

Supporting Information

Synthesis and Evaluation of Antimicrobial Activity of the Rearranged Abietane Prattinin A and its Synthetic Derivatives

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Table S1. Energies of the HOMO, LUMO, energy gap, and global chemical reactivity indices of the synthesized compounds.

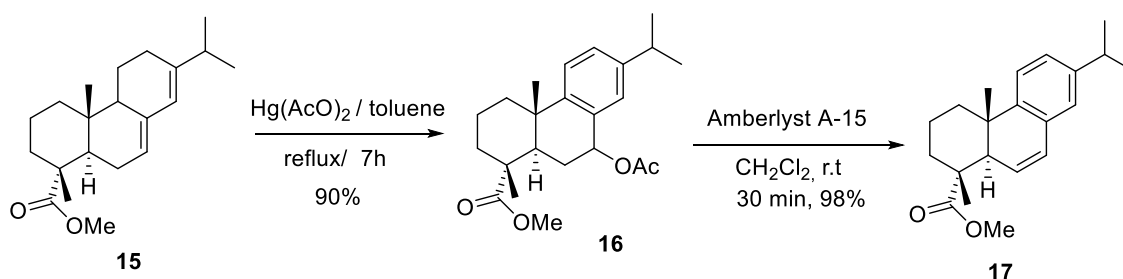
Compounds	E _{HOMO} (eV)	E _{LUMO} (eV)	ΔE	IP	EA	μ	η	σ	ω	χ
24	-5.58	0.064	5.644	5.58	-0.064	-2.758	2.822	0.354	0.673	2.758
25	-6.345	-3.217	3.128	6.345	3.217	-4.781	1.564	0.639	3.653	4.781
26	-6.553	-1.935	4.618	6.553	1.935	-4.244	2.309	0.433	1.950	4.244
27	-8.81	-1.195	7.615	8.81	1.195	-5.002	3.807	0.262	1.643	5.002
28	-5.603	-0.784	4.819	5.603	0.784	-3.193	2.409	0.415	1.058	3.193
29	-5.953	-1.346	4.607	5.953	1.346	-3.649	2.303	0.434	1.445	3.649
30	-5.522	-0.654	4.868	5.522	0.654	-3.088	2.434	0.410	0.979	3.088
31	-5.784	-1.22	4.564	5.784	1.22	-3.502	2.282	0.438	1.343	3.502
33	-5.339	-0.842	4.497	5.339	0.842	-3.090	2.248	0.444	1.061	3.090
34	-5.719	-1.412	4.307	5.719	1.412	-3.565	2.153	0.464	1.475	3.565

General Procedures

Except where otherwise indicated, The reactions were carried out under argon atmosphere using dry solvents. Solvents were dried as follows: THF and dioxane over Na–benzophenone, toluene over Na, dichloromethane (DCM) over CaH₂. Thin-layer chromatography (TLC) was performed using F254 precoated plates (0.25 mm) and visualized by UV fluorescence quenching and phosphomolybdic acid solution staining. Flash chromatography was performed on silica gel (230–400 mesh). Chromatography separations were carried out by conventional column on silica gel 60 (230–400 Mesh), using hexanes–AcOEt (AcOEt–hexane) mixtures of increasing polarity. ¹H and ¹³C NMR spectra were recorded at 500 and 400 MHz, and at 125 and 100 MHz, respectively. CDCl₃ was treated with K₂CO₃. Chemical shifts (δ H) are quoted in parts per million (ppm) referenced to the appropriate residual solvent peak and tetramethylsilane. Data for ¹H NMR spectra are reported as follows: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration), with the abbreviations s, br s, d, br d, t, q, sext and m denoting singlet, broad singlet, doublet, broad doublet, triplet, quartet, sextet and multiplet, respectively. J = coupling constant in Hertz (Hz). Data for ¹³C NMR spectra are reported in terms of chemical shift relative to Me₄Si (δ 0.0) and the signals were assigned utilizing DEPT experiments and on the basis of heteronuclear correlations. Infrared spectra (IR) were recorded as thin films or as solids on a FTIR spectrophotometer with samples between sodium chloride plates or as potassium bromide pellets and are reported in frequency of absorption (cm^{–1}). HRMS were recorded on a spectrometer, utilizing a Q-TOF analyzer, and ESI⁺ ionization.

