Supporting Information

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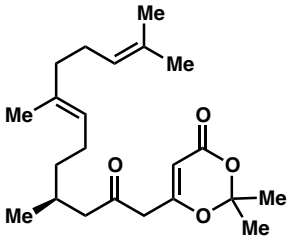
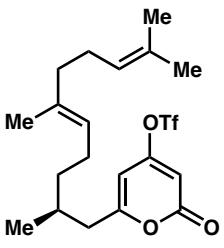
General Procedures

Unless otherwise stated, all reactions were performed in oven-dried or flame-dried glassware under an atmosphere of dry nitrogen or argon. Dry tetrahydrofuran (THF), dichloromethane, toluene, hexane, acetonitrile (MeCN), dimethylformamide (DMF), and diethyl ether (Et_2O) were obtained by passing these previously degassed solvents through activated alumina columns. Amines and alcohols were distilled from calcium hydride prior to use. Sulfuryl chloride (SO_2Cl_2) was distilled prior to use and the fraction boiling at 70 °C collected. The (*S*)-dihydrofarnesal employed displayed the following optical properties: $[\alpha]^{20}_D$ = -12.0° (c = 0.017 g/ml, $CHCl_3$); reduction of this material to (*S*)-dihydrofarnesol and protection as a *p*-methoxybenzyl (PMB) ether produced a compound with 90% enantiomeric excess (ee) as determined by chiral HPLC analysis (Chiralpak OJ column). Reactions were monitored by thin layer chromatography (TLC) on Silicycle Siliaplate^{TM} G TLC plates (250 μm thickness, 60 Å porosity, F-254 indicator) and visualized by UV irradiation and staining with *p*-anisaldehyde, phosphomolybdic acid, or potassium permanganate developing agents. Volatile solvents were removed under reduced pressure using a rotary evaporator. Flash column chromatography was performed using Silicycle F60 silica gel (60Å, 230-400 mesh, 40-63 μm). Proton nuclear magnetic resonance (^{1}H NMR) and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on Bruker AV-500 or AV-600 spectrometers operating respectively at 500, and 600 MHz for ^{1}H, and 125, and 151 MHz for ^{13}C. Chemical shifts are reported in parts per million (ppm) with respect to the residual solvent signal $CDCl_3$ (^{1}H NMR: δ = 7.26; ^{13}C NMR: δ = 77.16). Peak multiplicities are reported as follows: s = singlet, bs = broad singlet, d = doublet, t = triplet, p = pentet, dd = doublet of doublets, td = triplet of doublets, m = multiplet. app = apparent. Melting points were determined using MEl-TEMP™ apparatus and are uncorrected. IR spectra were recorded on a Nicolet 380 FT-IR spectrometer. High-resolution mass spectra (HRMS) were obtained by the qb3 mass spectrometry facility at the University of California, Berkeley. Optical rotations were measured on a Perkin-Elmer 241 polarimeter. X-ray crystallographic analyses were performed at the UC-Berkeley College of Chemistry X-ray crystallographic facility.

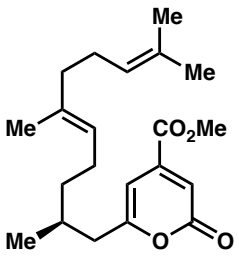


Ketone 9. BF_3•OEt_2 (1.0 mL, 8.1 mmol, 1.5 equiv) was added to a solution of aldehyde **6** (1.19 g, 5.4 mmol, 1 equiv) and silyl ketene acetal **7** (1.3 g, 6.1 mmol, 1.1 equiv) in CH_2Cl_2 (40 mL) over a period of 30 min at -78 °C. The reaction mixture was stirred for another 30 min at this temperature before solid $NaHCO_3$ (1.4 g, 16.7 mmol, 3 equiv) and Dess-Martin periodinane (3.4 g, 8.0 mmol, 1.5 equiv) were added. The resulting mixture was slowly warmed to room temperature and stirred overnight. After 8 hours, an additional portion of $NaHCO_3$ (1.4 g, 16.7 mmol, 3 equiv) and Dess-Martin periodinane (3.4 g, 8.0 mmol, 1.5 equiv) was added and the mixture stirred for an additional 1 hour at room temperature. A saturated solution of $Na_2S_2O_3$•$5H_2O$ (50 mL) was slowly added at 0 °C and the reaction mixture stirred for 30 min. The aqueous phase was extracted with CH_2Cl_2 (2 x 100 mL), washed with saturated aqueous $NaHCO_3$ (100 mL), brine (100 mL), and the combined organic phases dried ($MgSO_4$) and concentrated *in vacuo*. Purification by silica gel flash column chromatography (ethyl acetate/hexane) gave ketone **9** (1.2 g, 62%) as a colorless oil: $[\alpha]^{20}_D$ = -4.8° (c = 0.014 g/ml, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.32 (s, 1H), 5.07 (dddt, *J* = 7.0, 5.8, 3.0, 1.5 Hz, 2H), 3.29 (d, *J* = 1.2 Hz, 2H), 2.48 (dd, *J* = 16.4, 5.5 Hz, 1H), 2.30 (dd, *J* = 16.4, 8.1 Hz, 1H), 2.12 - 1.87 (m, 7H), 1.70 (s, 6H), 1.66 (s, 3H), 1.58 (dd, *J* = 2.7, 1.4 Hz, 6H), 1.38 - 1.26 (m, 1H), 1.26 - 1.12 (m, 1H), 0.91 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 203.1, 164.7, 160.8, 135.6, 131.5, 124.4, 124.0, 107.3, 96.8, 50.7, 47.6, 39.8, 36.9, 28.9, 26.8, 25.8, 25.4, 25.2, 25.2, 19.8, 17.8, 16.1; IR (thin film, cm^{-1}) 2962, 2920, 2852, 1732, 1638, 1391, 1376, 1272, 1015; HRMS (ESI) calcd. for $[C_{22}H_{35}O_4]^+$ $(M+H)^+$: *m/z* 363.2530, found 363.2533.



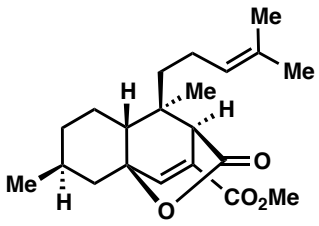
Triflate 11. Ketone **9** (600 mg, 1.66 mmol, 1 equiv) in toluene (20 mL) was added over a period of 50 minutes to refluxing toluene (145 mL). The solution was heated for an additional 30 minutes, cooled to room temperature, diluted with dry DCM (100 mL), and cooled to -78 °C. Et_3N (0.6 mL, 4.1 mmol, 2.5 equiv) was added, followed by the dropwise addition of Tf_2O (280 μL, 1.66 mmol, 1 equiv). The resulting mixture was stirred for 1 hour at -78 °C and then quenched with saturated aqueous $NaHCO_3$ solution (25 mL). The organic layer was separated and the aqueous layer was extracted with Et_2O (3 x 50 mL). The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated *in vacuo*. Purification by silica gel flash

column chromatography (ethyl acetate/hexane) afforded triflate **11** (484 mg, 67%) as a colorless oil: $[\alpha]^{20}_D$ = -6.0° (c = 0.014 g/ml, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.12 (d, *J* = 2.3 Hz, 1H), 6.03 (d, *J* = 2.2 Hz, 1H), 5.08 (dddq, *J* = 7.0, 5.7, 2.9, 1.6 Hz, 2H), 2.58 (dd, *J* = 14.3, 5.9 Hz, 1H), 2.31 (dd, *J* = 14.3, 8.4 Hz, 1H), 2.12 - 1.92 (m, 7H), 1.72 - 1.65 (m, 3H), 1.60 (s, 6H), 1.45 - 1.33 (m, 1H), 1.33 - 1.20 (m, 1H), 0.94 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.7, 161.8, 161.0, 135.8, 131.5, 124.4, 123.7, 121.7, 119.6, 117.5, 115.4, 102.5, 100.0, 41.74, 39.8, 36.7, 31.5, 26.8, 25.8, 25.3, 19.3, 17.8, 16.1; IR (thin film, cm^{-1}) 2963, 2921, 2854, 1753, 1643, 1576, 1435, 1249, 1215, 1140; HRMS (ESI) calcd. for $[C_{20}H_{28}O_5SF_3]^+$ $(M+H)^+$: *m/z* 437.1604, found 437.1602.

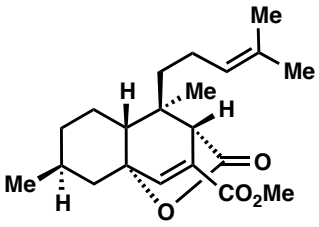


Ester S1. An oven-dried flask was charged with $Pd(OAc)_2$ (78 mg, 0.35 mmol, 10 mol %), DPEPhos (187 mg, 0.35 mmol, 10 mol %) and degased CH_3CN (5 mL). The resulting mixture was stirred for 15 min, and then a solution of triflate **11** (1.52 g, 3.47 mmol, 1 equiv) in degased CH_3CN (25 mL) was added, followed by degased MeOH (6 mL) and ^{i}Pr$_2$NEt (1.2 mL, 6.9 mmol, 2 equiv). CO gas was bubbled through the resulting mixture (via balloon) for approximately 5 minutes and the reaction stirred overnight under an atmosphere of CO. The reaction mixture was flushed thoroughly with a stream of nitrogen, diluted with Et_2O (100 mL), and washed with brine. The organic layer was dried over $MgSO_4$, and concentrated *in vacuo*. Purification by silica gel flash column chromatography (ethyl acetate/hexane) afforded ester **S1** (1.1 g, 90%) as a colorless oil: $[\alpha]^{20}_D$ = -13.6° (c = 0.018 g/ml, $CHCl_3$); ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.76 (s, 1H), 6.41 (s, 1H), 5.07 (t, *J* = 7.1 Hz, 2H), 3.90 (s, 3H), 2.54 (dd, *J* = 14.3, 6.0 Hz, 1H), 2.28 (dd, *J* = 14.2, 8.3 Hz, 1H), 2.09 – 2.00 (m, 3H), 2.00 – 1.92 (m, 4H), 1.66 (s, 3H), 1.58 (s, 6H), 1.43 – 1.31 (m, 1H), 1.28 – 1.15 (m, 1H), 0.92 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.3, 164.1, 162.7, 144.1, 135.5, 131.4, 124.4, 124.0, 115.3, 102.1, 53.3, 41.7, 39.8, 36.8, 31.5, 26.8, 25.8, 25.4, 19.4, 17.8, 16.1; IR (thin film, cm^{-1}) 2958, 2919, 2851, 1733, 1639, 1563, 1256; HRMS (ESI) calcd. for $[C_{21}H_{31}O_4]^+$ $(M+H)^+$: *m/z* 347.2217, found 347.2216.

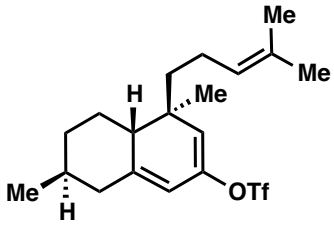
Cycloadducts 12 and **13.** A solution of ester **S1** (1.0 g, 2.9 mmol, 1 equiv) in toluene (60 mL) was heated to 100 °C for 4 days. Upon cooling, the reaction mixture was concentrated *in vacuo* and the crude residue purified by silica gel flash column chromatography (ethyl acetate/hexanes) affording cycloadducts **12** (451 mg, 45%) and **13** (450 mg, 45%).



Diastereomer **12**: White foam; $[\alpha]^{20}_{D}$ = -16.6° (c = 0.016 g/ml, $CHCl_3$); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.15 (d, *J* = 1.7 Hz, 1H), 5.07 (td, *J* = 7.2, 3.7 Hz, 1H), 3.80 (s, 3H), 3.69 (d, *J* = 1.8 Hz, 1H), 2.26 (ddd, *J* = 12.8, 3.4, 1.9 Hz, 1H), 2.14 (tt, *J* = 12.6, 6.5 Hz, 1H), 1.92 (tt, *J* = 13.1, 6.4 Hz, 1H), 1.74 (dq, *J* = 13.0, 3.1 Hz, 1H), 1.69 – 1.54 (m, 9H), 1.52 – 1.40 (m, 3H), 1.08 – 0.98 (m, 4H), 0.85 – 0.72 (m, 4H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.7, 163.9, 141.3, 136.1, 132.2, 123.7, 83.9, 53.1, 52.5, 50.2, 44.0, 40.9, 40.4, 34.2, 29.6, 28.2, 25.8, 23.3, 22.1, 18.9, 17.8; IR (thin film, cm^{-1}) 2926, 1757, 1724, 1220, 772; HRMS (ESI) calcd. for $[C_{21}H_{30}O_4Na]^+$ $(M+Na)^+$: *m/z* 369.2036, found 369.2038. Vapor diffusion of an ether solution of racemic **12** with pentane afforded X-ray quality crystals (m.p. = 92 - 94 °C).

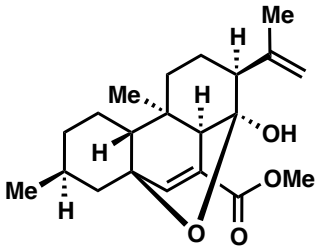


Diastereomer 13: colorless oil; $[\alpha]^{20}_{D}$ = +4.1° (c = 0.014 g/ml, $CHCl_3$); ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.94 (d, *J* = 1.9 Hz, 1H), 4.95 (tdd, *J* = 7.1, 2.9, 1.5 Hz, 1H), 3.80 (s, 3H), 3.63 (d, *J* = 1.9 Hz, 1H), 2.38 (ddd, *J* = 14.4, 3.5, 2.3 Hz, 1H), 2.05 – 1.97 (m, 1H), 1.86 – 1.75 (m, 3H), 1.67 – 1.61 (m, 4H), 1.56 (s, 3H), 1.45 (qd, *J* = 13.1, 3.2 Hz, 1H), 1.35 (dd, *J* = 14.4, 12.3 Hz, 1H), 1.29 – 1.14 (m, 2H), 1.14 – 1.07 (m, 1H), 1.06 (s, 3H), 1.03 – 0.95 (m, 1H), 0.94 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.4, 163.9, 143.3, 134.3, 132.1, 123.8, 82.9, 52.8, 52.5, 45.7, 42.2, 41.7, 38.7, 34.1, 27.1, 25.8, 25.3, 22.6, 22.0, 21.0, 17.7; IR (thin film, cm^{-1}) 2926, 1754, 1725, 1438, 1252; HRMS (EI) calcd. for $[C_{21}H_{30}O_4Na]^+$ $(M+Na)^+$: *m/z* 369.2036, found 369.2037.



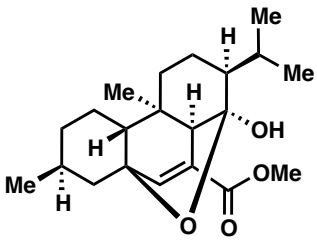
Dienol triflate 20: Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 5.48 (q, *J* = 1.8 Hz, 1H), 5.23 (d, *J* = 2.1 Hz, 1H), 5.05 (ddt, *J* = 8.5, 7.1, 1.5 Hz, 1H), 2.35 (ddd, *J* = 13.2, 4.3, 2.1 Hz, 1H), 2.02 (dd, *J* = 12.7, 4.5 Hz, 1H), 1.95 (dq, *J* = 11.4, 5.8 Hz, 2H), 1.85 - 1.78 (m, 1H), 1.78 - 1.71 (m, 2H), 1.67 (d, *J* = 1.5 Hz, 3H), 1.61 - 1.55 (m, 4H), 1.55 - 1.47 (m, 1H), 1.33 (qd, *J* = 12.8, 3.5 Hz, 1H), 1.28 - 1.20 (m, 1H), 1.06 (qd, *J* = 13.2, 3.7 Hz, 1H), 1.00 (s, 3H), 0.94 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.5, 144.8,

131.9, 124.4, 122.0, 120.9, 119.8, 117.7, 115.6, 111.8, 46.5, 44.0, 42.1, 38.4, 36.4, 35.3, 27.7, 25.8, 23.3, 22.4, 22.4, 17.7; IR (thin film, cm^{-1}) 2925, 1421, 1210, 965, 772.

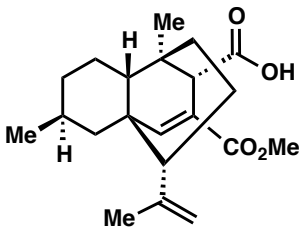


Hemiketal 17. *i.* A flame-dried round-bottom flask was charged with **12** (286 mg, 0.83 mmol, 1 equiv) and dry DCM (10 mL). The reaction was cooled to 0 °C and Na_2CO_3 (350 mg, 3.3 mmol, 4 equiv) was added, followed by the dropwise addition of freshly distilled SO_2Cl_2 (72 μL, 0.9 mmol, 1.1 equiv). The reaction mixture was stirred for 30 minutes at this temperature and quenched by the addition of saturated aqueous $NaHCO_3$ solution (10 mL). The organic layer was separated and the aqueous layer was extracted with Et_2O (30 mL). The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated *in vacuo* to give crude allylic chloride **16** (298 mg), which was sufficiently pure for the ensuing step.

ii. The above crude allylic chloride (220 mg, 0.58 mmol, 1 equiv) was dissolved in dry THF (10 mL) and treated with activated zinc (751 mg, 11.6 mmol, 20 equiv) under an atmosphere of nitrogen. The reaction vessel was sealed and heated to reflux for 24 hours. Upon cooling, the reaction mixture was filtered through a short plug of silica gel eluting with Et_2O (100 ml). The organic filtrate was concentrated *in vacuo* and the crude residue purified by silica gel flash column chromatography (ethyl acetate/hexanes) affording hemiketal **17** (162 mg, 80%) as a white foam: $[\alpha]^{20}_D$ = +42.3° (c = 0.012 g/ml, CH_2Cl_2); ^{1}H NMR (500 MHz, C_6D_6) δ 7.20 (d, *J* = 1.7 Hz, 1H), 4.90 (d, *J* = 2.5 Hz, 1H), 4.84 (dt, *J* = 2.9, 1.5 Hz, 1H), 3.46 (s, 3H), 3.02 (d, *J* = 1.8 Hz, 1H), 2.91 (s, 1H), 2.15 (dd, *J* = 12.7, 4.1 Hz, 1H), 1.99 (dt, *J* = 12.0, 2.4 Hz, 1H), 1.84 (s, 3H), 1.78 (td, *J* = 13.1, 4.2 Hz, 1H), 1.41 – 1.11 (m, 7H), 1.05 (td, *J* = 13.3, 4.4 Hz, 1H), 0.80 (d, *J* = 6.3 Hz, 3H), 0.73 (s, 3H), 0.70 – 0.57 (m, 1H), 0.49 (tt, *J* = 14.6, 11.0 Hz, 1H); ^{13}C NMR (126 MHz, C_6D_6) δ 165.0, 145.4, 142.4, 135.8, 115.2, 96.9, 75.6, 53.1, 51.0, 50.8, 47.9, 42.3, 37.4, 35.7, 34.5, 29.3, 27.1, 24.1, 24.0, 22.1, 21.1; IR (thin film, cm^{-1}) 2926, 1719, 1437, 1378, 1265, 1206; HRMS (ESI) calcd. for $[C_{21}H_{30}O_4Na]^+$ $(M+Na)^+$: *m/z* 369.2036, found 369.2040.

