
Me
O
O
O
Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4


8.65
7.44
7.42
7.40
7.38
7.13
7.11
7.09
7.07
6.46
6.23
6.23
6.21
6.17
5.98
5.50
5.09
5.08
4.01
3.97
3.92
3.70
3.48
3.44
3.38
3.37
2.13
1.98
1.92
1.92
1.90
1.86
1.85
1.84
O
Me
HO
Me
O
MeO
OMe
Me
OH
H
O
O
Me
3
1.04
1.05
1.10
1.12
4.36
1.10
0.97
1.03
2.92
1.24
3.10
1.08
1.08
3.10
3.03
6.36
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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198.79
197.20
196.78
159.92
146.71
145.87
145.53
145.18
142.21
141.65
138.77
133.68
130.57
130.19
126.55
126.25
123.70
120.55
119.90
60.81
60.27
59.41
58.12
54.72
50.61
18.92
18.88
10.10
9.61
O
Me
HO
Me
O
MeO
OMe
Me
OH
H
O
O
Me
3
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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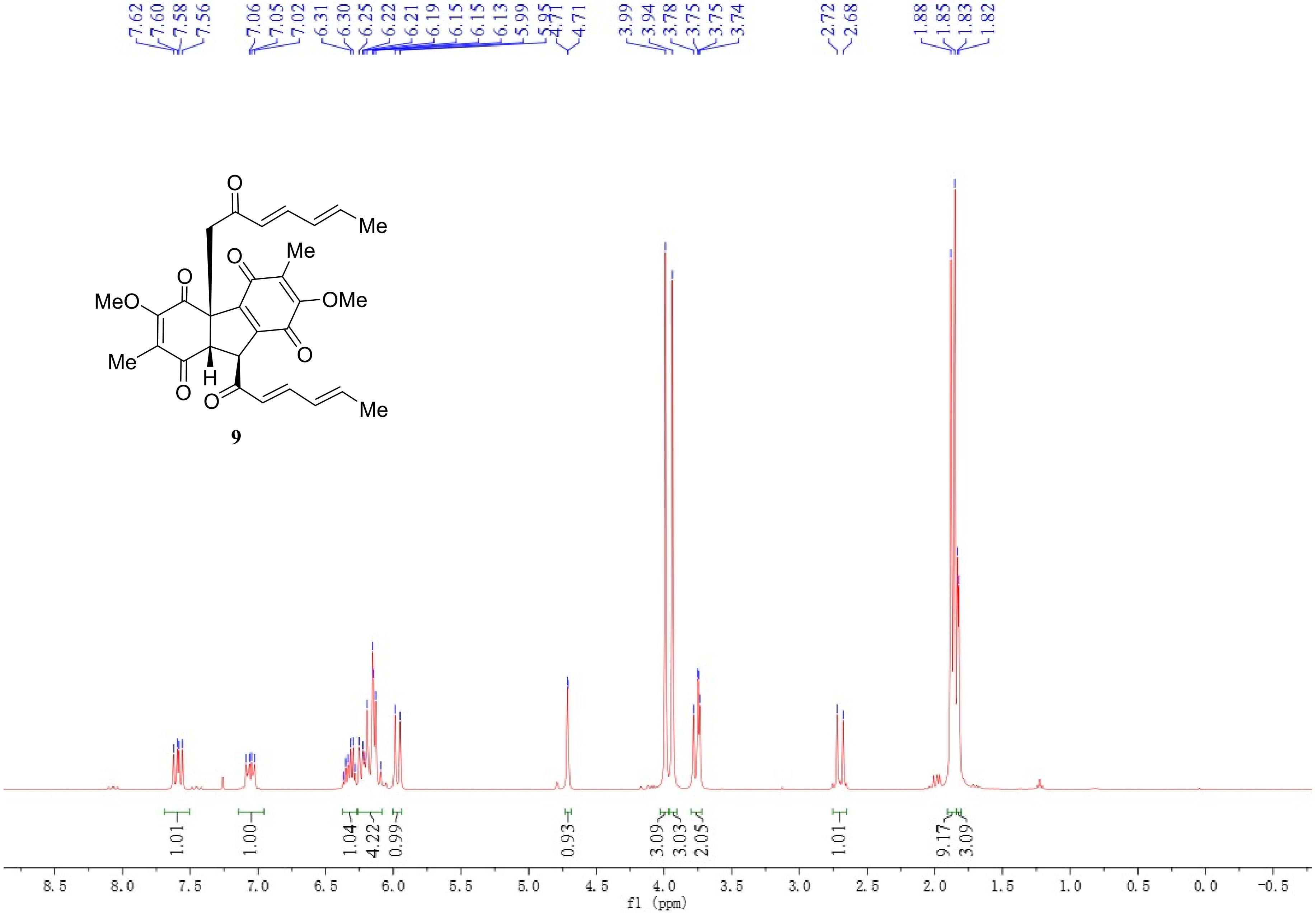
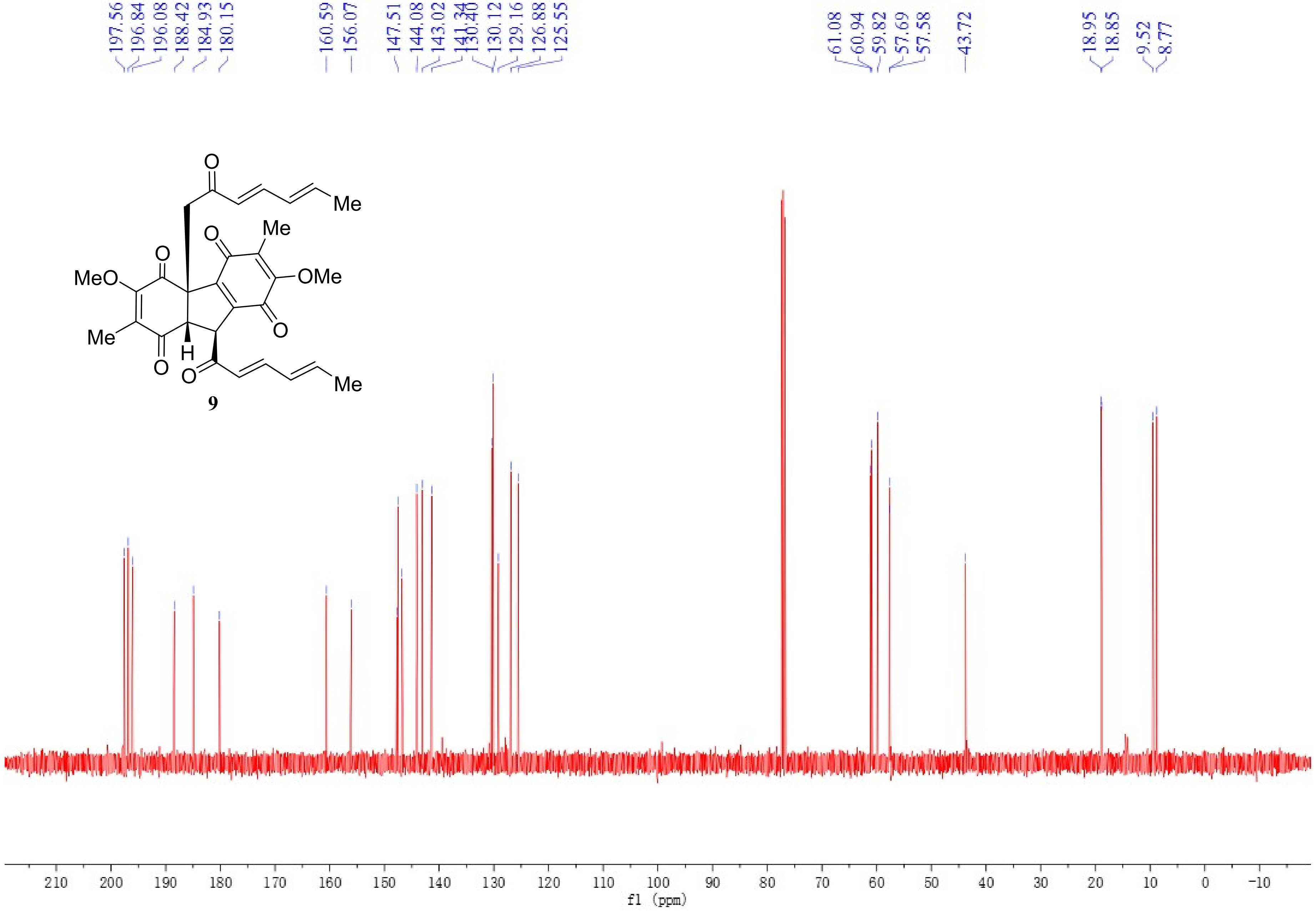
50
40
30
20
10
0
f1 (ppm)



9

7.62
7.60
7.58
7.56
7.06
7.05
7.02
6.31
6.30
6.25
6.22
6.21
6.19
6.15
6.15
6.13
5.99
5.95
4.71
4.71
3.99
3.94
3.78
3.75
3.75
3.74
2.72
2.68
1.88
1.85
1.83
1.82
O
Me
MeO
OMe
H
1.01
1.00
1.04
4.22
0.99
0.93
3.09
3.03
2.05
1.01
9.17
3.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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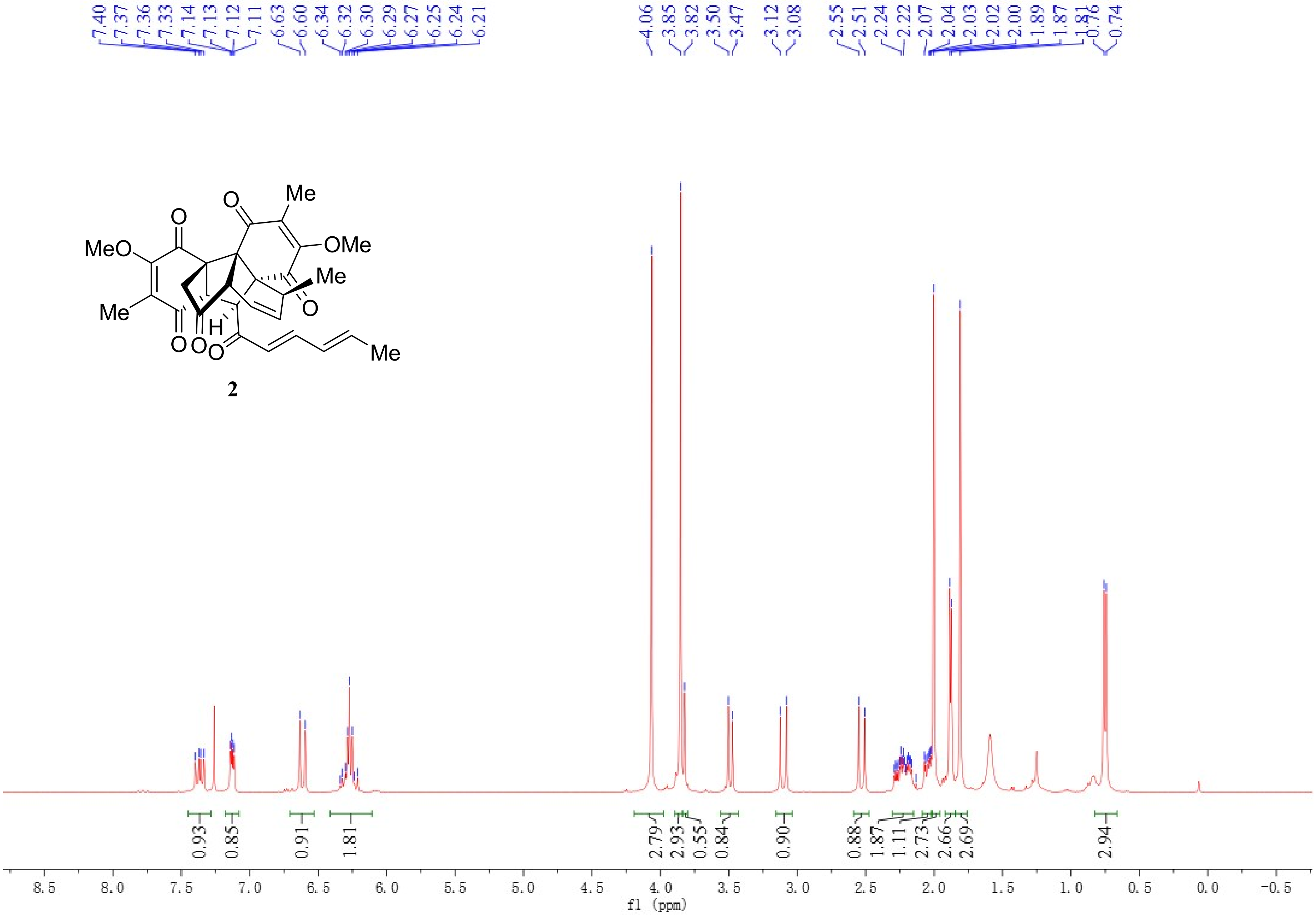