Experimental Procedures

Synthesis of compounds 16, and 17 from 15

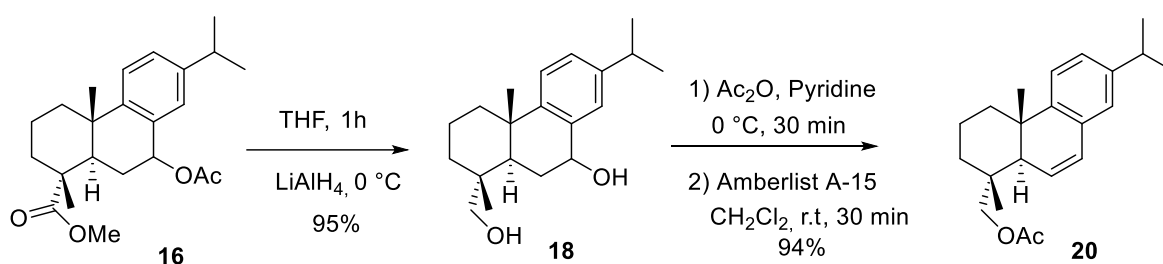


To a solution of compound **15** (1.3 g, 4.11 mmol) in toluene (10 mL) was added $\text{Hg}(\text{OAc})_2$ (2.65g, 8.28 mmol) and the mixture was stirred at reflux for 7 hours, at which time TLC showed no starting material. Then, the mixture was filtered, and the solvent was removed

under vacuum. The resulting crude product was purified by flash column chromatography, using 5% EtOAc/hexanes to afford product **16**¹ (1.37 g, 90%) as a white solid.

To a solution of **16** (0.5 g, 1.34 mmol) in DCM (8 mL), was added Amberlyst A-15 (0.3 g) and the mixture was stirred at room temperature for 30 min, at which time TLC showed no starting material. Then, the mixture was filtered and the solvent was removed under vacuum to give a crude product which was purified by column chromatography using 2% EtOAc/hexanes to afford product **17**² (410 mg, 98%) as a colourless syrup.

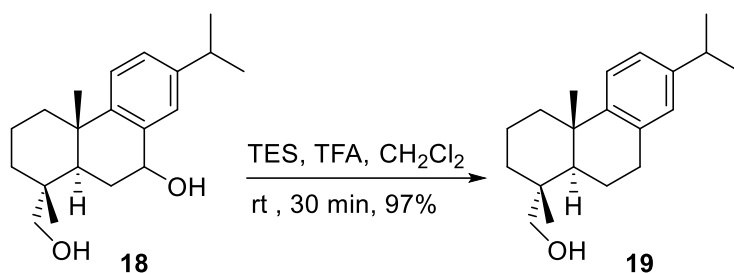
Synthesis of product **20** from **16**



To a solution of compound **16** (270 mg, 0.726 mmol) in anhydrous THF (5 ml) was added at 0°C LiAlH_4 (40 mg, 1.05 mmol) and the mixture was stirred at room temperature for one hour. After verifying by TLC that the reaction is complete, the reaction crude is poured slowly onto ice, and AcOEt (15 mL) was added. the phases were shaken and separated. The organic phase was washed with water (2 x 5 ml), brine (5 mL), and dried over anhydrous sodium sulfate. After filtration and evaporation of the solvent, the diol product **18**³ was obtained quantitatively (219 mg).