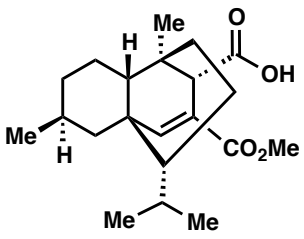


(+)-Chatancin (1). A solution of hemiketal **17** (100 mg, 0.29 mmol, 1 equiv) in anhydrous MeOH (6 mL) was treated with 5% Pd/C (62 mg, 0.03 mmol, 1 equiv) under an atmosphere of hydrogen (1 atm). The resulting heterogeneous mixture was stirred overnight at room temperature and then filtered through a short plug of silica gel eluting with Et_2O (50 mL). The organic filtrate was concentrated *in vacuo* and the crude material purified by silica gel flash column chromatography (ethyl acetate/hexane) affording (+)-chatancin (94 mg, 93%) as a white solid: $[\alpha]^{20}_D$ = +10.7° (c = 0.01 g/ml, $CHCl_3$); ^{1}H NMR (600 MHz, C_6D_6) δ 7.12 (d, *J* = 1.8 Hz, 1H), 3.43 (s, 3H), 2.93 (d, *J* = 1.8 Hz, 1H), 2.50 (pd, *J* = 7.0, 2.5 Hz, 1H), 1.92 - 1.79 (m, 2H), 1.49 (qd, *J* = 13.0, 4.1 Hz, 1H), 1.41 (ddd, *J* = 12.8, 3.8, 2.6 Hz, 1H), 1.38 - 1.22 (m, 4H), 1.22 - 1.12 (m, 3H), 1.11 (d, *J* = 6.9 Hz, 3H), 1.03 - 0.94 (m, 4H), 0.79 (d, *J* = 6.3 Hz, 3H), 0.67 (s, 3H), 0.58 (tdd, *J* = 12.9, 11.3, 3.4 Hz, 1H), 0.48 - 0.33 (m, 1H); ^{13}C NMR (151 MHz, C_6D_6) δ 164.9, 143.4, 135.9, 98.8, 75.4, 52.8, 51.0, 48.7, 47.5, 42.2, 37.6, 35.9, 34.4, 29.2, 27.0, 25.4, 24.1, 22.9, 22.0, 18.3; IR (thin film, cm^{-1}) 3494, 2953, 2928, 2870, 1719, 1456, 1438, 1268, 1209; HRMS (ESI) calcd. for $[C_{21}H_{32}O_4Na]^+$ $(M+Na)^+$: *m/z* 371.2193, found 371.2193. Vapor diffusion of an ether solution of (±)-chatancin with pentane afforded X-ray quality crystals (m.p = 106 – 108 °C).



Acid (±)-**14**: To a solution of lactone (±)-**13** (59 mg, 0.17 mmol, 1 equiv) in DCM (3 mL) was added TMSOTf (62 μL, 0.34 mmol, 2 equiv) dropwise at -78 °C. The reaction was slowly warmed to room temperature and quenched with saturated aqueous $NaHCO_3$ solution (5 mL). The organic layer was separated and the aqueous layer extracted with DCM (2 X 10 mL). The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated *in vacuo*. Purification by silica gel flash column chromatography (ethyl acetate/hexane) gave racemic **14** (20 mg, 34%) as a colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.93 (dd, *J* = 2.1, 1.2 Hz, 1H), 4.78 (t, *J* = 1.8 Hz, 1H), 4.65 - 4.56 (m, 1H), 3.75 (s, 3H), 3.09 (d, *J* = 2.1 Hz, 1H), 1.99 (dd, *J* = 10.5, 4.4 Hz, 1H), 1.79 (dt, *J* = 13.3, 2.8 Hz, 1H), 1.66 - 1.58 (m, 5H), 1.54 (qd, *J* = 13.2, 3.8 Hz, 1H), 1.48 - 1.36 (m, 5H), 1.33 (dddq, *J* = 12.5, 9.5, 6.3, 3.0 Hz, 1H), 1.27 - 1.22 (m, 1H), 1.15 - 1.05 (m, 4H), 0.85 (d, *J* = 6.5 Hz, 3H), 0.79 - 0.68 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 178.3, 166.6, 148.3, 146.5, 130.3, 113.4, 57.7,

52.0, 49.9, 49.8, 46.3, 45.6, 42.3, 36.2, 35.2, 29.6, 26.0, 25.9, 23.5, 22.9; IR (thin film, cm^{-1}) 2922, 1715, 1456, 1260; HRMS (ESI) calcd. for $[C_{21}H_{30}O_4Na]^+$ $(M + Na)^+$: *m/z* 369.2036, found 369.2034.



Acid (±)-**15**: A solution of acid (±)-**14** (12.4 mg, 0.036 mmol, 1 equiv) in anhydrous MeOH (2 mL) was treated with 5% Pd/C (7.6 mg, 0.0036 mmol, 10 mol%) under an atmosphere of hydrogen (balloon). The resulting heterogeneous mixture was stirred at room temperature for 8 hours and then filtered through a short plug of SiO_2 eluting with Et_2O (30 mL). The organic filtrate was concentrated *in vacuo* and the crude material purified by silica gel flash column chromatography (ethyl acetate/hexane) affording racemic acid **15** (10 mg, 80%) as a white foam; ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.97 (d, *J* = 2.1 Hz, 1H), 3.74 (d, *J* = 1.2 Hz, 3H), 3.04 (d, *J* = 1.9 Hz, 1H), 2.17 (p, *J* = 7.2 Hz, 1H), 2.11 – 2.02 (m, 1H), 1.69 – 1.57 (m, 2H), 1.57 – 1.29 (m, 6H), 1.29 – 1.18 (m, 3H), 1.12 – 0.99 (m, 4H), 0.90 – 0.81 (m, 6H), 0.73 (qd, *J* = 12.5, 3.8 Hz, 1H), 0.63 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 177.7, 166.7, 148.8, 129.8, 55.7, 51.9, 50.5, 49.7, 45.8, 45.7, 43.2, 36.2, 35.0, 29.8, 26.0, 25.4, 23.8, 23.6, 23.1, 18.7, 18.3; IR (thin film, cm^{-1}) 2953, 1711, 1436, 1260; HRMS (ESI) calcd. for $[C_{21}H_{31}O_4]^-$ $(M - H)^-$: *m/z* 347.2229, found 347.2228. Vapor diffusion of an ether solution of racemic **15** with pentane afforded X-ray quality crystals (m.p. = 118 – 120 °C).

X-ray Crystal Structure Determination of (±)-12

A colorless prism 0.050 x 0.030 x 0.030 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 5 seconds per frame using a scan width of 2.0°. Data collection was 100.0% complete to 67.000° in θ. A total of 40080 reflections were collected covering the indices, -10<=*h*<=11, -17<=*k*<=19, -15<=*l*<=14. 3448 reflections were found to be symmetry independent, with an R_{int} of 0.0254. Indexing and unit cell refinement indicated a primitive, monoclinic lattice. The space group was found to be P 21/n (No. 14). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014.

SI Table 1. Crystal data and structure refinement for (±)-**12**

X-ray ID	maimone37	
Sample/notebook ID	ZYM-889-3	
Empirical formula	C21 H30 O4	
Formula weight	346.45	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 9.9351(3) Å	α= 90°.
	b = 16.0173(4) Å	β= 108.5970(10)°.
	c = 12.5159(3) Å	γ = 90°.
Volume	1887.70(9) $Å^3$	
Z	4	
Density (calculated)	1.219 Mg/m^3	
Absorption coefficient	0.662 mm^{-1}	
F(000)	752	
Crystal size	0.050 x 0.030 x 0.030 mm^3	
Theta range for data collection	4.638 to 68.299°.	
Index ranges	-10<=h<=11, -17<=k<=19, -15<=l<=14	
Reflections collected	40080	
Independent reflections	3448 [R(int) = 0.0254]	
Completeness to theta = 67.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.851	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3448 / 0 / 231	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0347, wR2 = 0.0880	
R indices (all data)	R1 = 0.0368, wR2 = 0.0900	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.286 and -0.238 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for maimone37. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6051(1)	2325(1)	4692(1)	18(1)
C(2)	4646(1)	2066(1)	3741(1)	18(1)
C(3)	3787(1)	1511(1)	4333(1)	18(1)
C(4)	2258(1)	1782(1)	4187(1)	22(1)
C(5)	1548(1)	1180(1)	4789(1)	25(1)
C(6)	2361(1)	1131(1)	6048(1)	23(1)
C(7)	3897(1)	868(1)	6219(1)	21(1)
C(8)	4609(1)	1451(1)	5611(1)	18(1)
C(9)	4874(1)	2327(1)	6078(1)	18(1)
C(10)	5633(1)	2784(1)	5591(1)	18(1)
C(11)	6795(1)	1533(1)	5231(1)	20(1)
C(12)	3870(1)	2869(1)	3215(1)	21(1)
C(13)	5009(1)	1548(1)	2826(1)	21(1)
C(14)	5819(1)	2017(1)	2148(1)	27(1)
C(15)	6353(1)	1435(1)	1430(1)	26(1)
C(16)	5812(1)	1313(1)	325(1)	23(1)
C(17)	4525(1)	1754(1)	-431(1)	30(1)
C(18)	6447(2)	688(1)	-270(1)	34(1)
C(19)	1639(1)	536(1)	6647(1)	31(1)
C(20)	6007(1)	3679(1)	5794(1)	19(1)
C(21)	5994(2)	4865(1)	6897(1)	30(1)
O(1)	6004(1)	1074(1)	5718(1)	21(1)
O(2)	7952(1)	1297(1)	5251(1)	27(1)
O(3)	6568(1)	4077(1)	5239(1)	31(1)
O(4)	5640(1)	3993(1)	6648(1)	26(1)

Table 3. Bond lengths [Å] and angles [°] for maimone37.

C(1)-C(10)	1.5096(14)	C(12)-H(12A)	0.9800
C(1)-C(11)	1.5133(15)	C(12)-H(12B)	0.9800
C(1)-C(2)	1.5748(14)	C(12)-H(12C)	0.9800
C(1)-H(1)	1.0000	C(13)-C(14)	1.5389(15)
C(2)-C(12)	1.5352(15)	C(13)-H(13A)	0.9900
C(2)-C(13)	1.5458(14)	C(13)-H(13B)	0.9900
C(2)-C(3)	1.5723(14)	C(14)-C(15)	1.5029(16)
C(3)-C(4)	1.5331(15)	C(14)-H(14A)	0.9900
C(3)-C(8)	1.5491(15)	C(14)-H(14B)	0.9900
C(3)-H(3)	1.0000	C(15)-C(16)	1.3296(17)
C(4)-C(5)	1.5283(15)	C(15)-H(15)	0.9500
C(4)-H(4A)	0.9900	C(16)-C(18)	1.5021(16)
C(4)-H(4B)	0.9900	C(16)-C(17)	1.5022(17)
C(5)-C(6)	1.5264(16)	C(17)-H(17A)	0.9800
C(5)-H(5A)	0.9900	C(17)-H(17B)	0.9800
C(5)-H(5B)	0.9900	C(17)-H(17C)	0.9800
C(6)-C(19)	1.5250(16)	C(18)-H(18A)	0.9800
C(6)-C(7)	1.5308(16)	C(18)-H(18B)	0.9800
C(6)-H(6)	1.0000	C(18)-H(18C)	0.9800
C(7)-C(8)	1.5152(15)	C(19)-H(19A)	0.9800
C(7)-H(7A)	0.9900	C(19)-H(19B)	0.9800
C(7)-H(7B)	0.9900	C(19)-H(19C)	0.9800
C(8)-O(1)	1.4784(12)	C(20)-O(3)	1.2022(14)
C(8)-C(9)	1.5109(15)	C(20)-O(4)	1.3330(13)
C(9)-C(10)	1.3294(15)	C(21)-O(4)	1.4485(14)
C(9)-H(9)	0.9500	C(21)-H(21A)	0.9800
C(10)-C(20)	1.4835(15)	C(21)-H(21B)	0.9800
C(11)-O(2)	1.2032(14)	C(21)-H(21C)	0.9800
C(11)-O(1)	1.3539(14)		

C(10)-C(1)-C(11)	106.66(9)	C(11)-C(1)-H(1)	111.5
C(10)-C(1)-C(2)	107.66(8)	C(2)-C(1)-H(1)	111.5
C(11)-C(1)-C(2)	107.78(9)	C(12)-C(2)-C(13)	109.60(9)
C(10)-C(1)-H(1)	111.5	C(12)-C(2)-C(3)	113.68(9)

C(13)-C(2)-C(3)	109.67(8)	C(9)-C(8)-C(7)	115.47(9)
C(12)-C(2)-C(1)	107.82(9)	O(1)-C(8)-C(3)	106.82(8)
C(13)-C(2)-C(1)	109.94(9)	C(9)-C(8)-C(3)	108.11(8)
C(3)-C(2)-C(1)	106.03(8)	C(7)-C(8)-C(3)	112.35(9)
C(4)-C(3)-C(8)	108.51(9)	C(10)-C(9)-C(8)	112.88(9)
C(4)-C(3)-C(2)	116.70(9)	C(10)-C(9)-H(9)	123.6
C(8)-C(3)-C(2)	109.60(8)	C(8)-C(9)-H(9)	123.6
C(4)-C(3)-H(3)	107.2	C(9)-C(10)-C(20)	127.00(10)
C(8)-C(3)-H(3)	107.2	C(9)-C(10)-C(1)	113.87(10)
C(2)-C(3)-H(3)	107.2	C(20)-C(10)-C(1)	119.02(9)
C(5)-C(4)-C(3)	110.96(9)	O(2)-C(11)-O(1)	120.50(10)
C(5)-C(4)-H(4A)	109.4	O(2)-C(11)-C(1)	126.86(10)
C(3)-C(4)-H(4A)	109.4	O(1)-C(11)-C(1)	112.64(9)
C(5)-C(4)-H(4B)	109.4	C(2)-C(12)-H(12A)	109.5
C(3)-C(4)-H(4B)	109.4	C(2)-C(12)-H(12B)	109.5
H(4A)-C(4)-H(4B)	108.0	H(12A)-C(12)-H(12B)	109.5
C(6)-C(5)-C(4)	111.53(9)	C(2)-C(12)-H(12C)	109.5
C(6)-C(5)-H(5A)	109.3	H(12A)-C(12)-H(12C)	109.5
C(4)-C(5)-H(5A)	109.3	H(12B)-C(12)-H(12C)	109.5
C(6)-C(5)-H(5B)	109.3	C(14)-C(13)-C(2)	115.74(9)
C(4)-C(5)-H(5B)	109.3	C(14)-C(13)-H(13A)	108.3
H(5A)-C(5)-H(5B)	108.0	C(2)-C(13)-H(13A)	108.3
C(19)-C(6)-C(5)	111.31(10)	C(14)-C(13)-H(13B)	108.3
C(19)-C(6)-C(7)	111.28(10)	C(2)-C(13)-H(13B)	108.3
C(5)-C(6)-C(7)	109.53(9)	H(13A)-C(13)-H(13B)	107.4
C(19)-C(6)-H(6)	108.2	C(15)-C(14)-C(13)	111.96(10)
C(5)-C(6)-H(6)	108.2	C(15)-C(14)-H(14A)	109.2
C(7)-C(6)-H(6)	108.2	C(13)-C(14)-H(14A)	109.2
C(8)-C(7)-C(6)	111.38(9)	C(15)-C(14)-H(14B)	109.2
C(8)-C(7)-H(7A)	109.4	C(13)-C(14)-H(14B)	109.2
C(6)-C(7)-H(7A)	109.4	H(14A)-C(14)-H(14B)	107.9
C(8)-C(7)-H(7B)	109.4	C(16)-C(15)-C(14)	127.58(11)
C(6)-C(7)-H(7B)	109.4	C(16)-C(15)-H(15)	116.2
H(7A)-C(7)-H(7B)	108.0	C(14)-C(15)-H(15)	116.2
O(1)-C(8)-C(9)	107.50(8)	C(15)-C(16)-C(18)	121.27(12)
O(1)-C(8)-C(7)	106.14(8)	C(15)-C(16)-C(17)	124.51(11)