196.84
196.08
188.42
184.93
180.15
160.59
156.07
147.51
144.08
143.02
141.34
130.40
130.12
129.16
126.88
125.55
61.08
60.94
59.82
57.69
57.58
43.72
18.95
18.85
9.52
8.77
O
Me
O
Me
O
MeO
OMe
Me
O
O
H
O
Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

9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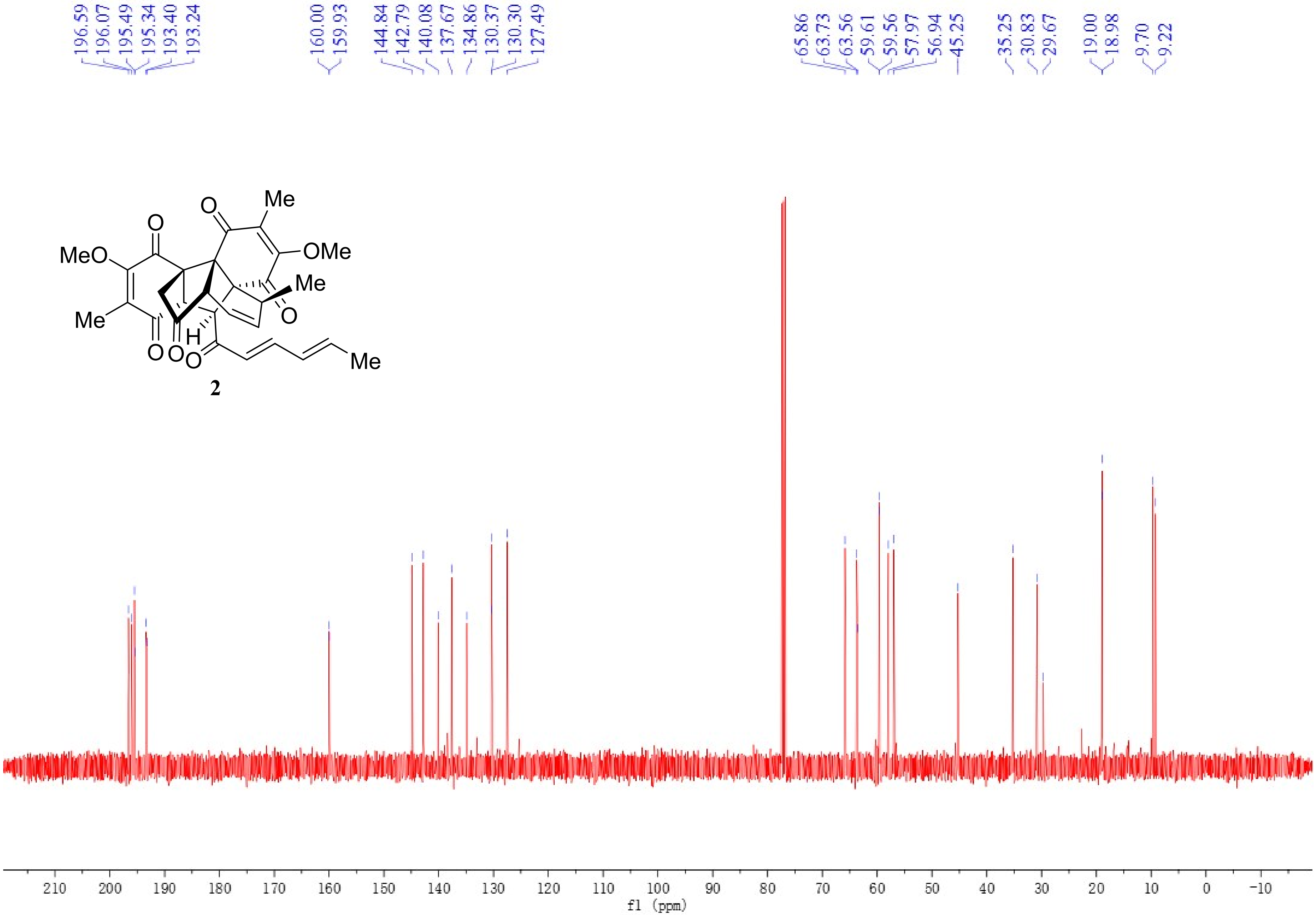
7.14
7.13
7.12
7.11
6.63
6.60
6.34
6.32
6.30
6.29
6.27
6.25
6.24
6.21
4.06
3.85
3.82
3.50
3.47
3.12
3.08
2.55
2.51
2.24
2.22
2.07
2.04
2.03
2.02
2.00
1.89
1.87
1.81
0.76
0.74
O
Me
O
MeO
OMe
Me
Me
O
H
O
O
O
Me
0.93
0.85
0.91
1.81