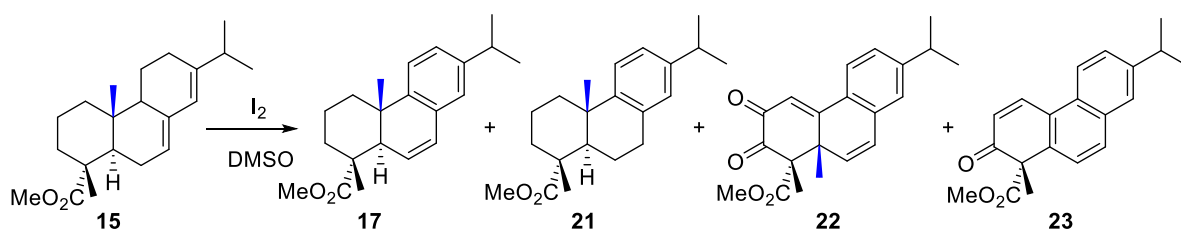
The latter diol **18** without purification was dissolved in pyridine (3 ml) and Ac_2O (2 ml) was added. The resulting mixture was stirred at room temperature for 30 minutes. After this time, TLC indicated the complete consumption of the starting material. Water was added and stirred for 6 minutes. Meanwhile, 20 ml of diethyl ether was added and the phases were shaken and separated. The organic phase was washed with 2 N HCl (5 x 10 ml), water (2 x 15 ml), saturated NaHCO_3 solution (3 x 10 ml), and brine (2 x 10 ml). The mixture was then dried over anhydrous Na_2SO_4 and filtered. The solvent was evaporated under vacuum to obtain the crude product which was dissolved in DCM (5 mL) and treated by Amberlyst A-15 (200 mg) for 30 min, to give, after filtration, compound **20**² (222 mg, 94%) as a colourless syrup.

Treatment of **18** with the system TES/TFA



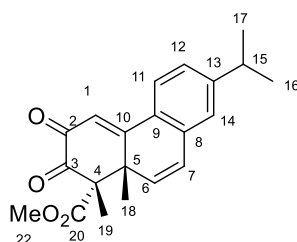
To a solution of **18** (158 mg, 0.52 mmol) in DCM (6 mL) were added Triethylsilane (TES) (0.5 mL) and TFA (0.2 mL) and the reaction mixture was stirred at room temperature for 30 min. Then, the solvent was removed under vacuum and the crude product was directly purified by column chromatography using 10% EtOAc/hexanes to give compound **19**⁴ (144 mg, 97%) as a colourless syrup.

Treatment of abietic methylester **15** by I₂/DMSO.(entry 4)



The action of 5% iodine (8 mg, 31.5 μmol) with abietic ester **15** (200 mg, 0.631 mmol), solubilized in the minimum amount of DMSO (4 ml) solvent at 160°C for 9 hours, leads to the complete transformation of the starting material. The reaction mixture is treated with water and dichloromethane. The organic phase is collected and dried over Na₂SO₄, and solvent concentration yields a crude product. The latter has been purified by column chromatography on silica gel, affording ester **21**⁵ (128 mg, 75%) eluted with 10% EtOAc/hexane, dioxo-ester **22** (21.4 mg, 10%), and one oxo-ester **23** (29.2 mg, 15%) eluted with 20% EtOAc/hexane.

Methyl (1S,10aS)-7-isopropyl-1,10a-dimethyl-2,3-dioxo-1,2,3,10a-tetrahydrophenanthrene-1-carboxylate (**22**)

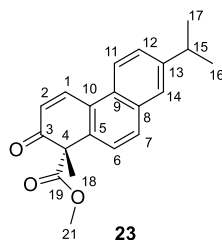


Viscous yellow. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.80 (d, J = 8.3 Hz, 1H, H-11), 7.25 (dd, J = 8.3, 1.9 Hz, 1H, H-12), 7.12 (d, J = 1.9 Hz, 1H, H-14), 7.08 (s, 1H, H-1), 6.67 (d, J = 9.8 Hz, 1H, H-6), 6.33 (d, J = 9.8 Hz, 1H, H-7), 3.58 (s, 3H, H-19), 2.97 (hept, J = 6.9 Hz, 1H, H-15), 1.70 (s, 3H, H-18), 1.30 (d, J = 6.9 Hz, 3H, H-16), 1.24 (d, J = 6.9 Hz, 3H, H-17), 1.18 (s, 3H, H-22). ^{13}C NMR (101 MHz, Chloroform-*d*) 192.79 (C=O, C-3), 181.21 (C=O, C-2), 170.65 (C=O, C-20), 166.00 (C, C-10), 154.75 (C, C-8), 133.83 (CH, C-12), 133.71 (C, C-13), 126.96 (CH, C-11), 126.03 (CH, C-14), 125.82 (CH, C-1), 125.20 (C, C-9), 124.75 (CH, C-6), 121.94 (CH, C-7), 66.56 (C, C-4), 52.93 (CH₃, C-22), 47.53 (C, C-5), 34.14 (CH, C-15), 27.01 (CH₃, C-19), 23.51 (2 \times CH₃, C-16, C-17), 13.18 (CH₃, C-18). HRMS (FAB-TOF) m/z : $[\text{M} + \text{H}]^+$ calcd for C₂₁H₂₂O₄; 339.1596 found, 339.1593.