C(18)-C(16)-C(17)	114.21(11)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(6)-C(19)-H(19A)	109.5
C(6)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(6)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
O(3)-C(20)-O(4)	124.03(10)
O(3)-C(20)-C(10)	123.39(10)
O(4)-C(20)-C(10)	112.57(9)
O(4)-C(21)-H(21A)	109.5
O(4)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(4)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(11)-O(1)-C(8)	113.55(8)
C(20)-O(4)-C(21)	115.18(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for maimone37. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	17(1)	18(1)	20(1)	-2(1)	7(1)	-1(1)
C(2)	19(1)	17(1)	19(1)	-1(1)	6(1)	-1(1)
C(3)	19(1)	17(1)	19(1)	-2(1)	6(1)	-2(1)
C(4)	17(1)	25(1)	22(1)	1(1)	4(1)	-1(1)
C(5)	19(1)	26(1)	31(1)	-1(1)	9(1)	-3(1)
C(6)	26(1)	20(1)	27(1)	-1(1)	14(1)	-3(1)
C(7)	25(1)	18(1)	22(1)	2(1)	8(1)	-1(1)
C(8)	16(1)	18(1)	20(1)	0(1)	5(1)	2(1)
C(9)	16(1)	19(1)	16(1)	0(1)	3(1)	1(1)
C(10)	15(1)	19(1)	17(1)	-1(1)	2(1)	1(1)
C(11)	18(1)	20(1)	21(1)	-4(1)	5(1)	-1(1)
C(12)	22(1)	21(1)	20(1)	1(1)	6(1)	0(1)
C(13)	25(1)	19(1)	20(1)	-1(1)	9(1)	-2(1)
C(14)	38(1)	24(1)	25(1)	-2(1)	17(1)	-5(1)
C(15)	29(1)	23(1)	30(1)	3(1)	15(1)	2(1)
C(16)	25(1)	19(1)	30(1)	-2(1)	17(1)	-2(1)
C(17)	26(1)	33(1)	33(1)	-5(1)	11(1)	-2(1)
C(18)	42(1)	27(1)	41(1)	-5(1)	27(1)	0(1)
C(19)	32(1)	30(1)	37(1)	3(1)	18(1)	-5(1)
C(20)	16(1)	20(1)	19(1)	0(1)	4(1)	1(1)
C(21)	46(1)	16(1)	30(1)	-4(1)	16(1)	-1(1)
O(1)	18(1)	18(1)	25(1)	2(1)	6(1)	3(1)
O(2)	19(1)	28(1)	35(1)	0(1)	10(1)	4(1)
O(3)	41(1)	22(1)	38(1)	-5(1)	23(1)	-9(1)
O(4)	39(1)	16(1)	25(1)	-2(1)	16(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for maimone37.

	x	y	z	U(eq)
H(1)	6676	2675	4385	22
H(3)	3741	935	4015	22
H(4A)	2263	2351	4496	26
H(4B)	1707	1799	3374	26
H(5A)	564	1369	4681	30
H(5B)	1499	618	4452	30
H(6)	2373	1700	6379	28
H(7A)	4436	869	7035	26
H(7B)	3908	292	5934	26
H(9)	4535	2530	6658	21
H(12A)	4503	3214	2938	32
H(12B)	3591	3179	3786	32
H(12C)	3021	2725	2586	32
H(13A)	5584	1061	3194	25
H(13B)	4112	1332	2292	25
H(14A)	5183	2437	1658	33
H(14B)	6634	2316	2674	33
H(15)	7173	1117	1812	31
H(17A)	3728	1362	-670	45
H(17B)	4731	1970	-1094	45
H(17C)	4276	2219	-20	45
H(18A)	7284	432	273	50
H(18B)	6728	969	-861	50
H(18C)	5745	254	-609	50
H(19A)	661	719	6525	47
H(19B)	2161	534	7457	47
H(19C)	1634	-29	6345	47
H(21A)	7007	4950	7013	45
H(21B)	5779	5024	7581	45
H(21C)	5433	5209	6264	45

X-ray Crystal Structure Determination of (±)-15

A colorless prism 0.060 x 0.040 x 0.030 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 5 seconds per frame using a scan width of 2.0°. Data collection was 98.6% complete to 67.000° in θ. A total of 35829 reflections were collected covering the indices, -8<=*h*<=8, -10<=*k*<=11, -18<=*l*<=18. 3359 reflections were found to be symmetry independent, with an R_{int} of 0.0342. Indexing and unit cell refinement indicated a primitive, triclinic lattice. The space group was found to be P -1 (No. 2). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014.

SI Table 2. Crystal data and structure refinement for (±)-**15**

X-ray ID	maimone36	
Sample/notebook ID	ZYM-931	
Empirical formula	C21 H32 O4	
Formula weight	348.46	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.2615(3) Å	α= 93.392(2)°.
	b = 9.1617(3) Å	β= 102.492(2)°.
	c = 15.4037(6) Å	γ = 109.220(2)°.
Volume	935.25(6) $Å^3$	
Z	2	
Density (calculated)	1.237 Mg/m^3	
Absorption coefficient	0.668 mm^{-1}	
F(000)	380	
Crystal size	0.060 x 0.040 x 0.030 mm^3	
Theta range for data collection	2.968 to 68.263°.	
Index ranges	-8<=h<=8, -10<=k<=11, -18<=l<=18	
Reflections collected	35829	
Independent reflections	3359 [R(int) = 0.0342]	
Completeness to theta = 67.000°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.870	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3359 / 0 / 232	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0410, wR2 = 0.1140	
R indices (all data)	R1 = 0.0464, wR2 = 0.1190	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.396 and -0.220 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for maimone36. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	164(2)	6224(2)	3115(1)	24(1)
C(2)	-1227(2)	6425(2)	2265(1)	25(1)
C(3)	-613(2)	8108(2)	2085(1)	25(1)
C(4)	1589(2)	8790(2)	2026(1)	20(1)
C(5)	2917(2)	8697(2)	2937(1)	19(1)
C(6)	5178(2)	9547(2)	3047(1)	22(1)
C(7)	6424(2)	9474(2)	3964(1)	28(1)
C(8)	6055(2)	7788(2)	4133(1)	27(1)
C(9)	3801(2)	6919(2)	4014(1)	25(1)
C(10)	2449(2)	6974(2)	3102(1)	20(1)
C(11)	2828(2)	6105(2)	2344(1)	19(1)
C(12)	2549(2)	6450(2)	1509(1)	18(1)
C(13)	1873(2)	7787(2)	1226(1)	19(1)
C(14)	-517(3)	4521(2)	3312(1)	30(1)
C(15)	-1089(3)	3269(2)	2501(1)	43(1)
C(16)	-2207(4)	4188(2)	3776(2)	50(1)
C(17)	1994(2)	10491(2)	1866(1)	25(1)
C(18)	7241(3)	7714(2)	5071(1)	38(1)
C(19)	2685(2)	5430(2)	759(1)	20(1)
C(20)	3439(2)	3189(2)	362(1)	24(1)
C(21)	3271(2)	8751(2)	694(1)	19(1)
O(1)	2197(2)	5584(1)	-22(1)	23(1)
O(2)	3399(2)	4318(1)	1045(1)	24(1)
O(3)	5089(2)	9060(1)	882(1)	22(1)
O(4)	2299(2)	9225(1)	4(1)	22(1)

Table 3. Bond lengths [Å] and angles [°] for maimone36.

C(1)-C(2)	1.531(2)	C(11)-H(11)	0.9500
C(1)-C(14)	1.544(2)	C(12)-C(19)	1.484(2)
C(1)-C(10)	1.579(2)	C(12)-C(13)	1.516(2)
C(1)-H(1)	1.0000	C(13)-C(21)	1.5291(19)
C(2)-C(3)	1.518(2)	C(13)-H(13)	1.0000
C(2)-H(2A)	0.9900	C(14)-C(16)	1.506(3)
C(2)-H(2B)	0.9900	C(14)-C(15)	1.530(2)
C(3)-C(4)	1.539(2)	C(14)-H(14)	1.0000
C(3)-H(3A)	0.9900	C(15)-H(15A)	0.9800
C(3)-H(3B)	0.9900	C(15)-H(15B)	0.9800
C(4)-C(17)	1.533(2)	C(15)-H(15C)	0.9800
C(4)-C(5)	1.545(2)	C(16)-H(16A)	0.9800
C(4)-C(13)	1.583(2)	C(16)-H(16B)	0.9800
C(5)-C(6)	1.534(2)	C(16)-H(16C)	0.9800
C(5)-C(10)	1.5500(19)	C(17)-H(17A)	0.9800
C(5)-H(5)	1.0000	C(17)-H(17B)	0.9800
C(6)-C(7)	1.523(2)	C(17)-H(17C)	0.9800
C(6)-H(6A)	0.9900	C(18)-H(18A)	0.9800
C(6)-H(6B)	0.9900	C(18)-H(18B)	0.9800
C(7)-C(8)	1.526(2)	C(18)-H(18C)	0.9800
C(7)-H(7A)	0.9900	C(19)-O(1)	1.2087(18)
C(7)-H(7B)	0.9900	C(19)-O(2)	1.3429(18)
C(8)-C(9)	1.530(2)	C(20)-O(2)	1.4435(18)
C(8)-C(18)	1.532(2)	C(20)-H(20A)	0.9800
C(8)-H(8)	1.0000	C(20)-H(20B)	0.9800
C(9)-C(10)	1.544(2)	C(20)-H(20C)	0.9800
C(9)-H(9A)	0.9900	C(21)-O(3)	1.2191(17)
C(9)-H(9B)	0.9900	C(21)-O(4)	1.3219(17)
C(10)-C(11)	1.498(2)	O(4)-H(4)	0.8400
C(11)-C(12)	1.331(2)		

C(2)-C(1)-C(14)	111.66(13)	C(2)-C(1)-H(1)	105.8
C(2)-C(1)-C(10)	111.27(12)	C(14)-C(1)-H(1)	105.8
C(14)-C(1)-C(10)	115.79(13)	C(10)-C(1)-H(1)	105.8

C(3)-C(2)-C(1)	112.00(12)	C(7)-C(8)-C(9)	109.91(13)
C(3)-C(2)-H(2A)	109.2	C(7)-C(8)-C(18)	111.33(13)
C(1)-C(2)-H(2A)	109.2	C(9)-C(8)-C(18)	110.44(14)
C(3)-C(2)-H(2B)	109.2	C(7)-C(8)-H(8)	108.4
C(1)-C(2)-H(2B)	109.2	C(9)-C(8)-H(8)	108.4
H(2A)-C(2)-H(2B)	107.9	C(18)-C(8)-H(8)	108.4
C(2)-C(3)-C(4)	113.21(13)	C(8)-C(9)-C(10)	114.83(12)
C(2)-C(3)-H(3A)	108.9	C(8)-C(9)-H(9A)	108.6
C(4)-C(3)-H(3A)	108.9	C(10)-C(9)-H(9A)	108.6
C(2)-C(3)-H(3B)	108.9	C(8)-C(9)-H(9B)	108.6
C(4)-C(3)-H(3B)	108.9	C(10)-C(9)-H(9B)	108.6
H(3A)-C(3)-H(3B)	107.7	H(9A)-C(9)-H(9B)	107.5
C(17)-C(4)-C(3)	107.08(12)	C(11)-C(10)-C(9)	111.30(12)
C(17)-C(4)-C(5)	111.01(12)	C(11)-C(10)-C(5)	108.12(11)
C(3)-C(4)-C(5)	106.81(11)	C(9)-C(10)-C(5)	109.26(11)
C(17)-C(4)-C(13)	111.64(11)	C(11)-C(10)-C(1)	109.03(11)
C(3)-C(4)-C(13)	108.70(11)	C(9)-C(10)-C(1)	109.54(12)
C(5)-C(4)-C(13)	111.36(12)	C(5)-C(10)-C(1)	109.56(12)
C(6)-C(5)-C(4)	113.74(11)	C(12)-C(11)-C(10)	123.41(14)
C(6)-C(5)-C(10)	111.66(12)	C(12)-C(11)-H(11)	118.3
C(4)-C(5)-C(10)	110.48(11)	C(10)-C(11)-H(11)	118.3
C(6)-C(5)-H(5)	106.8	C(11)-C(12)-C(19)	121.30(13)
C(4)-C(5)-H(5)	106.8	C(11)-C(12)-C(13)	123.93(13)
C(10)-C(5)-H(5)	106.8	C(19)-C(12)-C(13)	114.49(12)
C(7)-C(6)-C(5)	112.06(12)	C(12)-C(13)-C(21)	109.32(12)
C(7)-C(6)-H(6A)	109.2	C(12)-C(13)-C(4)	113.72(11)
C(5)-C(6)-H(6A)	109.2	C(21)-C(13)-C(4)	113.93(11)
C(7)-C(6)-H(6B)	109.2	C(12)-C(13)-H(13)	106.4
C(5)-C(6)-H(6B)	109.2	C(21)-C(13)-H(13)	106.4
H(6A)-C(6)-H(6B)	107.9	C(4)-C(13)-H(13)	106.4
C(6)-C(7)-C(8)	111.30(12)	C(16)-C(14)-C(15)	109.77(14)
C(6)-C(7)-H(7A)	109.4	C(16)-C(14)-C(1)	111.40(15)
C(8)-C(7)-H(7A)	109.4	C(15)-C(14)-C(1)	115.39(14)
C(6)-C(7)-H(7B)	109.4	C(16)-C(14)-H(14)	106.6
C(8)-C(7)-H(7B)	109.4	C(15)-C(14)-H(14)	106.6
H(7A)-C(7)-H(7B)	108.0	C(1)-C(14)-H(14)	106.6

C(14)-C(15)-H(15A)	109.5	C(19)-O(2)-C(20)	116.67(11)
C(14)-C(15)-H(15B)	109.5	C(21)-O(4)-H(4)	109.5
H(15A)-C(15)-H(15B)	109.5		
C(14)-C(15)-H(15C)	109.5		
H(15A)-C(15)-H(15C)	109.5		
H(15B)-C(15)-H(15C)	109.5		
C(14)-C(16)-H(16A)	109.5		
C(14)-C(16)-H(16B)	109.5		
H(16A)-C(16)-H(16B)	109.5		
C(14)-C(16)-H(16C)	109.5		
H(16A)-C(16)-H(16C)	109.5		
H(16B)-C(16)-H(16C)	109.5		
C(4)-C(17)-H(17A)	109.5		
C(4)-C(17)-H(17B)	109.5		
H(17A)-C(17)-H(17B)	109.5		
C(4)-C(17)-H(17C)	109.5		
H(17A)-C(17)-H(17C)	109.5		
H(17B)-C(17)-H(17C)	109.5		
C(8)-C(18)-H(18A)	109.5		
C(8)-C(18)-H(18B)	109.5		
H(18A)-C(18)-H(18B)	109.5		
C(8)-C(18)-H(18C)	109.5		
H(18A)-C(18)-H(18C)	109.5		
H(18B)-C(18)-H(18C)	109.5		
O(1)-C(19)-O(2)	124.06(14)		
O(1)-C(19)-C(12)	123.48(13)		
O(2)-C(19)-C(12)	112.45(12)		
O(2)-C(20)-H(20A)	109.5		
O(2)-C(20)-H(20B)	109.5		
H(20A)-C(20)-H(20B)	109.5		
O(2)-C(20)-H(20C)	109.5		
H(20A)-C(20)-H(20C)	109.5		
H(20B)-C(20)-H(20C)	109.5		
O(3)-C(21)-O(4)	123.14(13)		
O(3)-C(21)-C(13)	124.03(13)		
O(4)-C(21)-C(13)	112.82(12)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for maimone36. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	24(1)	23(1)	24(1)	3(1)	9(1)	2(1)
C(2)	17(1)	30(1)	25(1)	3(1)	7(1)	3(1)
C(3)	22(1)	32(1)	23(1)	4(1)	7(1)	11(1)
C(4)	21(1)	20(1)	20(1)	5(1)	6(1)	8(1)
C(5)	21(1)	17(1)	18(1)	2(1)	5(1)	4(1)
C(6)	22(1)	17(1)	24(1)	4(1)	4(1)	2(1)
C(7)	24(1)	24(1)	26(1)	1(1)	0(1)	1(1)
C(8)	28(1)	25(1)	24(1)	3(1)	-1(1)	7(1)
C(9)	30(1)	20(1)	20(1)	5(1)	3(1)	5(1)
C(10)	20(1)	17(1)	19(1)	4(1)	4(1)	2(1)
C(11)	17(1)	15(1)	24(1)	5(1)	4(1)	3(1)
C(12)	15(1)	15(1)	22(1)	3(1)	5(1)	2(1)
C(13)	18(1)	19(1)	18(1)	4(1)	4(1)	6(1)
C(14)	28(1)	23(1)	34(1)	7(1)	9(1)	2(1)
C(15)	51(1)	22(1)	56(1)	3(1)	31(1)	2(1)
C(16)	69(1)	30(1)	52(1)	7(1)	39(1)	4(1)
C(17)	33(1)	24(1)	24(1)	6(1)	8(1)	15(1)
C(18)	37(1)	35(1)	32(1)	5(1)	-6(1)	10(1)
C(19)	15(1)	18(1)	23(1)	4(1)	5(1)	2(1)
C(20)	27(1)	21(1)	26(1)	3(1)	8(1)	11(1)
C(21)	22(1)	16(1)	19(1)	3(1)	5(1)	7(1)
O(1)	24(1)	26(1)	20(1)	5(1)	6(1)	9(1)
O(2)	31(1)	21(1)	24(1)	4(1)	7(1)	13(1)
O(3)	19(1)	24(1)	24(1)	9(1)	6(1)	7(1)
O(4)	21(1)	26(1)	22(1)	11(1)	7(1)	10(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for maimone36.

	x	y	z	U(eq)
H(1)	-12	6855	3622	29
H(2A)	-1195	5754	1745	30
H(2B)	-2626	6078	2332	30
H(3A)	-808	8754	2572	30
H(3B)	-1507	8168	1514	30
H(5)	2523	9229	3414	23
H(6A)	5617	9070	2573	27
H(6B)	5422	10654	2966	27
H(7A)	6071	10032	4436	33
H(7B)	7872	10005	3998	33
H(8)	6517	7265	3678	33
H(9A)	3367	7370	4499	30
H(9B)	3586	5813	4086	30
H(11)	3292	5264	2466	23
H(13)	515	7303	797	22
H(14)	655	4410	3746	36
H(15A)	-1286	2248	2704	65
H(15B)	-7	3514	2188	65
H(15C)	-2339	3245	2091	65
H(16A)	-3398	4275	3371	75
H(16B)	-1792	4944	4321	75
H(16C)	-2530	3130	3936	75
H(17A)	1021	10526	1324	38
H(17B)	3363	10947	1789	38
H(17C)	1857	11086	2383	38
H(18A)	8685	8241	5128	57
H(18B)	6980	6620	5158	57
H(18C)	6819	8234	5525	57
H(20A)	2170	2297	219	36
H(20B)	4564	2830	582	36

H(20C)	3610	3672	-180	36
H(4)	3117	9717	-280	34

X-ray Crystal Structure Determination of (±)-1

A colorless plate 0.050 x 0.040 x 0.020 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 5 seconds per frame using a scan width of 2.0°. Data collection was 99.6% complete to 67.000° in θ. A total of 56859 reflections were collected covering the indices, -13<=*h*<=13, -19<=*k*<=19, -12<=*l*<=10. 3415 reflections were found to be symmetry independent, with an R_{int} of 0.0324. Indexing and unit cell refinement indicated a primitive, monoclinic lattice. The space group was found to be P 21/c (No. 14). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014.