2.79
2.93
0.55
0.84
0.90
0.88
1.87
1.11
2.73
2.66
2.69
2.94
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

2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195.34
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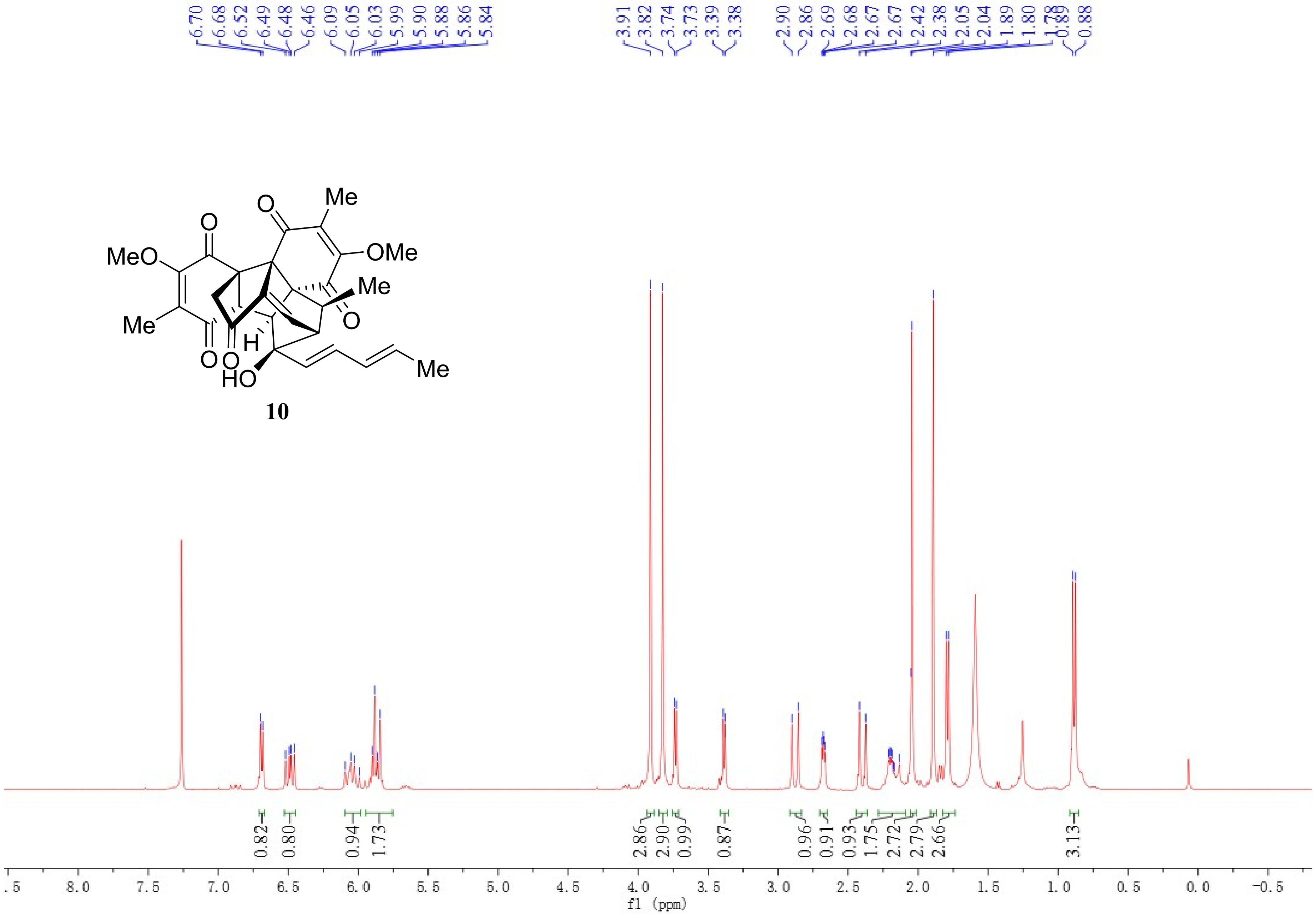
193.24
160.00
159.93
144.84
142.79
140.08
137.67
134.86
130.37
130.30
127.49
65.86
63.73
63.56
59.61
59.56
57.97
56.94
45.25
35.25
30.83
29.67
19.00
18.98
9.70
9.22
MeO
O
O
Me
OMe
Me
O
Me
H
O
O
O
Me
2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


6.70
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6.49
6.48
6.46
6.09
6.05
6.03
5.99
5.90