Summary table of assignment of NMR data of compound 22

Atom	δ (ppm)	HMBC	Atom	δ (ppm)	HMBC
1 C	121.94		13 C	154.90	15
1 H	7.00	3, 5, 9	14 C	126.03	
2 C	181.21		14 H	7.04	7, 12, 15
3 C	192.79	1, 18	15 C	34.14	12, 14
4 C	66.56	6, 18, 19	15 H	2.89	12, 13, 16
5 C	47.53	1, 6, 7, 18, 19	16 C	23.51	15
6 C	133.96	19	16 H3	1.21	
6 H	6.25	4, 5, 8, 10	17 C	23.51	
7 C	124.88	14, 18	17 H3	1.21	
7 H	6.59	5, 9	18 C	13.18	
8 C	133.71	6	18 H3	1.62	3, 4, 5, 7, 10, 20
9 C	125.30	1, 7, 12	19 C	27.01	
10 C	166.00	6, 18, 19	19 H3	1.10	4, 5, 6, 10
11 C	125.95		20 C	170.65	18, 22
11 H			22 C	52.93	
12 C	126.96	14, 15	22 H3	3.50	20

Methyl (S)-7-isopropyl-1-methyl-2-oxo-1,2-dihydrophenanthrene-1-carboxylate (23)

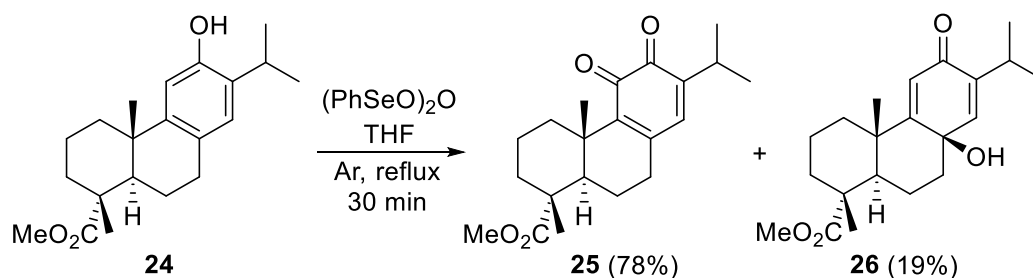


Viscous yellow. ^1H NMR (500 MHz, Chloroform-*d*) δ 8.30 (d, $J = 15.9$ Hz, 1H, H-1), 7.97 (d, $J = 8.85$ Hz, 1H, H-11), 7.71 (d, $J = 8.4$ Hz, 1H, H-7), 7.63 (d, $J = 1.9$ Hz, 1H, H-14), 7.42 (dd, $J = 8.8, 1.9$ Hz, 1H, H-12), 7.33 (d, $J = 8.4$ Hz, 1H, H-6), 6.93 (d, $J = 15.9$ Hz, 1H, H-2), 3.83 (s, 3H, H-21), 3.07 (hept, $J = 9.6$ Hz, 1H, H-15), 2.08 (s, 3H, H-18), 1.35 (d, $J = 6.9$ Hz, 6H, H-16, H-17). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 190.03 (C=O, C-3), 170.81 (C=O, C-19), 130.74 (C, C-10), 124.51 (CH, C-11), 130.27 (C, C-9), 145.74 (C, C-13), 132.44 (C, C-8), 133.9 (C, C-5), 124.64 (CH, C-14), 126.56 (CH, C-12), 128.29 (CH, C-2), 141.87 (CH, C-1), 128.7 (CH, C-7), 128.96 (CH, C-6), 61.4 (C, C-4), 170.8 (CH₃, C-19), 33.93 (CH, C-15), 19.65 (CH₃, C-18), 23.87 (CH₃, C-17), 23.88 (CH₃, C-16). IR (film): 2957, 2925, 2868, 1737, 1688, 1610, 1446, 1247, 1118, 1029, 823 cm^{-1} . HRMS (FAB-TOF) m/z : $[\text{M} + \text{H}]^+$ calcd for C₂₀H₂₁O₃; 309.1412 found, 309.1513.