SI Table 3. Crystal data and structure refinement for (±)-**1**

X-ray ID	maimone38	
Sample/notebook ID	ZYM-964	
Empirical formula	C21 H32 O4	
Formula weight	348.46	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 11.5012(6) Å	α= 90°.
	b = 15.9349(8) Å	β= 97.550(2)°.
	c = 10.3245(5) Å	γ = 90°.
Volume	1875.77(16) $Å^3$	
Z	4	
Density (calculated)	1.234 Mg/m^3	
Absorption coefficient	0.666 mm^{-1}	
F(000)	760	
Crystal size	0.050 x 0.040 x 0.020 mm^3	
Theta range for data collection	3.877 to 68.237°.	
Index ranges	-13<=h<=13, -19<=k<=19, -12<=l<=10	
Reflections collected	56859	
Independent reflections	3415 [R(int) = 0.0324]	
Completeness to theta = 67.000°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.829	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3415 / 0 / 232	
Goodness-of-fit on F^2	1.082	
Final R indices [I>2sigma(I)]	R1 = 0.0452, wR2 = 0.1269	
R indices (all data)	R1 = 0.0465, wR2 = 0.1284	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.360 and -0.233 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for maimone38. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8412(1)	6097(1)	6713(1)	21(1)
C(2)	9131(1)	6309(1)	5594(2)	24(1)
C(3)	8709(1)	5850(1)	4322(1)	24(1)
C(4)	7400(1)	5972(1)	3880(1)	22(1)
C(5)	6700(1)	5749(1)	5004(1)	21(1)
C(6)	7097(1)	6291(1)	6223(1)	22(1)
C(7)	6373(1)	6034(1)	7266(1)	22(1)
C(8)	6447(1)	5218(1)	7546(1)	21(1)
C(9)	7252(1)	4747(1)	6766(1)	22(1)
C(10)	7259(1)	3806(1)	6980(2)	23(1)
C(11)	7850(1)	3570(1)	8352(2)	24(1)
C(12)	9084(1)	3941(1)	8589(2)	26(1)
C(13)	9076(1)	4895(1)	8416(2)	24(1)
C(14)	8494(1)	5136(1)	7046(1)	21(1)
C(15)	8829(2)	6673(1)	7872(2)	27(1)
C(16)	6967(1)	5540(1)	2569(2)	25(1)
C(17)	7395(2)	6020(1)	1433(2)	29(1)
C(18)	7300(2)	4615(1)	2498(2)	37(1)
C(19)	5657(1)	6657(1)	7877(2)	23(1)
C(20)	4590(2)	6934(1)	9622(2)	28(1)
C(21)	7859(2)	2620(1)	8535(2)	30(1)
O(1)	6860(1)	4884(1)	5369(1)	21(1)
O(2)	5506(1)	5883(1)	4536(1)	24(1)
O(3)	5480(1)	7363(1)	7478(1)	35(1)
O(4)	5246(1)	6350(1)	8928(1)	25(1)

Table 3. Bond lengths [Å] and angles [°] for maimone38.

C(1)-C(15)	1.535(2)	C(11)-H(11)	1.0000
C(1)-C(2)	1.544(2)	C(12)-C(13)	1.531(2)
C(1)-C(6)	1.562(2)	C(12)-H(12A)	0.9900
C(1)-C(14)	1.569(2)	C(12)-H(12B)	0.9900
C(2)-C(3)	1.526(2)	C(13)-C(14)	1.531(2)
C(2)-H(2A)	0.9900	C(13)-H(13A)	0.9900
C(2)-H(2B)	0.9900	C(13)-H(13B)	0.9900
C(3)-C(4)	1.527(2)	C(14)-H(14)	1.0000
C(3)-H(3A)	0.9900	C(15)-H(15A)	0.9800
C(3)-H(3B)	0.9900	C(15)-H(15B)	0.9800
C(4)-C(5)	1.537(2)	C(15)-H(15C)	0.9800
C(4)-C(16)	1.542(2)	C(16)-C(18)	1.526(2)
C(4)-H(4)	1.0000	C(16)-C(17)	1.534(2)
C(5)-O(2)	1.4116(18)	C(16)-H(16)	1.0000
C(5)-O(1)	1.4346(17)	C(17)-H(17A)	0.9800
C(5)-C(6)	1.546(2)	C(17)-H(17B)	0.9800
C(6)-C(7)	1.502(2)	C(17)-H(17C)	0.9800
C(6)-H(6)	1.0000	C(18)-H(18A)	0.9800
C(7)-C(8)	1.332(2)	C(18)-H(18B)	0.9800
C(7)-C(19)	1.482(2)	C(18)-H(18C)	0.9800
C(8)-C(9)	1.505(2)	C(19)-O(3)	1.2057(19)
C(8)-H(8)	0.9500	C(19)-O(4)	1.3328(18)
C(9)-O(1)	1.4689(17)	C(20)-O(4)	1.4458(18)
C(9)-C(10)	1.516(2)	C(20)-H(20A)	0.9800
C(9)-C(14)	1.549(2)	C(20)-H(20B)	0.9800
C(10)-C(11)	1.535(2)	C(20)-H(20C)	0.9800
C(10)-H(10A)	0.9900	C(21)-H(21A)	0.9800
C(10)-H(10B)	0.9900	C(21)-H(21B)	0.9800
C(11)-C(21)	1.527(2)	C(21)-H(21C)	0.9800
C(11)-C(12)	1.528(2)	O(2)-H(2)	0.8400
C(15)-C(1)-C(2)	107.98(12)	C(15)-C(1)-C(14)	114.18(12)
C(15)-C(1)-C(6)	108.89(12)	C(2)-C(1)-C(14)	110.84(12)
C(2)-C(1)-C(6)	107.79(12)	C(6)-C(1)-C(14)	106.97(11)

C(3)-C(2)-C(1)	113.43(12)	O(1)-C(9)-C(8)	108.71(11)
C(3)-C(2)-H(2A)	108.9	O(1)-C(9)-C(10)	106.55(11)
C(1)-C(2)-H(2A)	108.9	C(8)-C(9)-C(10)	114.04(12)
C(3)-C(2)-H(2B)	108.9	O(1)-C(9)-C(14)	106.32(11)
C(1)-C(2)-H(2B)	108.9	C(8)-C(9)-C(14)	108.48(12)
H(2A)-C(2)-H(2B)	107.7	C(10)-C(9)-C(14)	112.40(12)
C(2)-C(3)-C(4)	112.69(12)	C(9)-C(10)-C(11)	111.73(12)
C(2)-C(3)-H(3A)	109.1	C(9)-C(10)-H(10A)	109.3
C(4)-C(3)-H(3A)	109.1	C(11)-C(10)-H(10A)	109.3
C(2)-C(3)-H(3B)	109.1	C(9)-C(10)-H(10B)	109.3
C(4)-C(3)-H(3B)	109.1	C(11)-C(10)-H(10B)	109.3
H(3A)-C(3)-H(3B)	107.8	H(10A)-C(10)-H(10B)	107.9
C(3)-C(4)-C(5)	109.79(12)	C(21)-C(11)-C(12)	111.86(13)
C(3)-C(4)-C(16)	113.39(12)	C(21)-C(11)-C(10)	110.61(13)
C(5)-C(4)-C(16)	114.76(12)	C(12)-C(11)-C(10)	110.01(12)
C(3)-C(4)-H(4)	106.1	C(21)-C(11)-H(11)	108.1
C(5)-C(4)-H(4)	106.1	C(12)-C(11)-H(11)	108.1
C(16)-C(4)-H(4)	106.1	C(10)-C(11)-H(11)	108.1
O(2)-C(5)-O(1)	108.70(11)	C(11)-C(12)-C(13)	111.93(12)
O(2)-C(5)-C(4)	106.82(11)	C(11)-C(12)-H(12A)	109.2
O(1)-C(5)-C(4)	111.05(11)	C(13)-C(12)-H(12A)	109.2
O(2)-C(5)-C(6)	111.33(12)	C(11)-C(12)-H(12B)	109.2
O(1)-C(5)-C(6)	107.99(11)	C(13)-C(12)-H(12B)	109.2
C(4)-C(5)-C(6)	110.95(12)	H(12A)-C(12)-H(12B)	107.9
C(7)-C(6)-C(5)	107.43(12)	C(12)-C(13)-C(14)	110.62(12)
C(7)-C(6)-C(1)	108.57(12)	C(12)-C(13)-H(13A)	109.5
C(5)-C(6)-C(1)	108.81(12)	C(14)-C(13)-H(13A)	109.5
C(7)-C(6)-H(6)	110.6	C(12)-C(13)-H(13B)	109.5
C(5)-C(6)-H(6)	110.6	C(14)-C(13)-H(13B)	109.5
C(1)-C(6)-H(6)	110.6	H(13A)-C(13)-H(13B)	108.1
C(8)-C(7)-C(19)	125.81(14)	C(13)-C(14)-C(9)	110.68(12)
C(8)-C(7)-C(6)	113.30(13)	C(13)-C(14)-C(1)	116.95(12)
C(19)-C(7)-C(6)	120.88(13)	C(9)-C(14)-C(1)	108.80(11)
C(7)-C(8)-C(9)	113.40(13)	C(13)-C(14)-H(14)	106.6
C(7)-C(8)-H(8)	123.3	C(9)-C(14)-H(14)	106.6
C(9)-C(8)-H(8)	123.3	C(1)-C(14)-H(14)	106.6

C(1)-C(15)-H(15A)	109.5	C(11)-C(21)-H(21C)	109.5
C(1)-C(15)-H(15B)	109.5	H(21A)-C(21)-H(21C)	109.5
H(15A)-C(15)-H(15B)	109.5	H(21B)-C(21)-H(21C)	109.5
C(1)-C(15)-H(15C)	109.5	C(5)-O(1)-C(9)	114.37(10)
H(15A)-C(15)-H(15C)	109.5	C(5)-O(2)-H(2)	109.5
H(15B)-C(15)-H(15C)	109.5	C(19)-O(4)-C(20)	115.56(12)
C(18)-C(16)-C(17)	109.70(13)		
C(18)-C(16)-C(4)	114.77(13)		
C(17)-C(16)-C(4)	110.49(12)		
C(18)-C(16)-H(16)	107.2		
C(17)-C(16)-H(16)	107.2		
C(4)-C(16)-H(16)	107.2		
C(16)-C(17)-H(17A)	109.5		
C(16)-C(17)-H(17B)	109.5		
H(17A)-C(17)-H(17B)	109.5		
C(16)-C(17)-H(17C)	109.5		
H(17A)-C(17)-H(17C)	109.5		
H(17B)-C(17)-H(17C)	109.5		
C(16)-C(18)-H(18A)	109.5		
C(16)-C(18)-H(18B)	109.5		
H(18A)-C(18)-H(18B)	109.5		
C(16)-C(18)-H(18C)	109.5		
H(18A)-C(18)-H(18C)	109.5		
H(18B)-C(18)-H(18C)	109.5		
O(3)-C(19)-O(4)	123.98(14)		
O(3)-C(19)-C(7)	123.90(14)		
O(4)-C(19)-C(7)	112.12(13)		
O(4)-C(20)-H(20A)	109.5		
O(4)-C(20)-H(20B)	109.5		
H(20A)-C(20)-H(20B)	109.5		
O(4)-C(20)-H(20C)	109.5		
H(20A)-C(20)-H(20C)	109.5		
H(20B)-C(20)-H(20C)	109.5		
C(11)-C(21)-H(21A)	109.5		
C(11)-C(21)-H(21B)	109.5		
H(21A)-C(21)-H(21B)	109.5		

Symmetry transformations used to generate equivalent atoms:

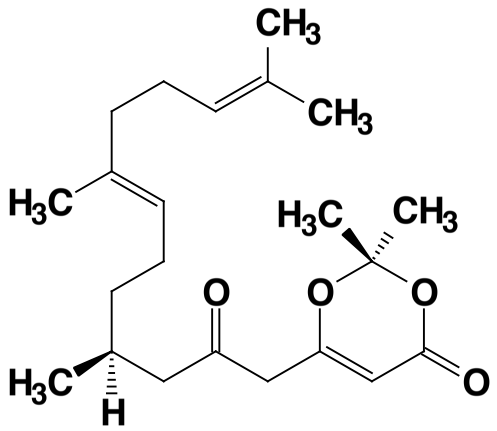
Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for maimone38. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	25(1)	20(1)	19(1)	0(1)	2(1)	-2(1)
C(2)	24(1)	24(1)	23(1)	2(1)	3(1)	-3(1)
C(3)	27(1)	25(1)	20(1)	2(1)	6(1)	-1(1)
C(4)	26(1)	19(1)	20(1)	2(1)	4(1)	-1(1)
C(5)	24(1)	18(1)	21(1)	2(1)	3(1)	1(1)
C(6)	26(1)	19(1)	21(1)	2(1)	4(1)	0(1)
C(7)	24(1)	23(1)	19(1)	1(1)	3(1)	0(1)
C(8)	23(1)	23(1)	18(1)	2(1)	2(1)	-1(1)
C(9)	25(1)	21(1)	19(1)	2(1)	2(1)	0(1)
C(10)	26(1)	20(1)	24(1)	1(1)	4(1)	0(1)
C(11)	26(1)	23(1)	23(1)	4(1)	7(1)	2(1)
C(12)	27(1)	28(1)	22(1)	5(1)	2(1)	2(1)
C(13)	26(1)	27(1)	20(1)	2(1)	0(1)	-1(1)
C(14)	23(1)	21(1)	18(1)	1(1)	3(1)	0(1)
C(15)	35(1)	23(1)	23(1)	-2(1)	1(1)	-4(1)
C(16)	26(1)	26(1)	23(1)	-1(1)	3(1)	-3(1)
C(17)	37(1)	32(1)	19(1)	0(1)	2(1)	1(1)
C(18)	57(1)	26(1)	27(1)	-5(1)	5(1)	-6(1)
C(19)	26(1)	22(1)	21(1)	0(1)	2(1)	0(1)
C(20)	33(1)	27(1)	26(1)	-4(1)	10(1)	1(1)
C(21)	34(1)	26(1)	31(1)	7(1)	6(1)	3(1)
O(1)	27(1)	19(1)	17(1)	1(1)	2(1)	0(1)
O(2)	22(1)	26(1)	23(1)	4(1)	4(1)	1(1)
O(3)	51(1)	24(1)	33(1)	4(1)	18(1)	9(1)
O(4)	31(1)	23(1)	22(1)	2(1)	9(1)	4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for maimone38.

	x	y	z	U(eq)
H(2A)	9088	6922	5432	28
H(2B)	9963	6164	5873	28
H(3A)	8874	5243	4442	28
H(3B)	9155	6056	3629	28
H(4)	7285	6587	3725	26
H(6)	6986	6901	6015	26
H(8)	6033	4959	8177	26
H(10A)	7682	3532	6319	28
H(10B)	6442	3595	6860	28
H(11)	7380	3822	9003	29
H(12A)	9570	3685	7971	31
H(12B)	9446	3801	9486	31
H(13A)	9891	5109	8550	29
H(13B)	8643	5157	9079	29
H(14)	8974	4874	6414	25
H(15A)	9664	6575	8159	41
H(15B)	8379	6553	8593	41
H(15C)	8710	7260	7604	41
H(16)	6091	5570	2443	30
H(17A)	8254	6001	1522	44
H(17B)	7135	6605	1447	44
H(17C)	7070	5760	603	44
H(18A)	6930	4377	1670	55
H(18B)	7029	4311	3228	55
H(18C)	8154	4564	2551	55
H(20A)	4991	7478	9689	42
H(20B)	4536	6717	10501	42
H(20C)	3800	7003	9148	42
H(21A)	8275	2357	7870	45
H(21B)	7051	2411	8445	45
H(21C)	8258	2480	9406	45