5.88
5.86
5.84
3.91
3.82
3.74
3.73
3.39
3.38
2.90
2.86
2.69
2.68
2.67
2.67
2.42
2.38
2.05
2.04
1.89
1.80
1.78
0.89
0.88
MeO
O
O
Me
OMe
Me
O
Me
O
O
H
HO
Me
0.82
0.80
0.94
1.73
2.86
2.90
0.99
0.87
0.96
0.91
0.93
1.75
2.72
2.79
2.66
3.13
.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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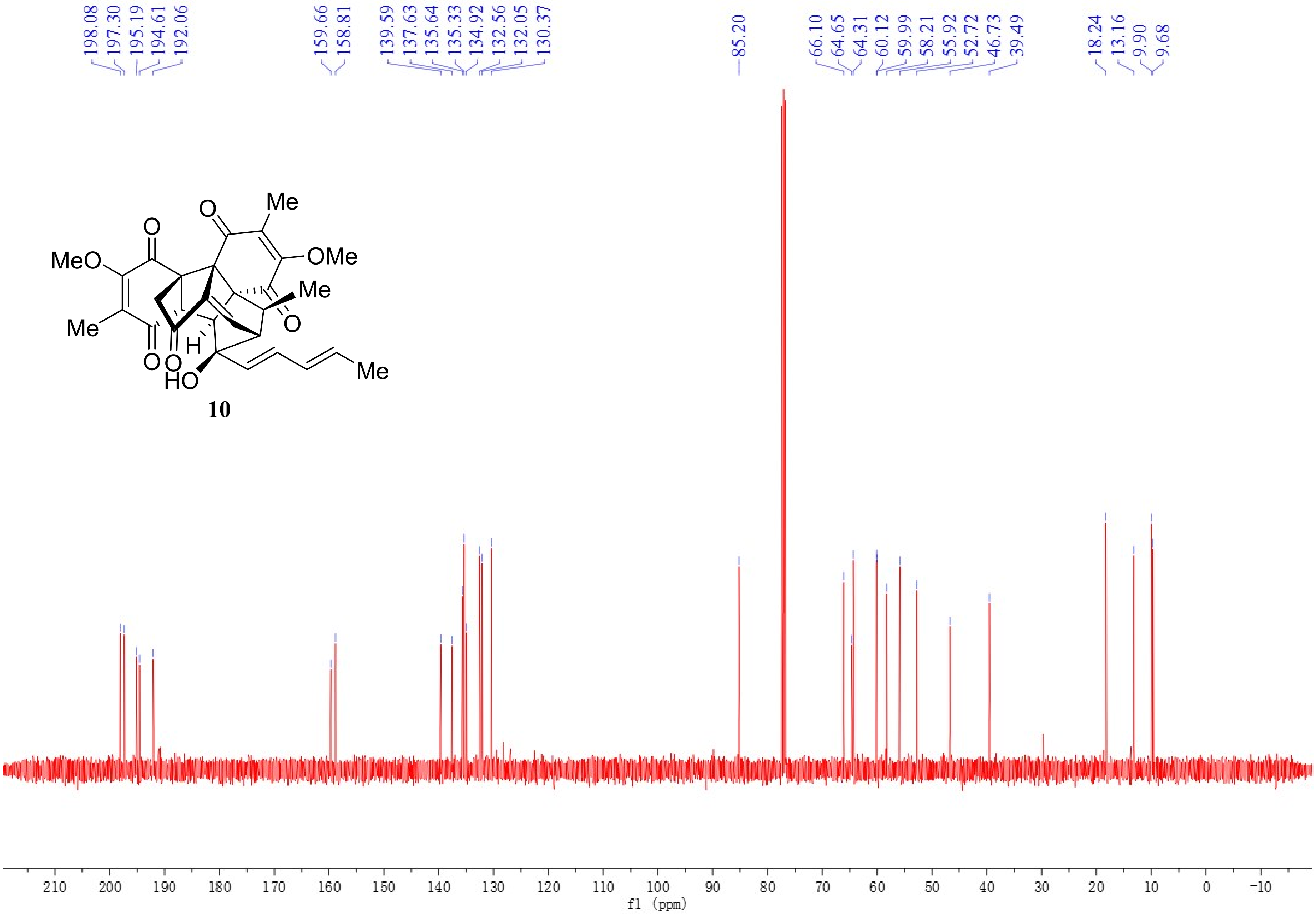
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

10



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198.08
197.30
195.19
194.61
192.06
159.66
158.81
139.59
137.63
135.64
135.33
134.92
132.56
132.05
130.37
85.20
66.10
64.65