Summary table of assignment of NMR data of compound **23**

Atom	δ (ppm)	HMBC	Atom	δ (ppm)	HMBC
1 C	141.87		12 C	126.56	
1 H	8.26	3, 5	12 H	7.38	10
2 C	128.29		13 C	145.74	11, 15
2 H	6.89	3, 10	14 C	124.64	
3 C	190.03	1, 2, 18	14 H	7.59	10
4 C	61.4	18	15 C	33.93	
5 C	133.9	1, 7	15 H	3.02	13
6 C	128.96		16 C	23.88	
6 H	7.29	8, 10	16 H3	1.31	17
7 C	128.7		17 C	23.87	16
7 H	7.67	5, 10, 11	17 H3	1.31	
8 C	132.44	6, 11	18 C	19.65	
9 C	130.27		18 H3	1.72	3, 4, 19
10 C	130.74	2, 6, 7, 11, 12, 14	19 C	170.8	18, 21
11 C	124.51	7	21 C	53.18	
11 H	7.93	8, 10, 13	21 H3	3.79	19

Treatment of phenol **24** with (PhSeO)₂O.

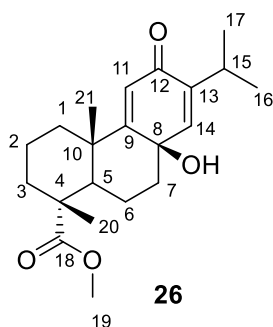


(PhSeO)₂O (217 mg, 0.61 mmol) was added to a solution of phenol **24** (200 mg, 0.61 mmol) in anhydrous THF (7 mL) under an argon atmosphere, and the reaction was kept stirring at reflux for 15 min. The solvent was evaporated under vacuum to give a crude product, which after column chromatography on silica gel, afforded quinone **25** (168 mg, 80%), eluted with 5% EtOAc/hexane, and hydroxy dienone **26** (42.3 mg, 20%), eluted with 10% EtOAc/hexane).

Methyl (1R,4aS,10aR)-7-isopropyl-1,4a-dimethyl-5,6-dioxo-1,2,3,4,4a,5,6,9,10,10a-decahydrophenanthrene-1-carboxylate (**25**)

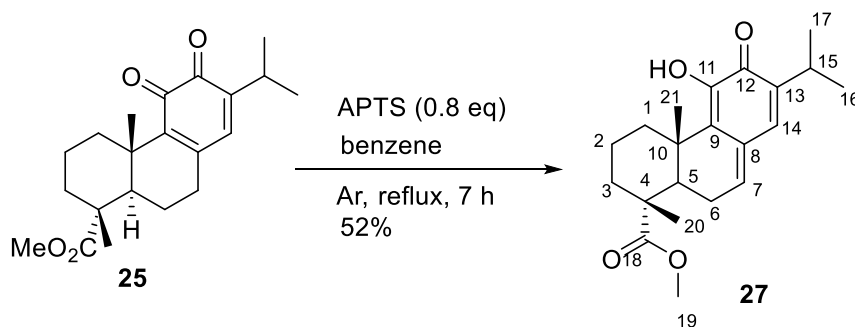
Green solid, ¹H NMR (400 MHz, Chloroform-*d*) δ 6.40 (s, 1H), 3.70 (s, 3H), 2.91 (hept, *J* = 6.9 Hz, 1H), 2.78 (d, *J* = 12.6 Hz, 1H), 2.57 – 2.38 (m, 2H), 2.03 (dd, *J* = 12.4, 1.8 Hz, 1H), 1.76 – 1.55 (m, 4H), 1.45 – 1.31 (m, 1H), 1.27 (s, 3H), 1.25 (s, 3H), 1.12 (d, *J* = 2.5 Hz, 3H), 1.10 (d, *J* = 2.5 Hz, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 180.93 (C=O), 179.91 (C=O), 178.77 (C=O), 147.93 (C), 146.95 (C), 144.10 (C), 137.57 (CH), 52.00 (CH), 47.57 (C), 45.47 (CH₃), 37.38 (C), 36.65 (CH₂), 35.21 (CH₂), 33.24 (CH₂), 26.89 (CH), 21.37 (2 × CH₃), 20.79 (CH₂), 20.18 (CH₃), 18.00 (CH₂), 16.51 (CH₃). IR (film): 1728, 1439, 1376, 1228, 1118 cm⁻¹. HRMS (FAB-TOF) *m/z*: [M + H]⁺ calcd for C₂₁H₂₈O₄, 344.20, found: 345.2051.