H(2)	5088	5689	5075	36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H3C
CH3
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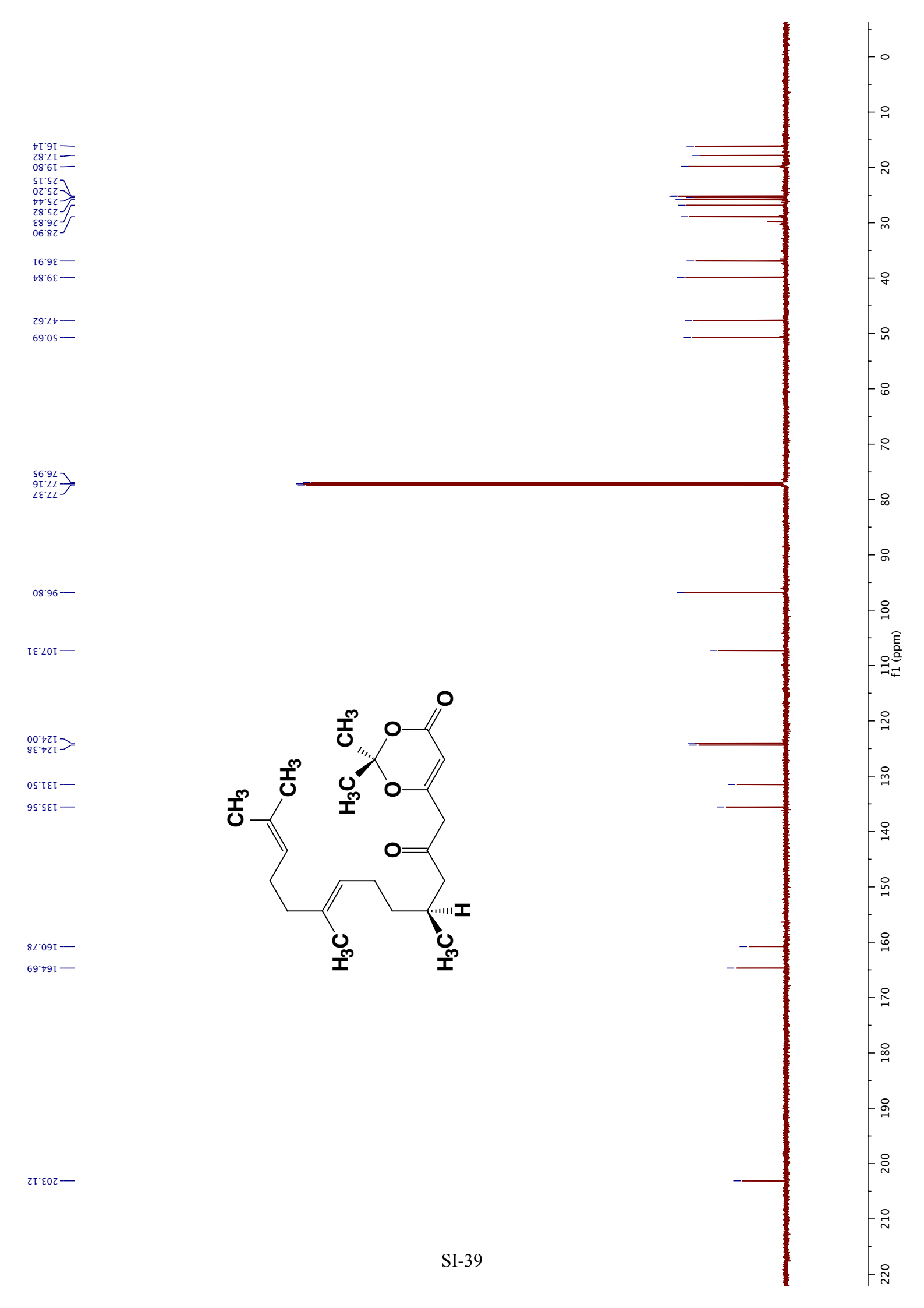
O
O
O
H3C
H