64.31
60.12
59.99
58.21
55.92
52.72
46.73
39.49
18.24
13.16
9.90
9.68
O
Me
O
OMe
MeO
Me
Me
O
H
O
O
HO
Me
210
200
190
180
170
160
150
140
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120
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100
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80
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30
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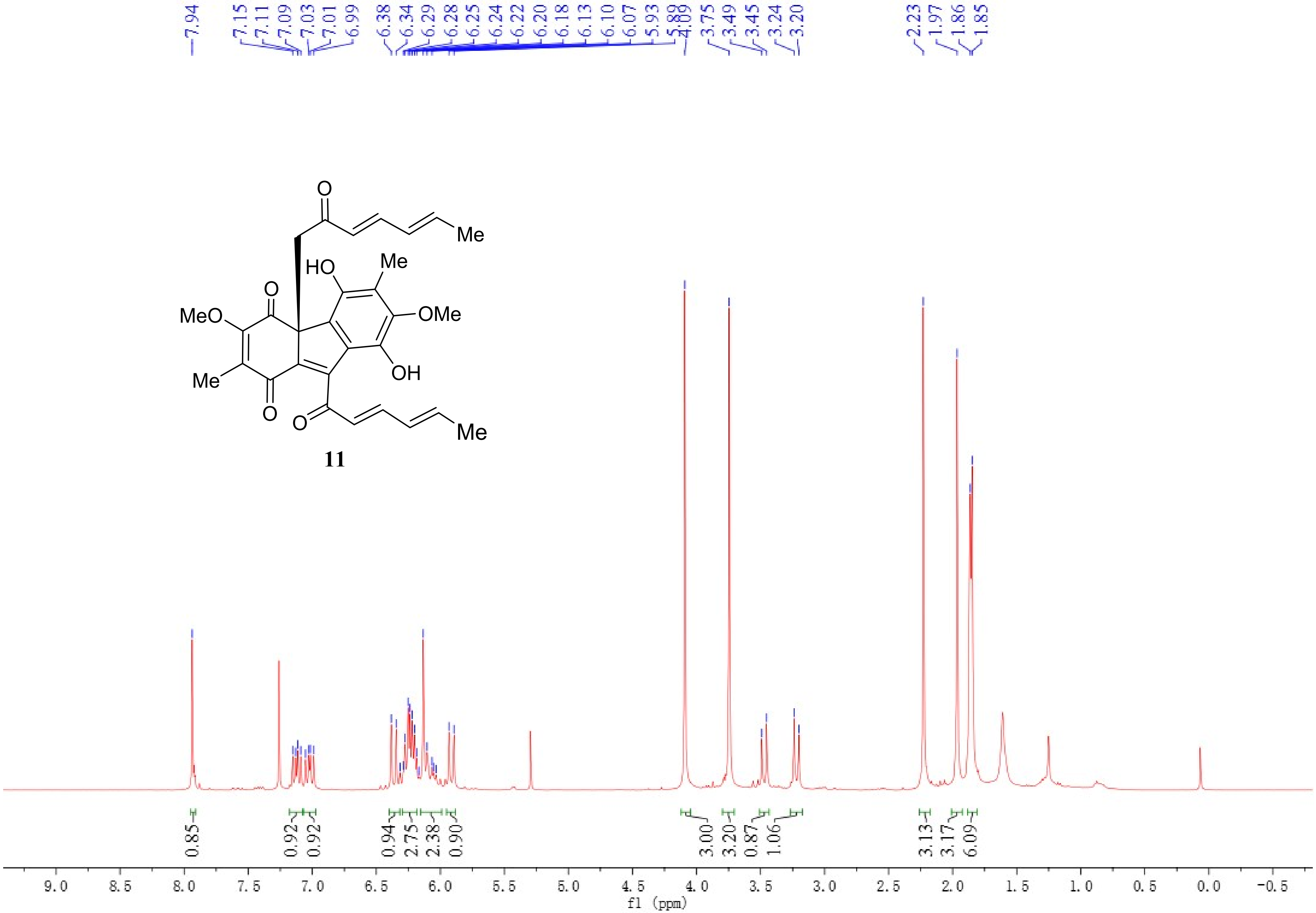
f1 (ppm)



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7.03
7.01
6.99
6.38
6.34
6.29
6.28
6.25
6.24
6.22
6.20
6.18
6.13
6.10
6.07
5.93
5.89
4.09
3.75
3.49
3.45