Methyl (1R,4aS,8aR,10aR)-8a-hydroxy-7-isopropyl-1,4a-dimethyl-6-oxo-1,2,3,4,4a,6,8a,9,10,10a-decahydrophenanthrene-1-carboxylate (**26**)



Colorless crystal, ^1H NMR (500 MHz, Chloroform-*d*) δ 6.37 (s, 1H, H-14), 6.00 (s, 1H, H-11), 3.64 (s, 3H, H-19), 2.88 (hept, $J = 6.9$ Hz, 1H, H-15), 2.10 – 1.95 (m, 2H), 1.83 – 1.65 (m, 5H), 1.63 – 1.44 (m, 3H), 1.39 (s, 3H, H-21), 1.28 (s, 3H, H-20), 1.06 (d, $J = 6.9$ Hz, 3H, H-16), 1.03 (d, $J = 6.9$ Hz, 3H, H-17). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 187.19 (C=O, C-12), 178.58 (C=O, C-18), 168.01 (C, C-9), 145.27 (CH, C-14), 141.97 (C, C-13), 122.08 (CH, C-11), 69.29 (C-OH), 52.03 (CH₃, C-19), 48.79 (CH, C-5), 47.98 (C, C-10), 40.47 (C, C-4), 39.21 (CH₂), 36.97 (CH₂), 36.82 (CH₂), 25.61 (CH, C-15), 21.77 (CH₃, C-20), 21.33 (CH₃, C-21), 20.56 (CH₃, C-16), 20.28 (CH₂), 17.81 (CH₂), 16.65 (CH₃, C-17). IR (film): 3446; 2926, 2870, 1726, 1664, 1632, 1460, 1388, 1250, 1179, 1132, 1104, 1045 cm^{-1} . HRMS (FAB-TOF) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{21}\text{H}_{30}\text{O}_4$, 347.2222; found, 347.2213.

Synthesis of 6-deoxytaxodione derivative 27

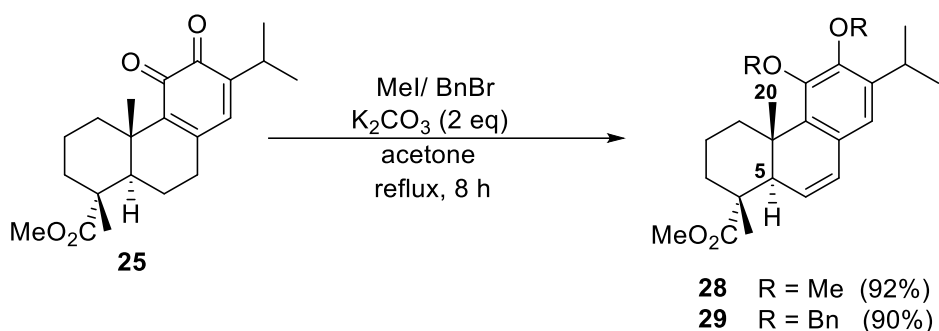


The compound **25** (50 mg, 0.145 mmol) was dissolved in benzene (8 mL), and then APTS (20 mg, 0.116 mmol) was added. After refluxing for 7 hours under argon atmosphere, the solution was concentrated. The residue was purified by silica gel column chromatography using a 10% EtOAc/hexane mixture to yield **27** (26 mg, 52%).