7.26 5.32 5.09 5.09 5.08 5.08 5.08 5.07 5.07 5.07 5.06 5.06 5.06 5.06 5.05 5.05 3.32 3.29 3.26 2.50 2.49 2.47 2.46 2.32 2.31 2.29 2.27 2.07 2.07 2.07 2.07 2.05 2.04 2.04 2.04 2.03 2.03 2.02 2.02 2.01 2.01 2.01 2.01 2.00 1.99 1.99 1.98 1.98 1.97 1.96 1.95 1.95 1.94 1.94 1.92 1.70 1.67 1.66 1.66 1.66 1.59 1.58 1.58 1.58 1.35 1.33 1.33 1.32 1.32 1.32 1.31 1.31 1.30 1.30 1.30 1.29 1.29 1.28 1.24 1.24 1.23 1.23 1.22 1.22 1.21 1.21 1.20 1.20 1.20 1.19 1.19 1.18 1.17 0.91 0.90
0.95
1.97
2.02
1.00
1.00
7.14
6.13
3.12
6.08
1.06
1.10
3.07
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
f1 (ppm)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76.95
77.16
77.37
96.80
107.31
124.00
124.38
131.50
135.56
160.78
164.69
203.12
CH3
CH3
CH3
H3C
H3C
H
O
O
O
O
220
210
200
190
180
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110
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90
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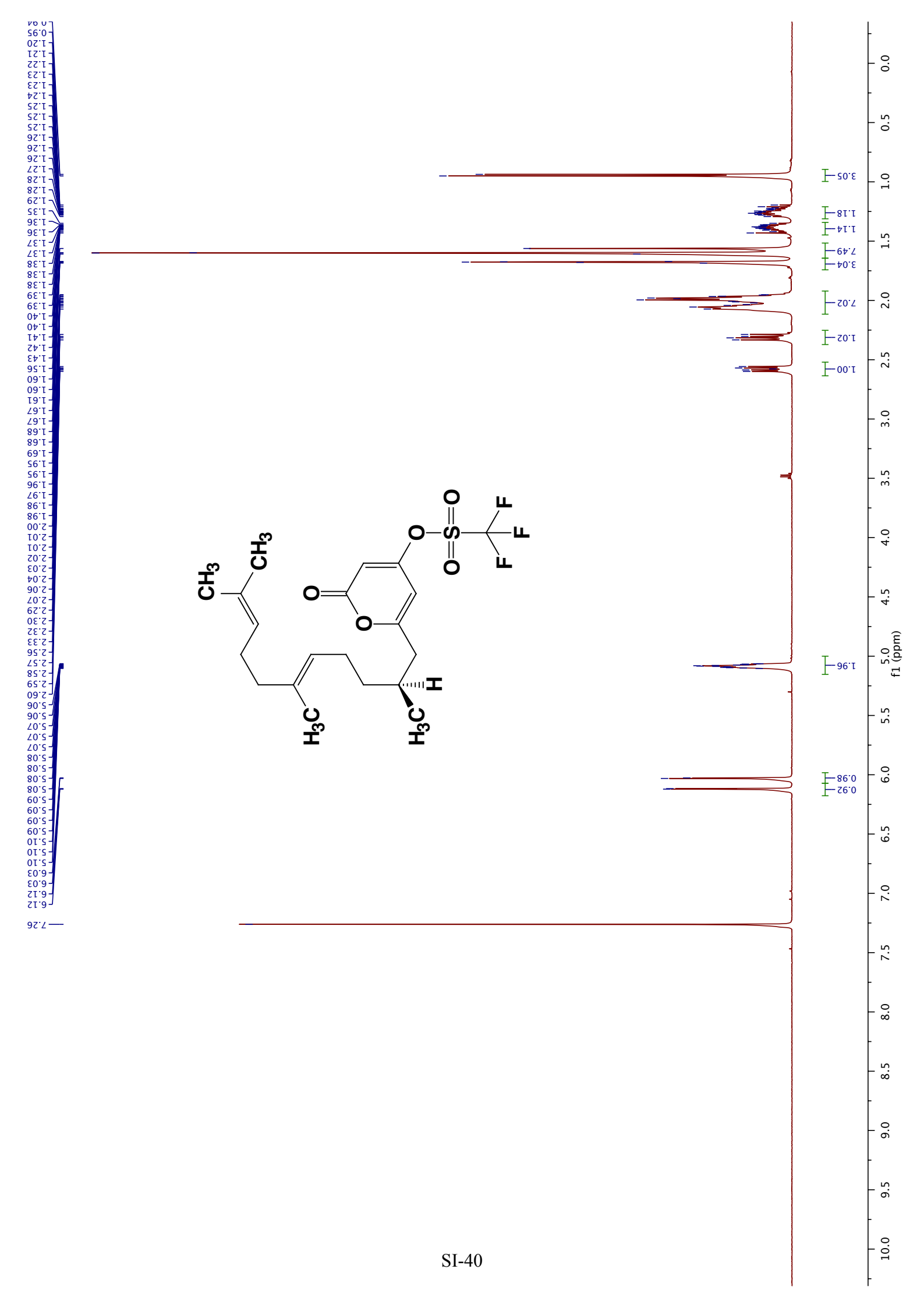
50
40
30
20
10
0
f1 (ppm)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1.00
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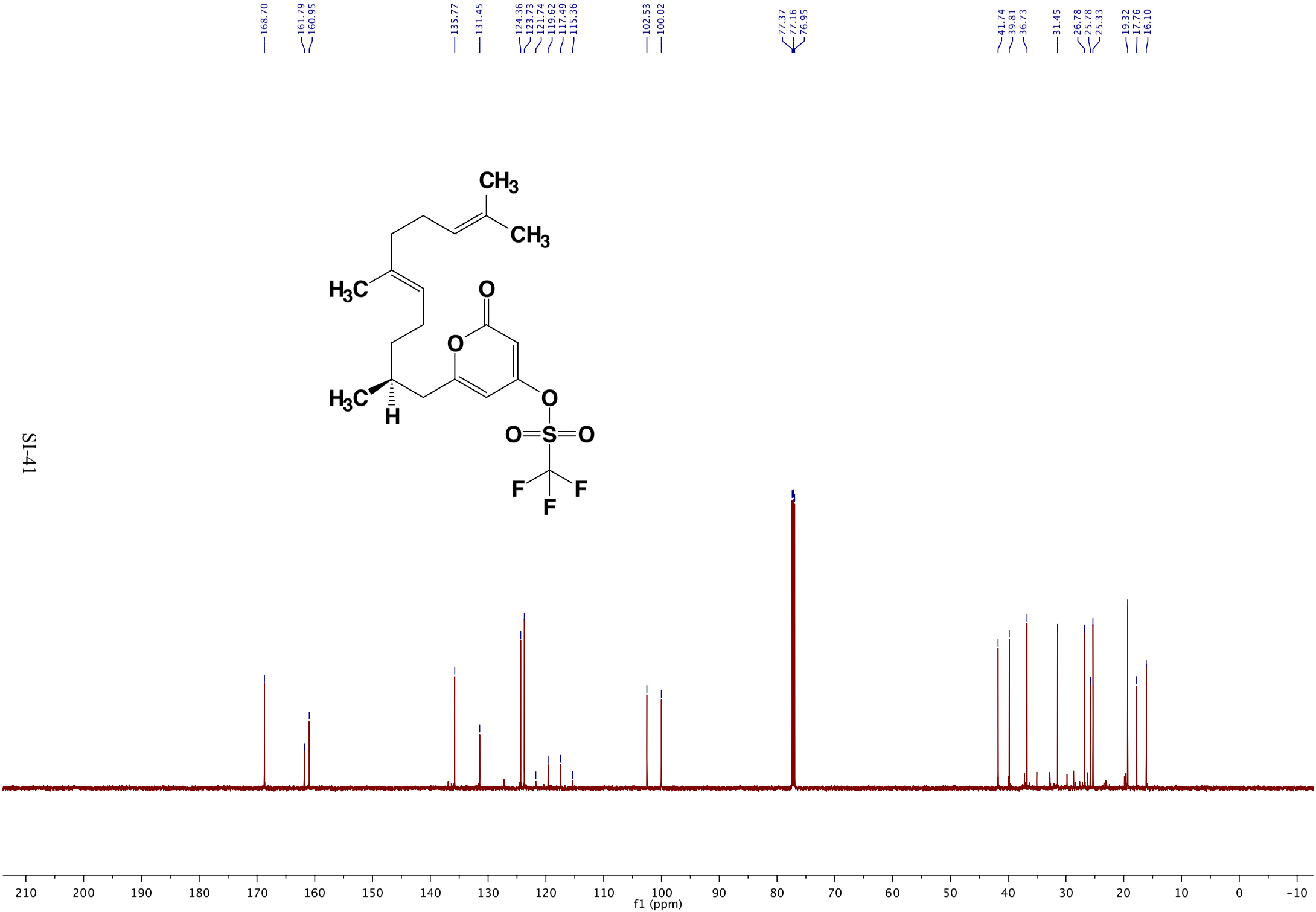
0.98
0.92
f1 (ppm)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124.36
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121.74
119.62
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115.36
102.53
100.02
77.37
77.16
76.95
41.74
39.81
36.73
31.45
26.78
25.78
25.33
19.32
17.76
16.10
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CH3
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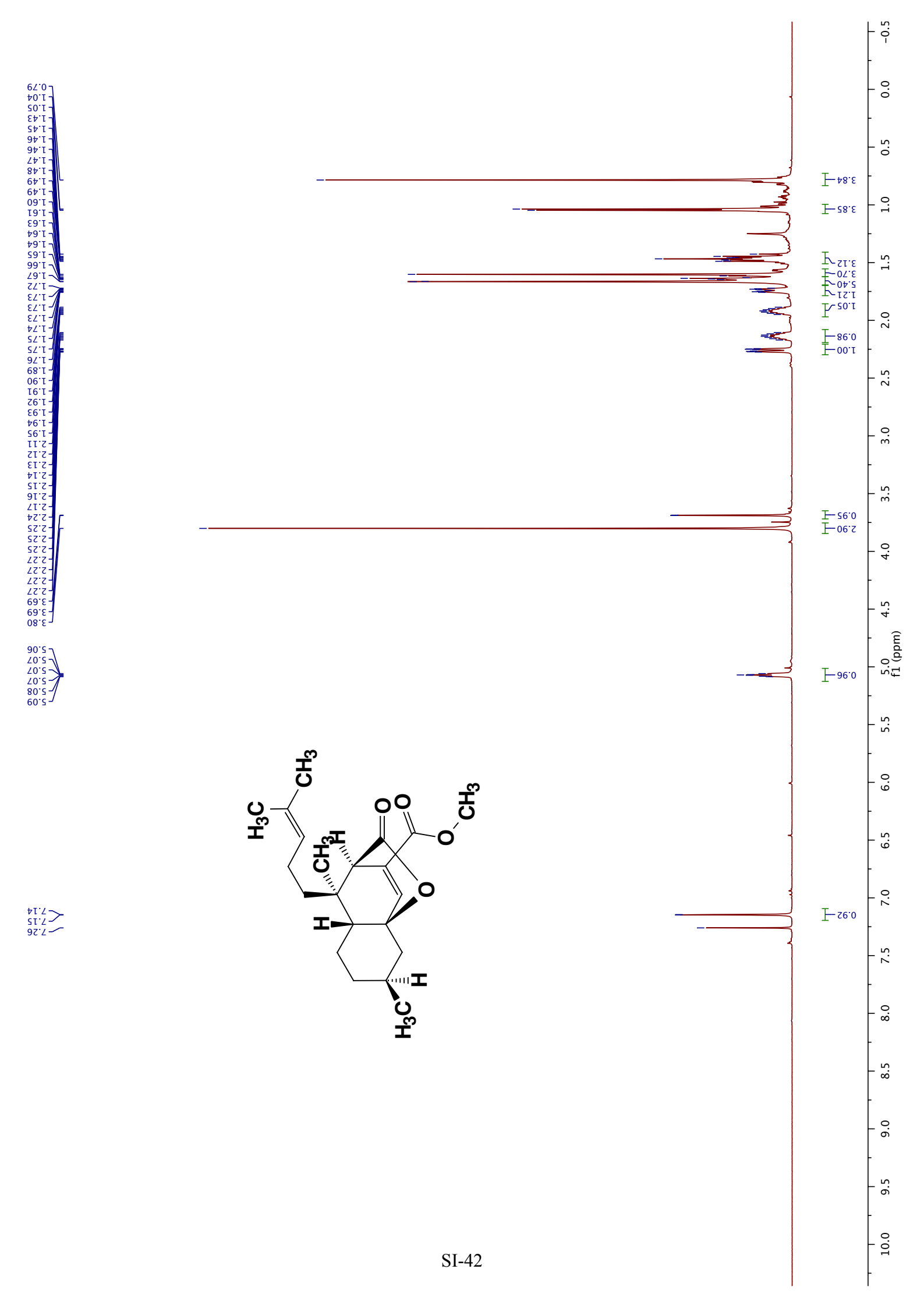
O
O
H3C
H
O
O=S=O
F
F
F
f1 (ppm)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1.94
1.95
2.11
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2.13
2.14
2.15
2.16
2.17
2.24
2.25
2.25
2.25
2.27
2.27
2.27
2.27
3.69
3.69
3.80
5.06
5.07
5.07
5.07
5.08
5.09
7.14
7.15
7.26
3.84
3.85
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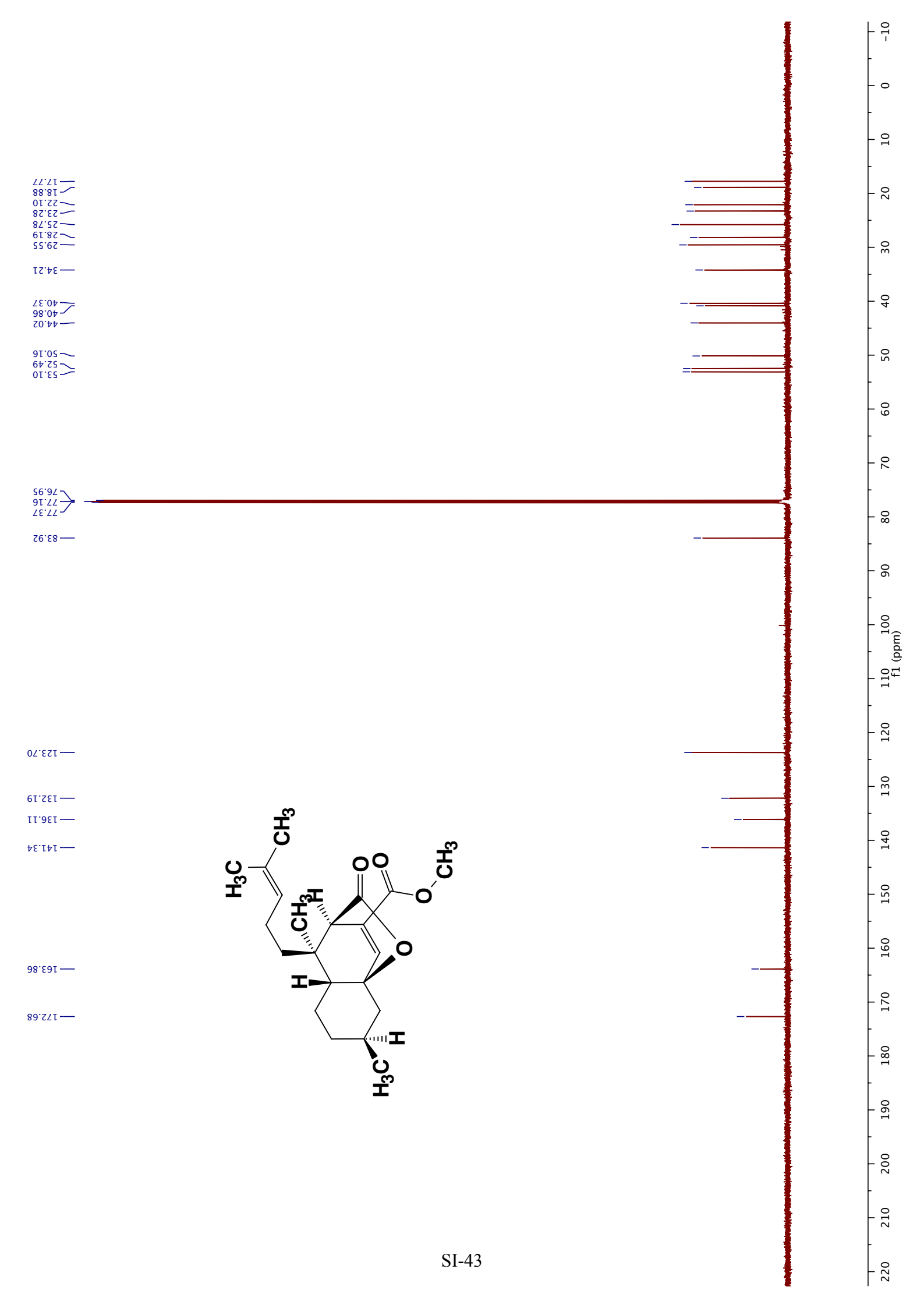
1.05
0.98
1.00
0.95
2.90
0.96
0.92
f1 (ppm)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44.02
50.16
52.49
53.10
76.95
77.16
77.37
83.92
123.70
132.19
136.11
141.34
163.86
172.68
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CH3
CH3
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H
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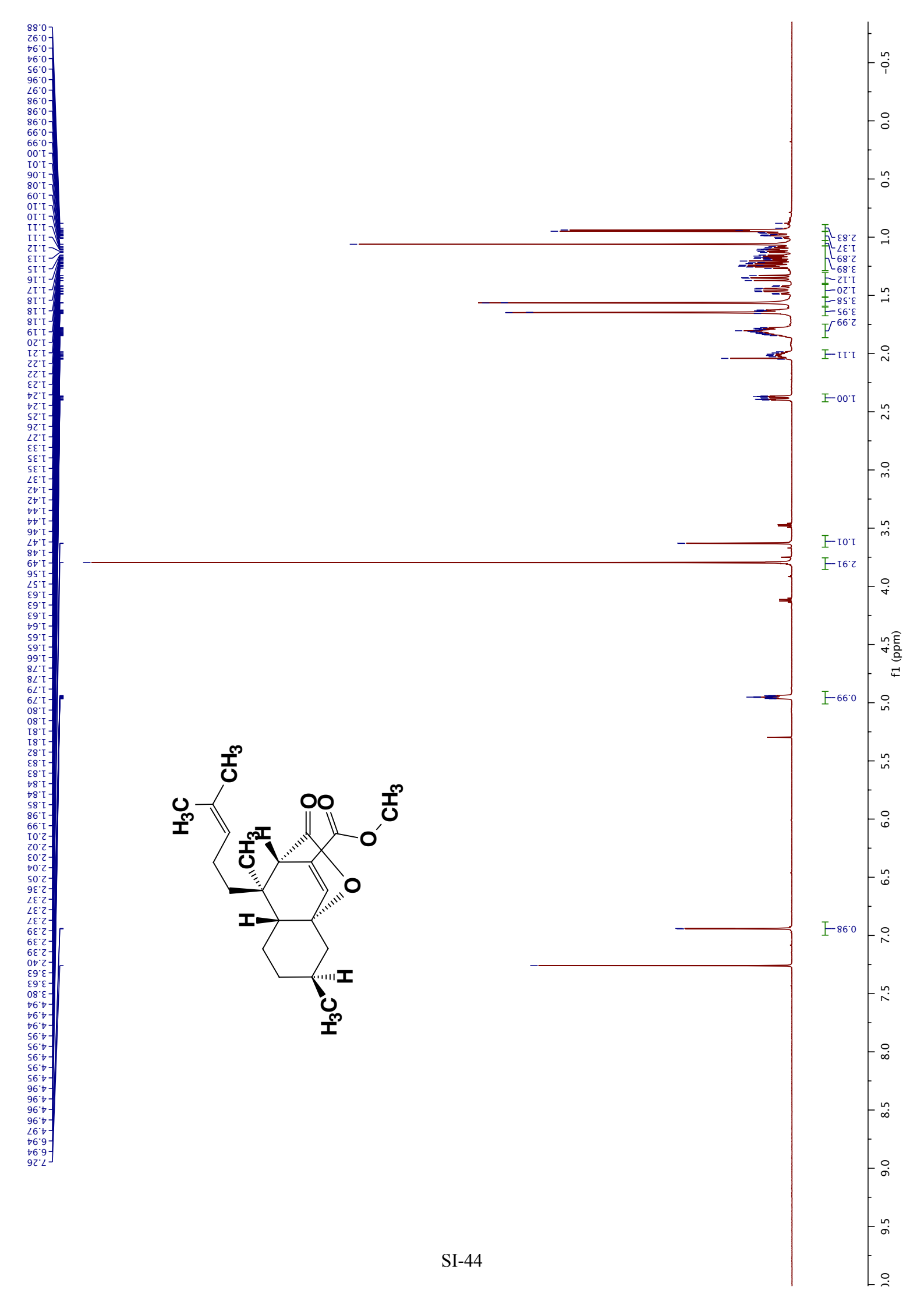
O
O
O
CH3
H3C
f1 (ppm)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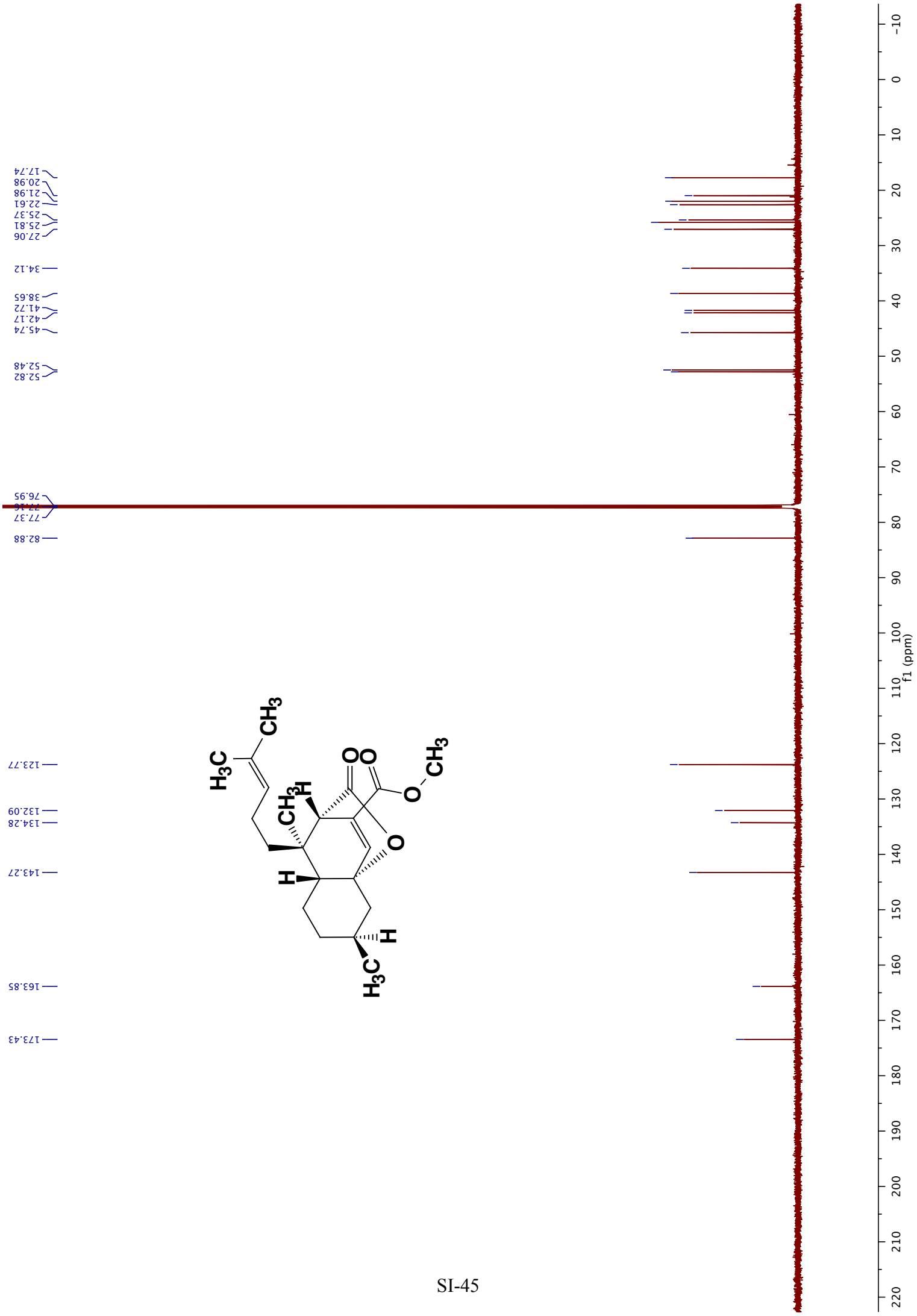
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34.12
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42.17
45.74
52.48
52.82
76.95
77.16
77.37
82.88
123.77
132.09
134.28
143.27
163.85
173.43
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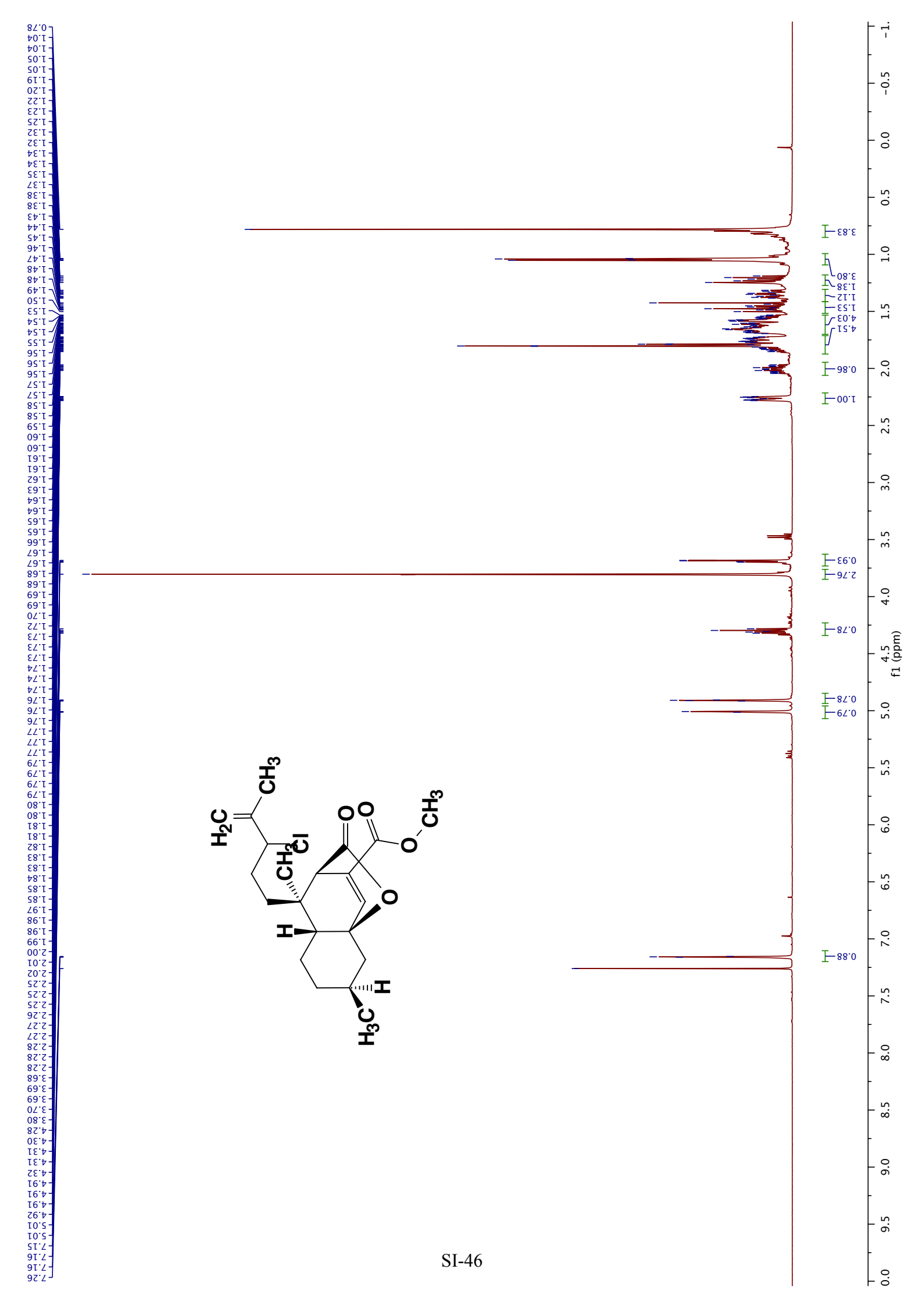
CH3
CH3
H
H
H3C
O
O
O
O
CH3
f1 (ppm)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4.51
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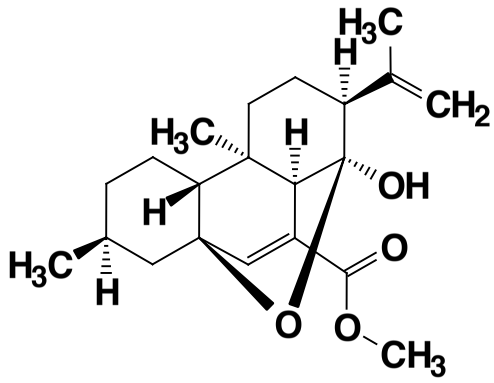
1.00
0.93
2.76
0.78
0.78
0.79
0.88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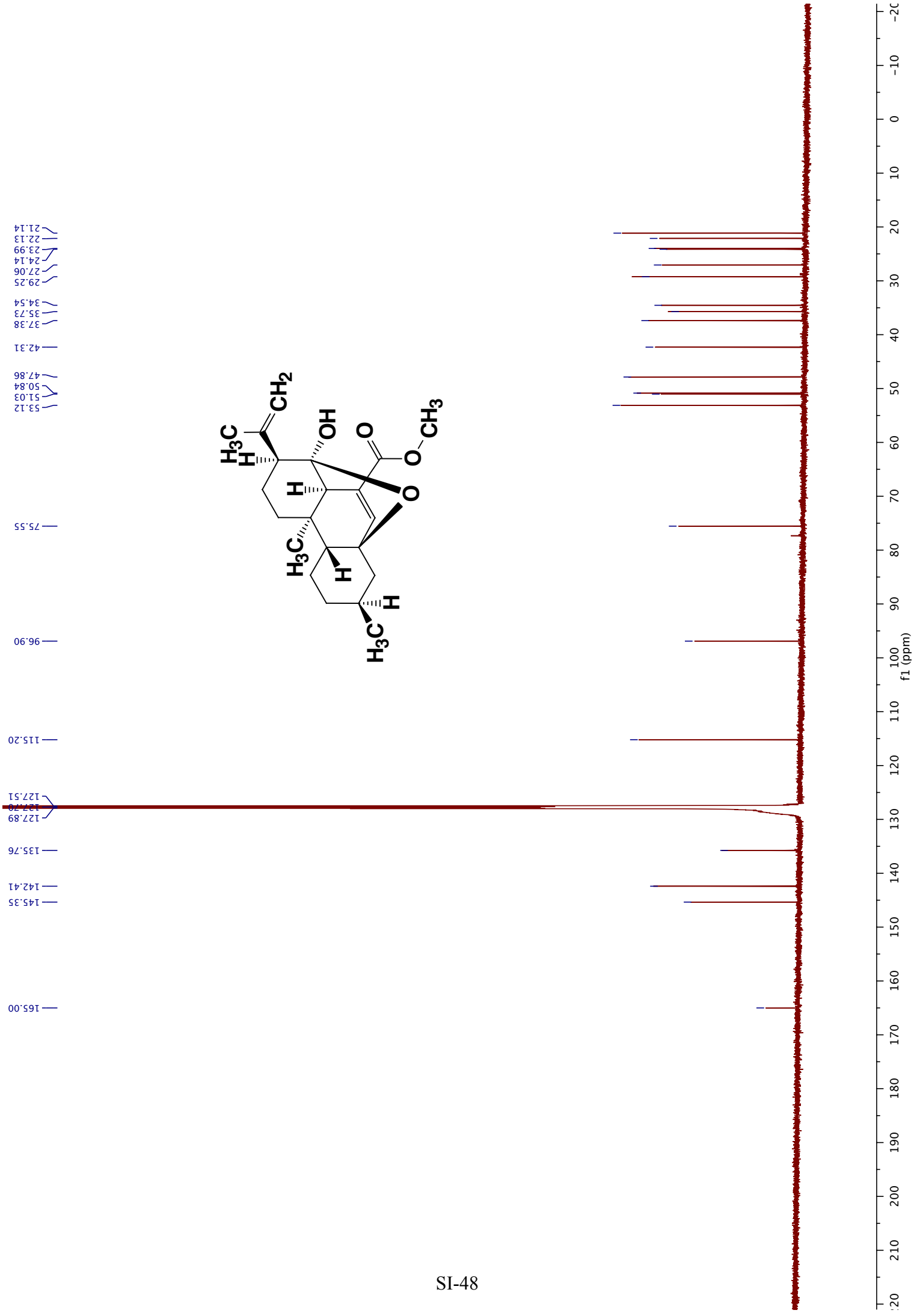
H3C
H
OH
H
H3C
H
O
O
O
CH3