3.24
3.20
2.23
1.97
1.86
1.85
O
Me
HO
Me
MeO
OMe
Me
OH
O
Me
0.85
0.92
0.92
0.94
2.75
2.38
0.90
3.00
3.20
0.87
1.06
3.13
3.17
6.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
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2.0
1.5
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0.5
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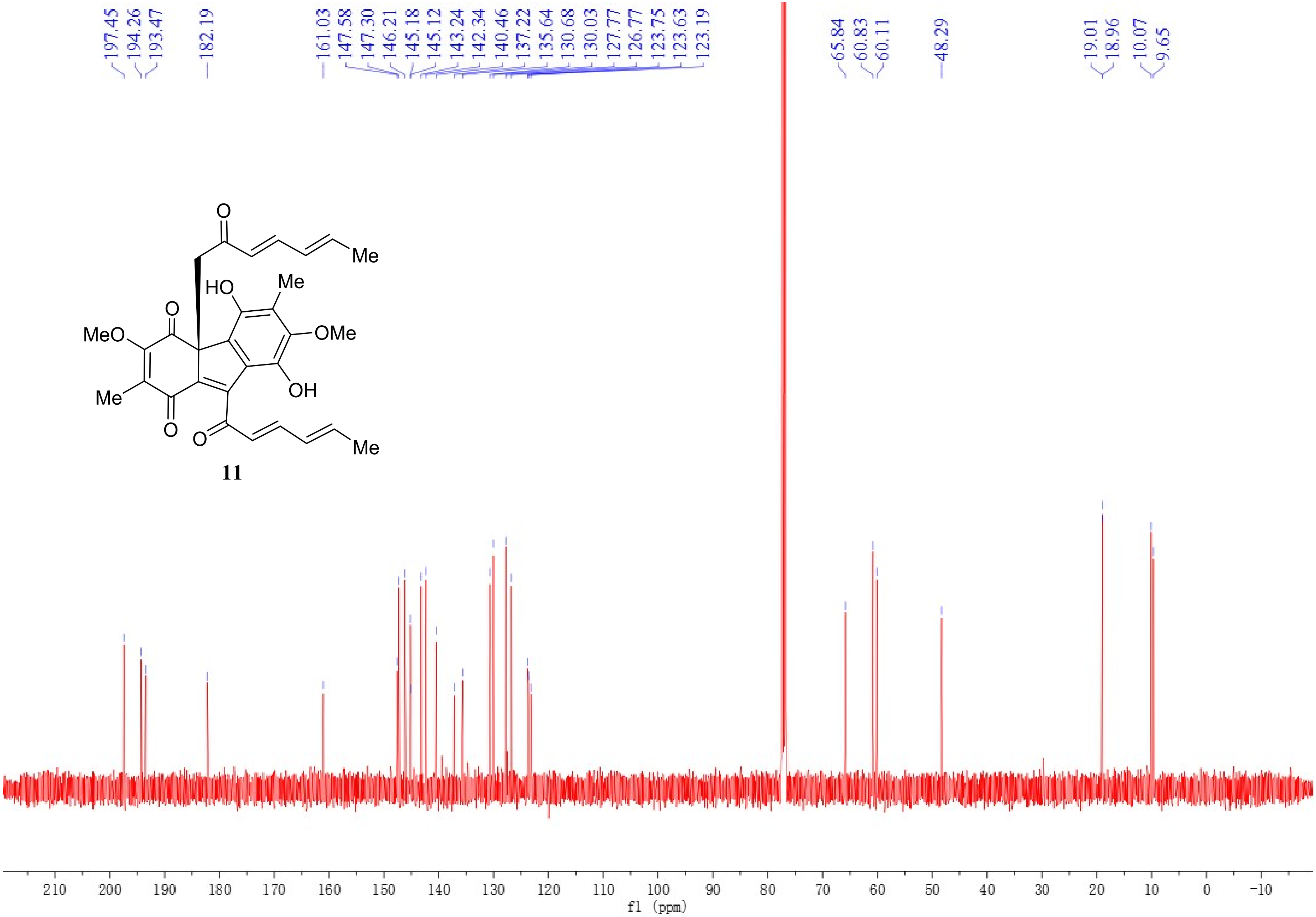
-0.5
f1 (ppm)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193.47
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161.03
147.58
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146.21
145.18
145.12
143.24
142.34