f1 (ppm)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23.99
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27.06
29.25
34.54
35.73
37.38
42.31
47.86
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53.12
75.55
96.90
115.20
127.51
127.70
127.89
135.76
142.41
145.35
165.00
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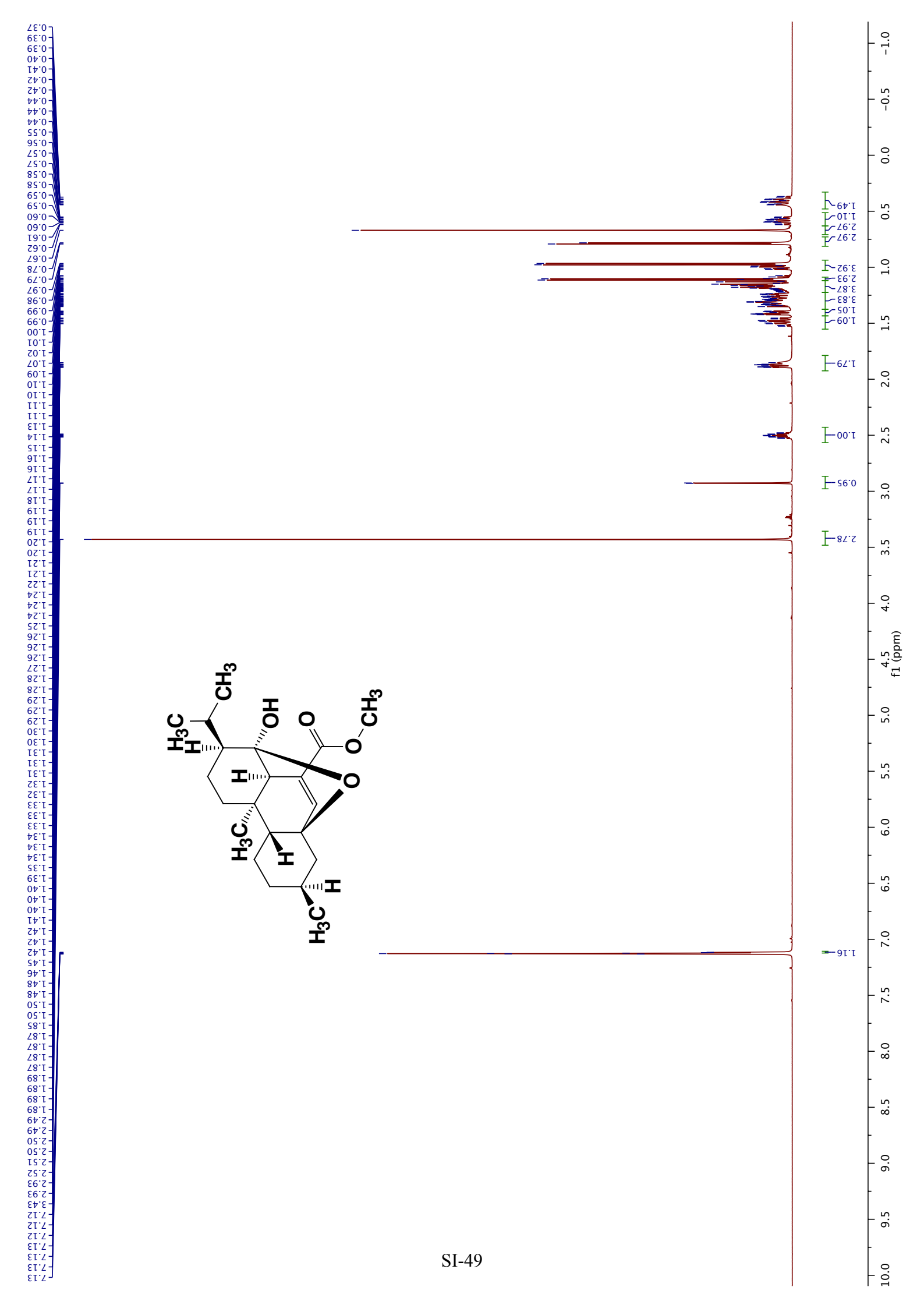
OH
O
O
CH3
H3C
H
H
H3C
H
H3C
H
f1 (ppm)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H
OH
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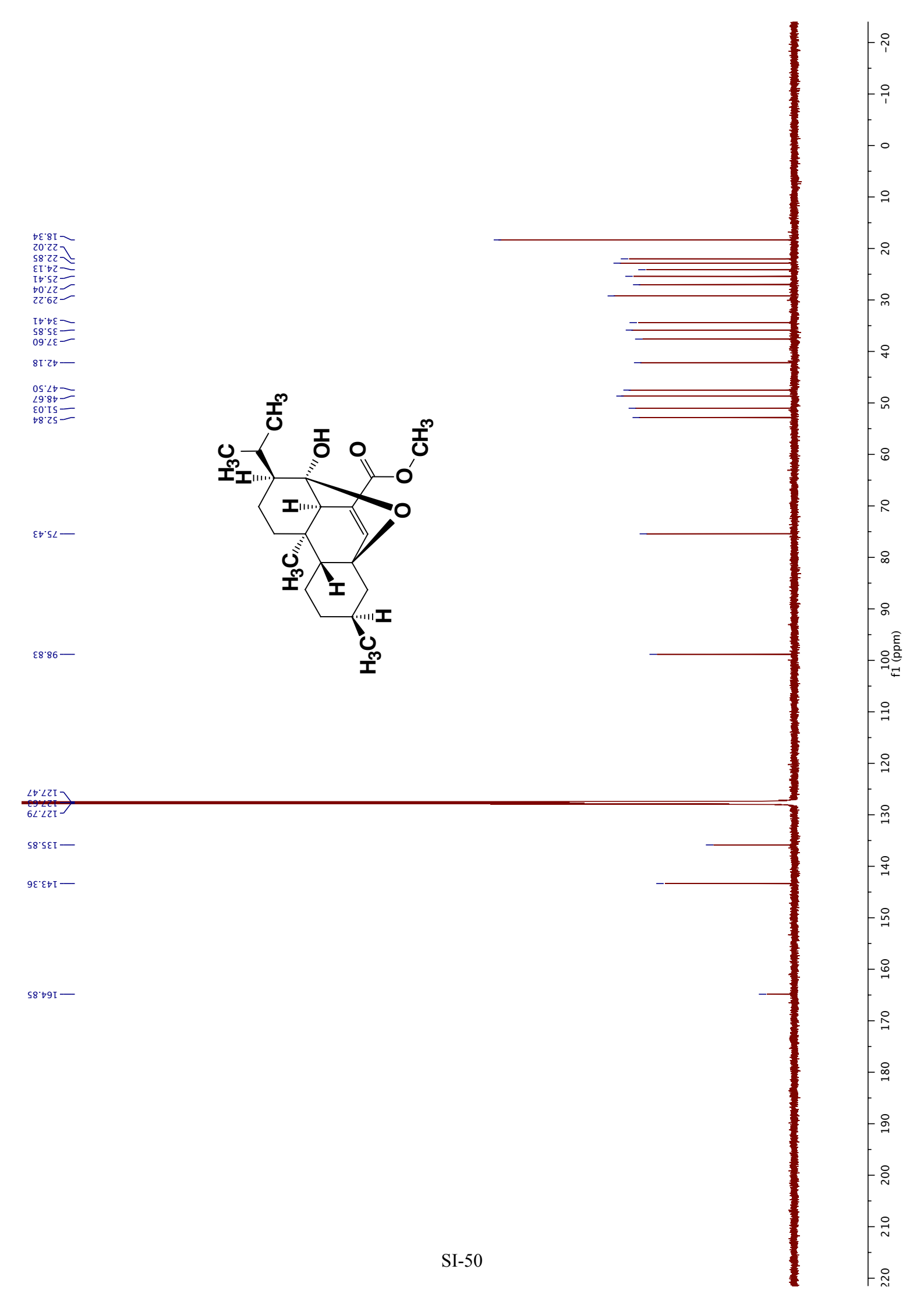
O
H
H3C
H
H3C
H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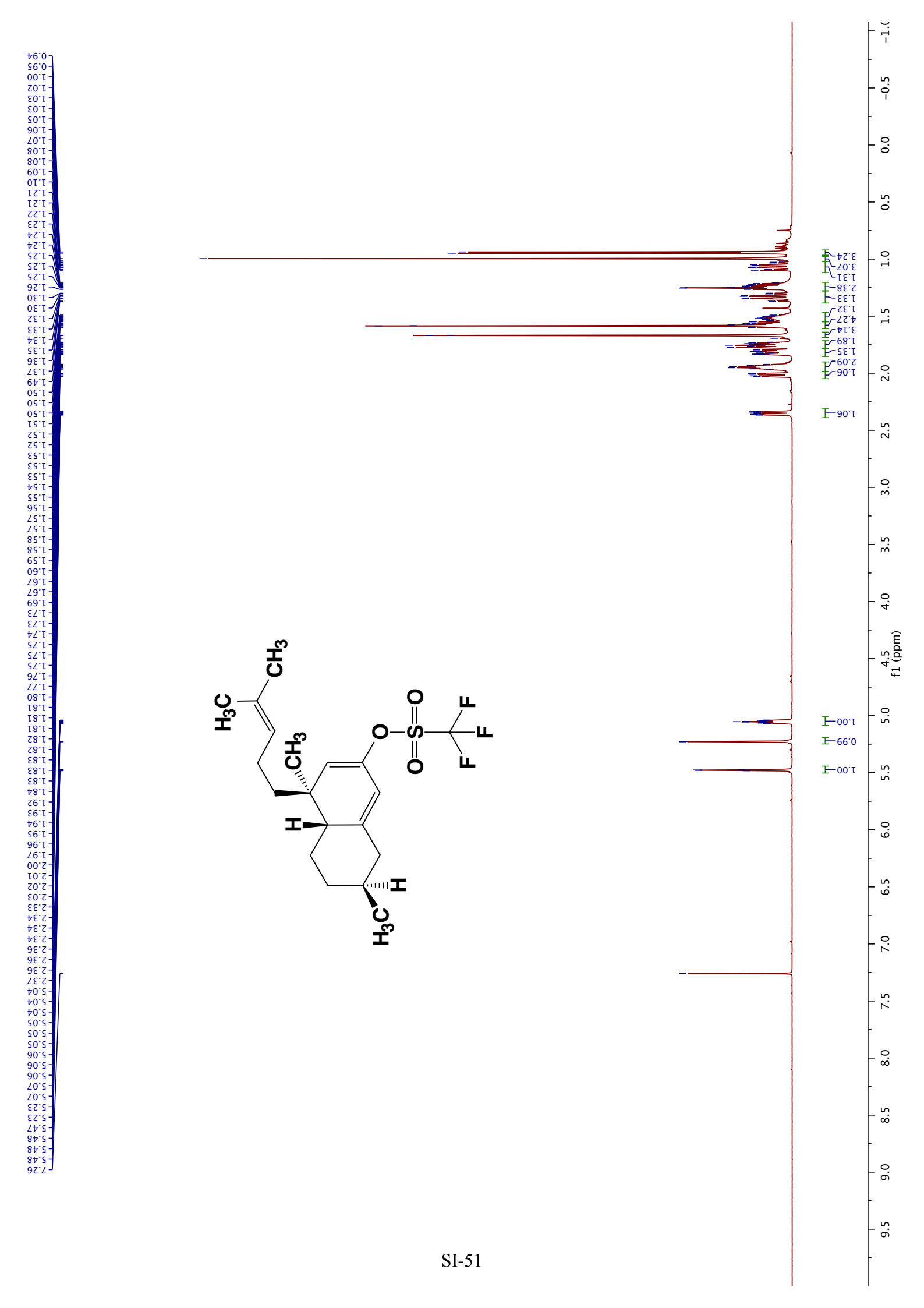
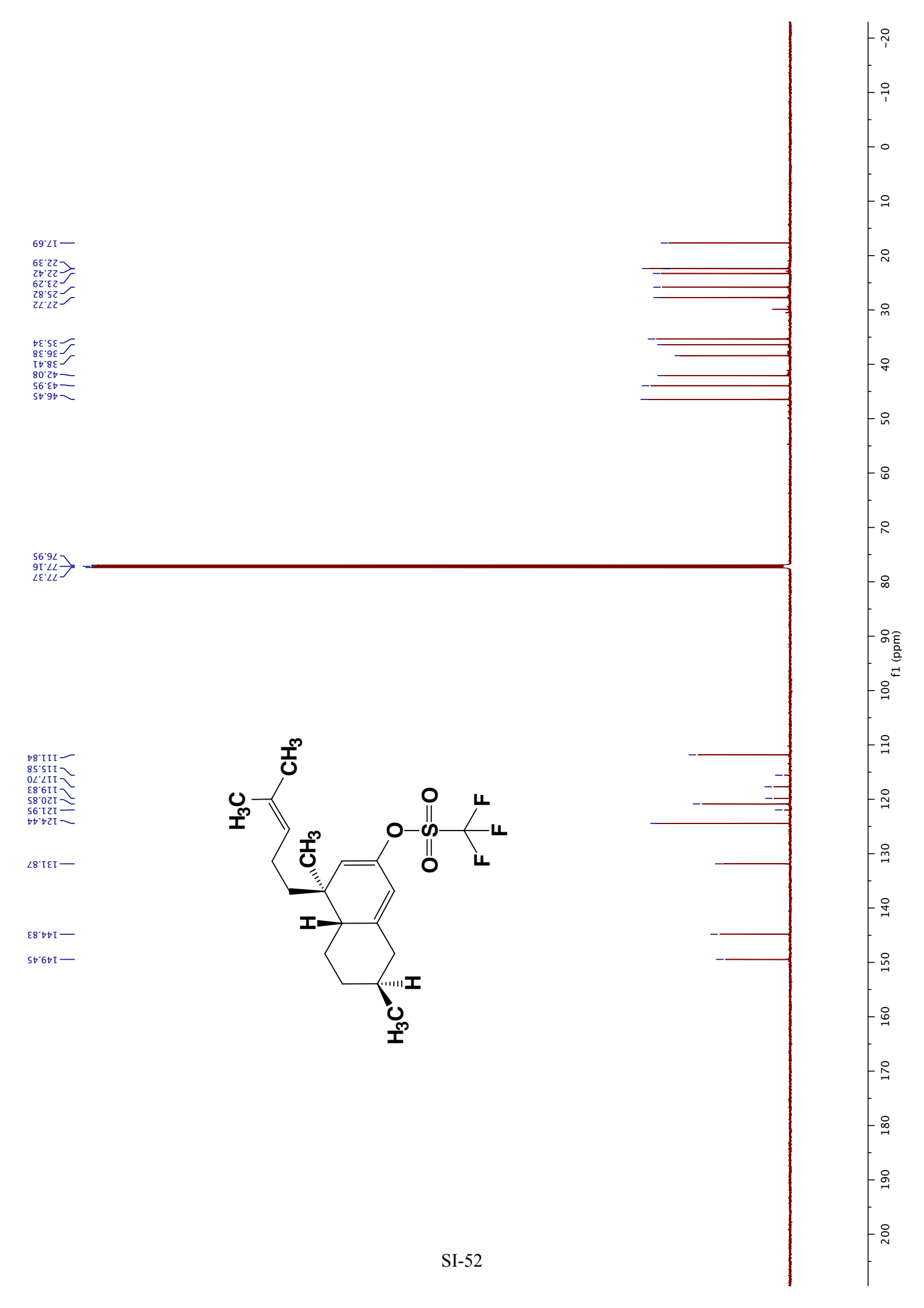
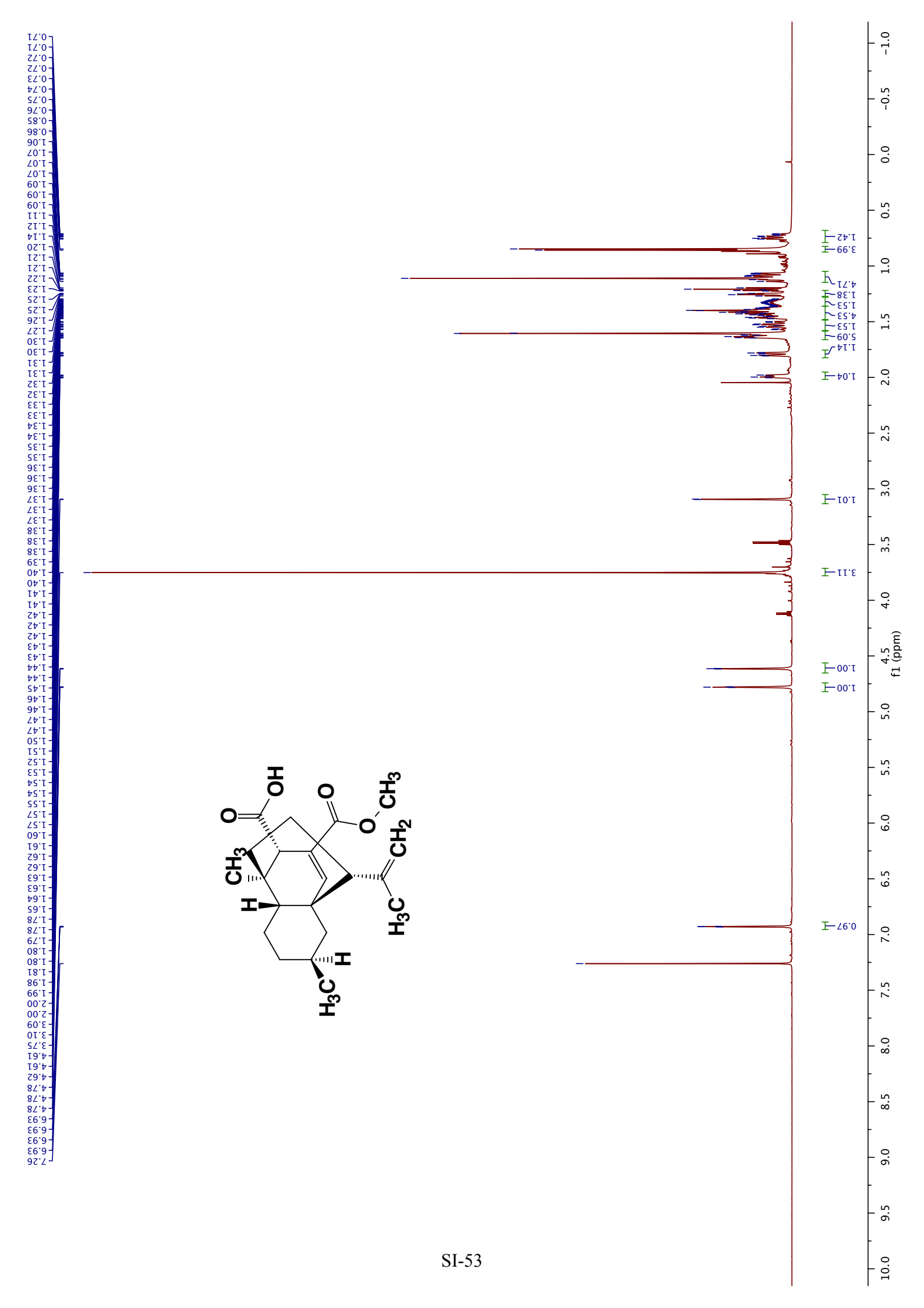
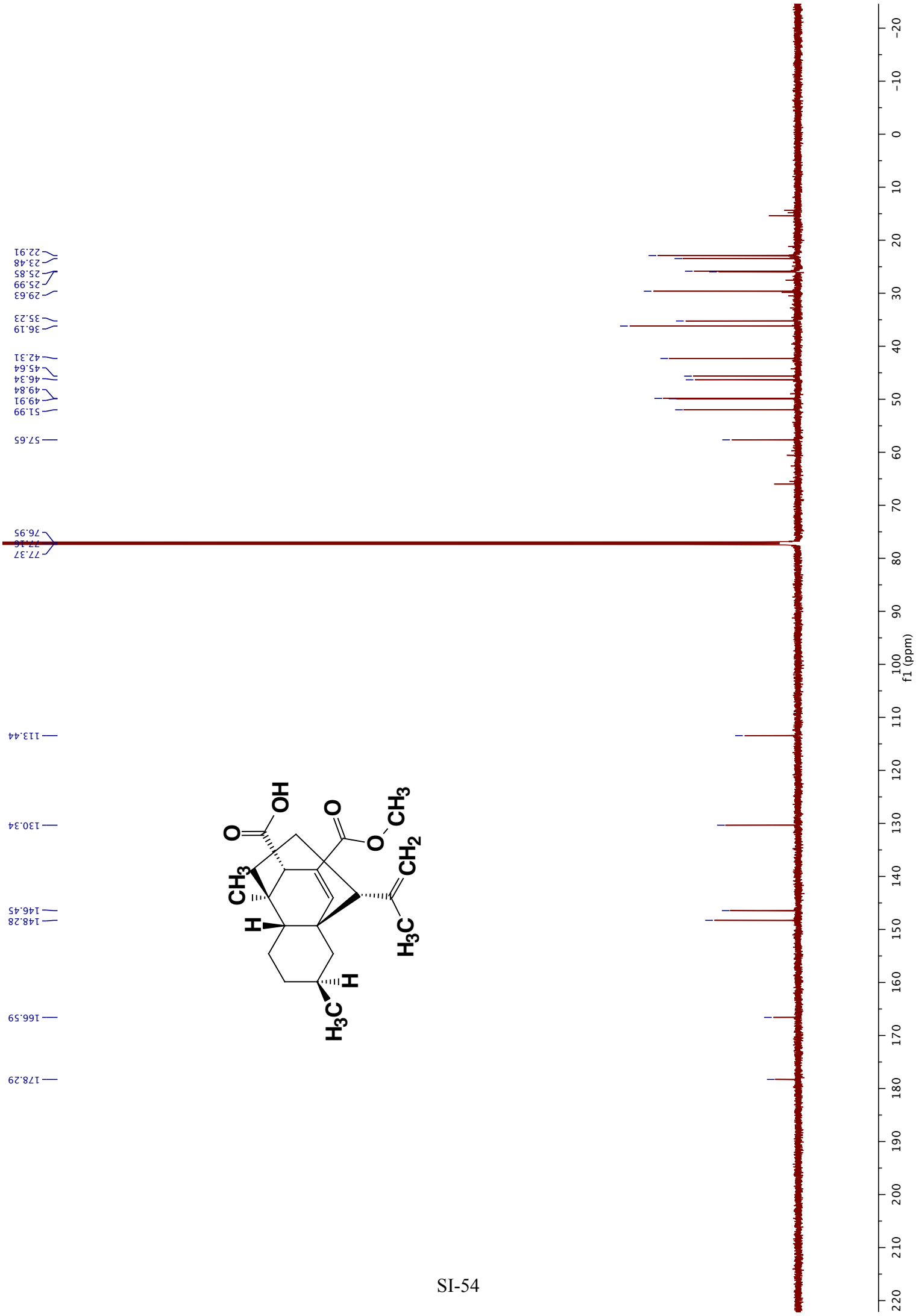
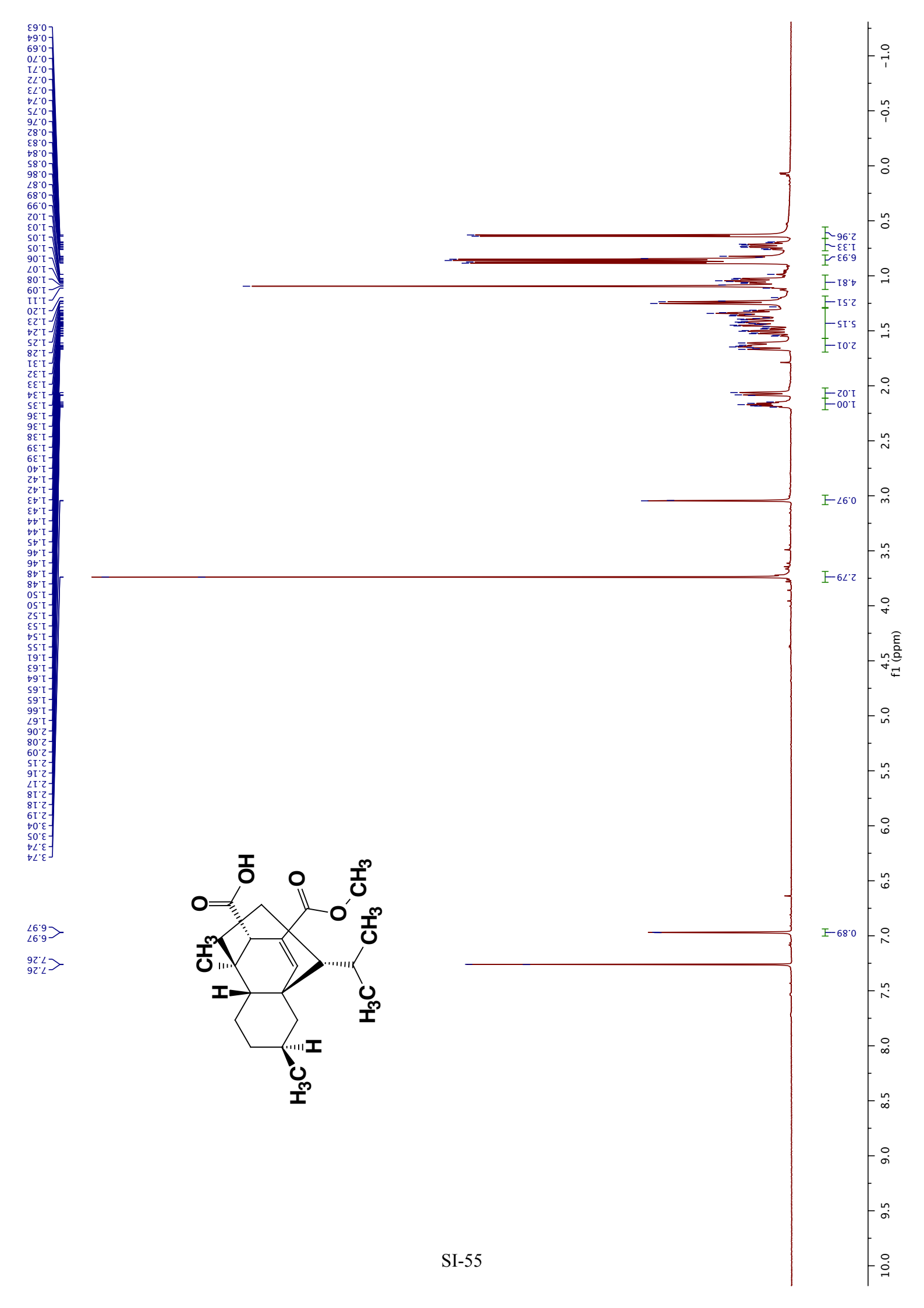
51.03
52.84
75.43
98.83
127.47
127.63
127.79
135.85
143.36
164.85
H3C
CH3
H
OH
O
O
CH3
H
H3C
H
H3C
H
-20
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
f1 (ppm)

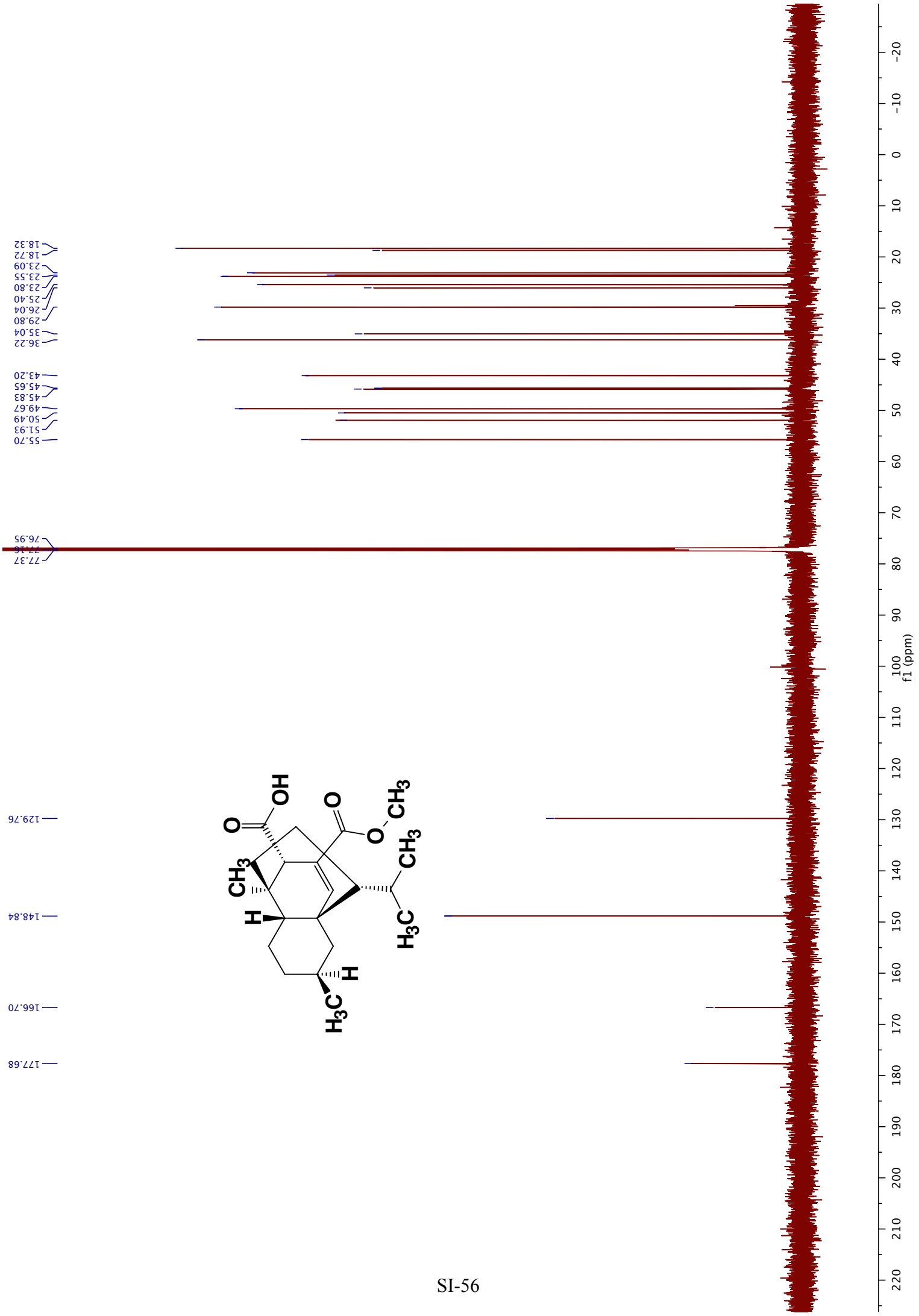

f1 (ppm)


17.69
22.39
22.42
23.29
25.82
27.72
35.34
36.38
38.41
42.08
43.95
46.45
76.95
77.16
77.37
111.84
115.58
117.70
119.83
120.85
121.95
124.44
131.87
144.83
149.45
H3C
CH3
CH3
H
H3C
O
S
O
O
F
F
F
f1 (ppm)

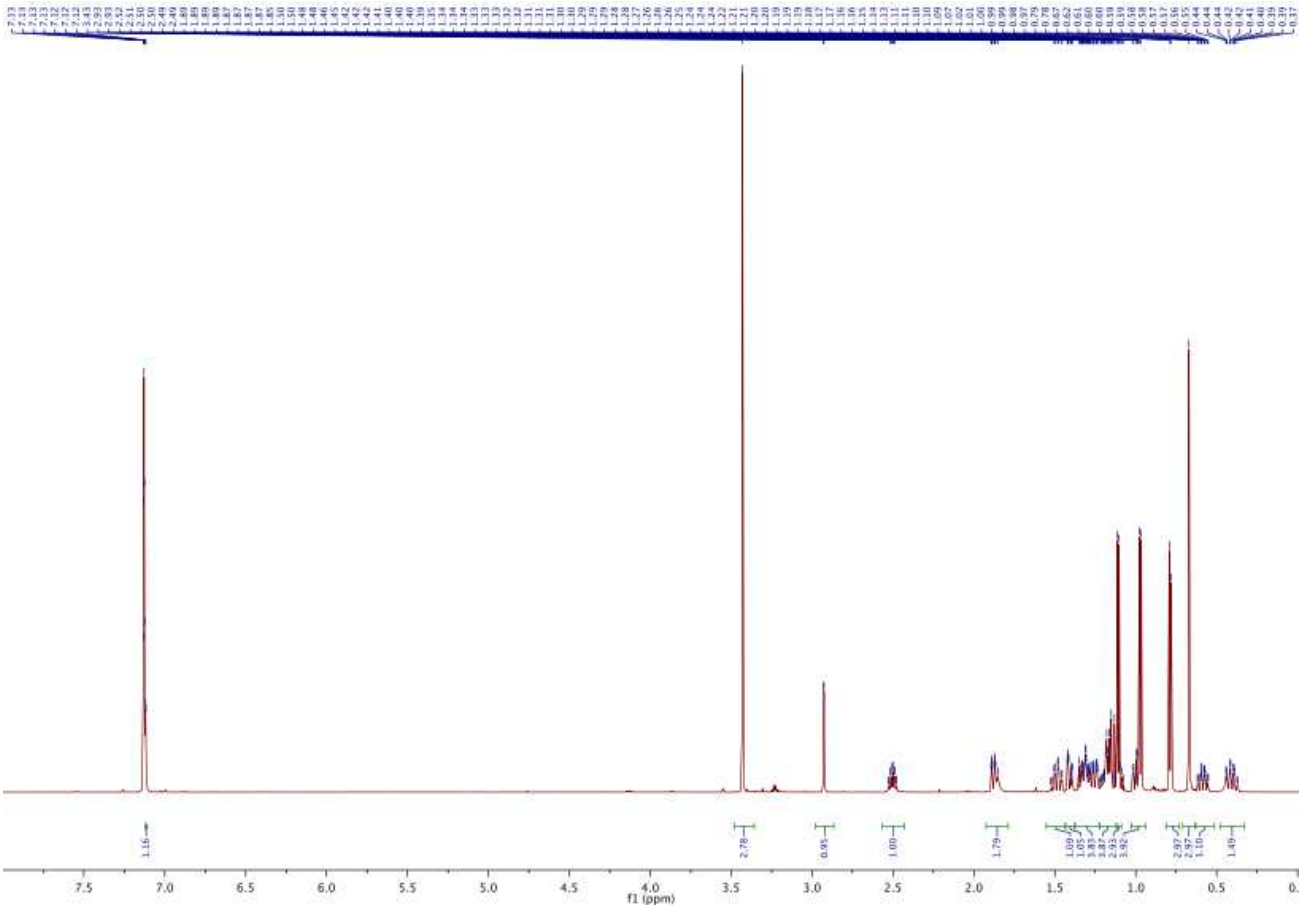

O
OH
O
O
CH3
CH3
H
CH2
H3C
H3C
H
f1 (ppm)


22.91
23.48
25.85
25.99
29.63
35.23
36.19
42.31
45.64
46.34
49.84
49.91
51.99
57.65
76.95
77.16
77.37
113.44
130.34
146.45
148.28
166.59
178.29
O
OH
O
O
CH3
CH3
CH2
H
H3C
H3C
H
-20
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
f1 (ppm)


f1 (ppm)
2.96
1.33
6.93
4.81
2.51
5.15
2.01
1.02
1.00
0.97
2.79
0.89
O
OH
O
O
CH3
CH3
H
H3C
H3C
H


18.32
18.72
23.09
23.55
23.80
25.40
26.04
29.80
35.04
36.22
43.20
45.65
45.83
49.67
50.49
51.93
55.70
76.95
77.16
77.37
129.76
148.84
166.70
177.68
OH
O
O
O
CH3
CH3
H
H3C
H3C
H
f1 (ppm)

Synthetic Chatancin: ^{1}H NMR in C_6D_6 (this work)



Synthetic Chatancin: ^{1}H NMR in C_6D_6 (from Ref. 9)