140.46
137.22
135.64
130.68
130.03
127.77
126.77
123.75
123.63
123.19
65.84
60.83
60.11
48.29
19.01
18.96
10.07
9.65
O
Me
HO
Me
O
MeO
OMe
Me
OH
O
O
Me
210
200
190
180
170
160
150
140
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120
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100
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80
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60
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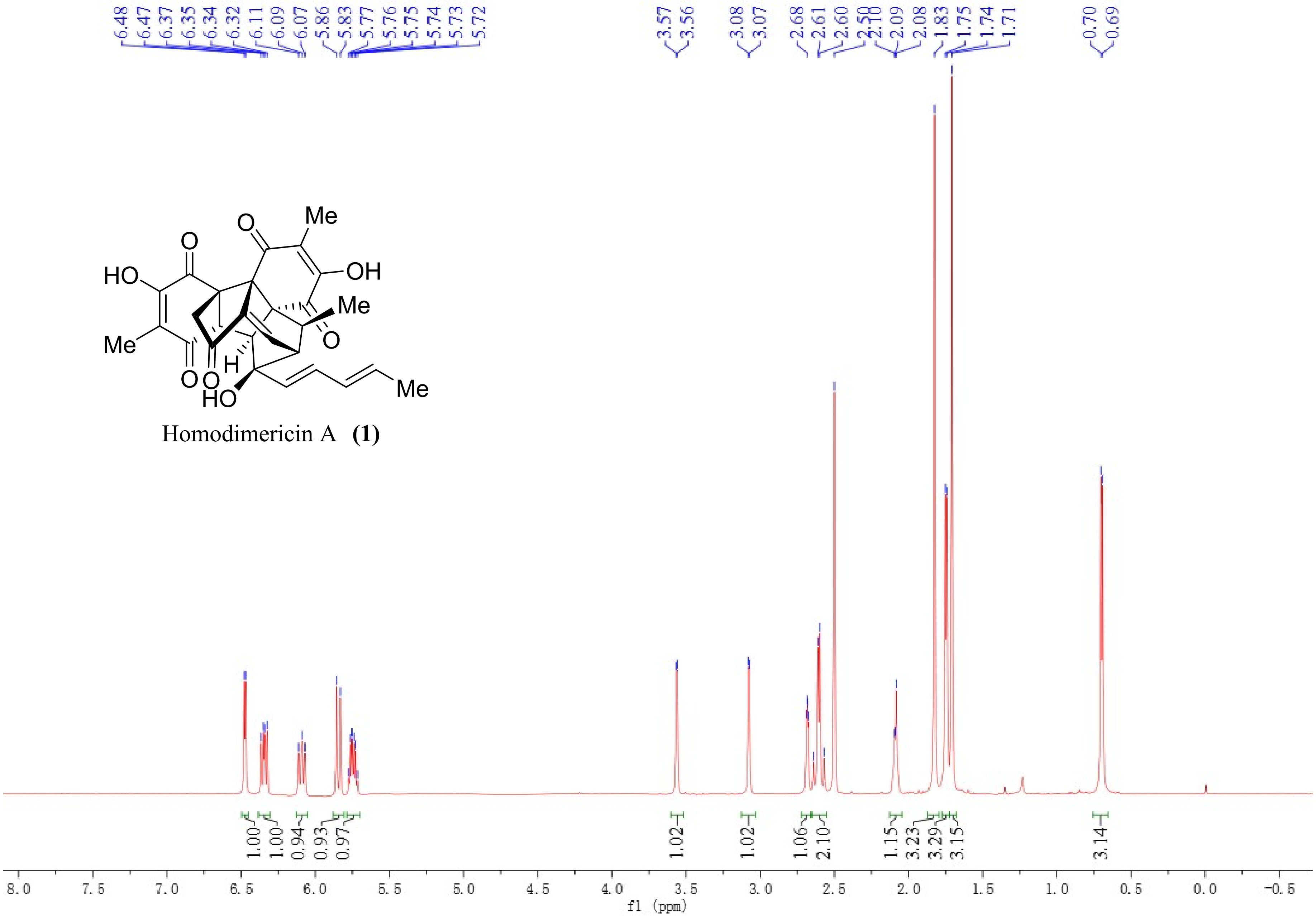
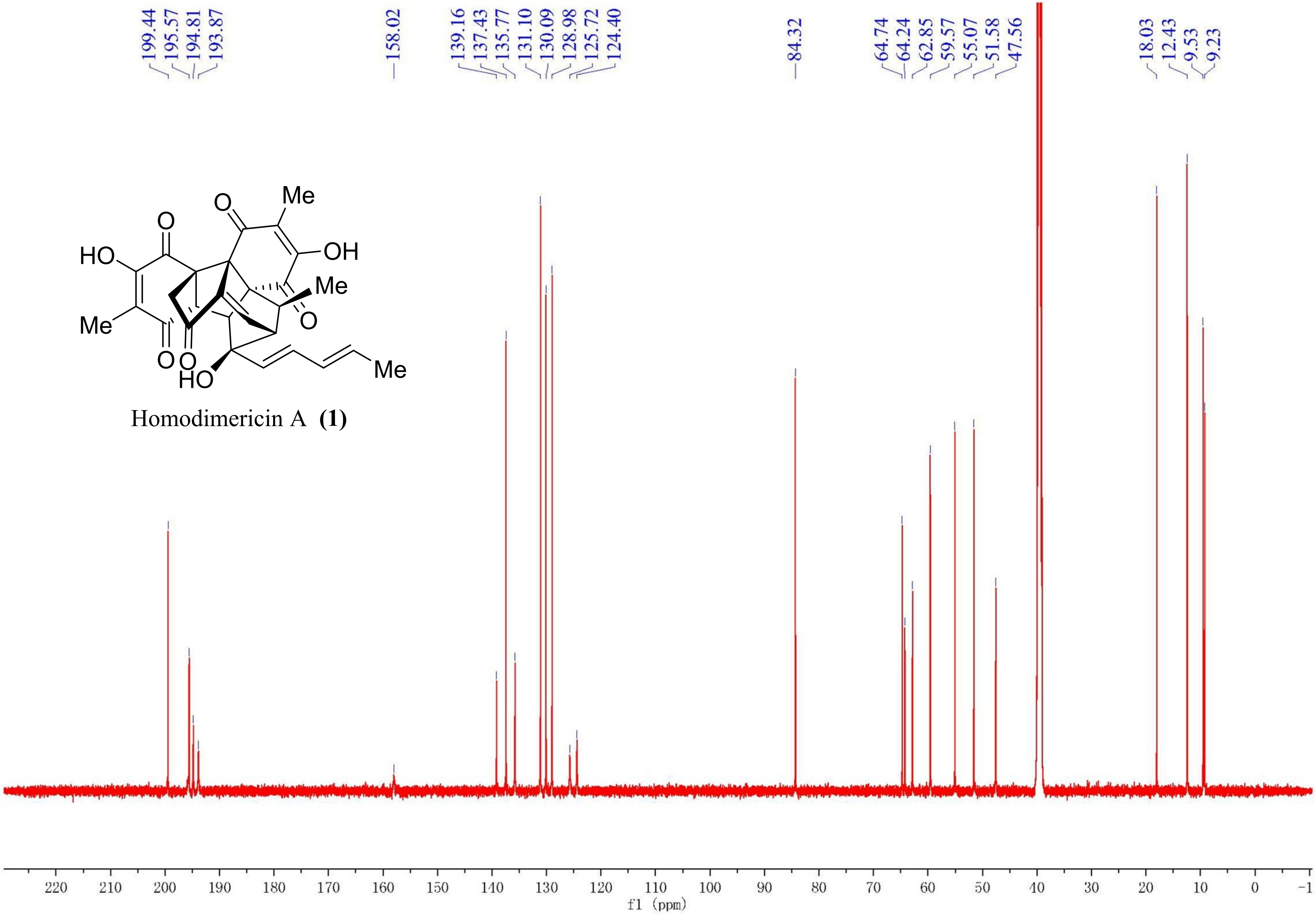
40
30
20
10
0
-10
f1 (ppm)



Homodimericin A **(1)**



Homodimericin A **(1)**