6-Deoxytaxodione derivative 27: ^1H NMR (500 MHz, Chloroform-*d*) δ 7.48 (s, 1H, H-14), 6.79 (s, 1H), 6.74 (dd, $J = 6.9, 3.0$ Hz, 1H, H-7), 3.68 (s, 3H, H-19), 3.08 (hept, $J = 6.7$ Hz, 1H, H-15), 3.06 – 3.01 (m, 2H), 2.55 – 2.38 (m, 1H), 2.20 – 2.00 (m, 1H), 1.87 – 1.53 (m, 5H), 1.32 (s, 3H, H-21), 1.23 (s, 3H, H-20), 1.16 (d, $J = 6.7$ Hz, 3H, H-16), 1.15 (d, $J = 6.7$

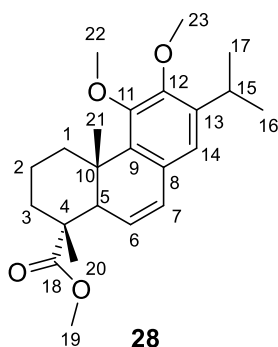
Hz, 3H, H-17). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 181.34 (C=O, C-12), 178.47 (C=O, C-18), 147.69 (CH, C-11), 143.83 (C, C-13), 140.71 (C, C-8), 136.12 (CH, C-14), 131.61 (C, C-9), 126.54 (C), 52.09 (CH₃, C-19), 47.30 (C, C-4), 45.01 (CH, C-5), 38.09 (C, C-10), 36.80 (CH₂), 35.96 (CH₂), 27.72 (CH₂), 26.62 (CH, C-15), 21.80 (CH₃, C-21), 21.46 (CH₃, C-20), 18.84 (CH₃, C-16), 18.20 (CH₂), 17.13 (CH₃, C-17). HRMS (FAB-TOF) m/z : $[\text{M} + \text{H}]^+$ calcd for C₂₀H₂₉O₃, 317.2117; found, 317.2106.

Synthesis of compounds **28** and **29**.



The treatment of quinone **25** (100 mg, 0.290 mmol) with 0.638 mmol of MeI or (BnBr) in the presence of K₂CO₃ (88.2 mg, 0.638 mmol) in acetone, under reflux for 8 hours, leads to the complete transformation of the initial product. Subsequently, the solvent is evaporated, and the reaction is treated with water and ethyl acetate. The organic phase is collected and dried with Na₂SO₄. Separation by column chromatography filled with silica gel and a mixture of 10% AcOEt/hexane yields the pure product **28** (99.4 mg, 92%) or **29** (137 mg, 90%)

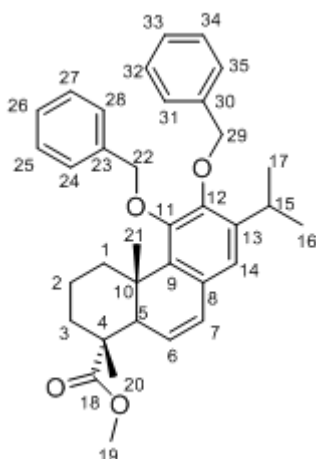
Methyl (1R,4aS,10aR)-7-isopropyl-5,6-dimethoxy-1,4a-dimethyl-1,2,3,4,4a,10a-hexahydrophenanthrene-1-carboxylate (**28**)



Colourless oil, ^1H NMR (500 MHz, Chloroform-*d*) δ 6.67 (s, 1H, H-14), 6.42 (dd, $J = 9.5, 3.1$ Hz, 1H, H-7), 5.58 (dd, $J = 9.4, 2.8$ Hz, 1H, H-6), 3.82 (s, 3H, H-22), 3.81 (s, 3H, H-23), 3.66

(s, 3H, H-19), 3.26 (hept, $J = 7.1$ Hz, 1H, H-15), 3.00 (t, $J = 3.1$ Hz, 1H, H-5), 2.95 (dd, $J = 13.5, 3.7$ Hz, 2H), 1.95 – 1.68 (m, 2H), 1.67 – 1.61 (m, 2H), 1.39 (s, 3H, H-21), 1.21 (dd, $J = 24.0, 6.8$ Hz, 6H, H-17, H-16), 1.18 (s, 3H, H-20). ^{13}C NMR (126 MHz, Chloroform- d) δ 178.58 (C=O, C-18), 150.86 (C, C-11), 150.74 (C, C-12), 140.25 (C, C-13), 137.18 (C, C-9), 130.27 (C, C-8), 128.51 (CH, C-14), 128.36 (CH, C-6), 120.32 (CH, C-7), 60.37 (CH₃, C-22), 60.10 (CH₃, C-23), 52.01 (CH₃, C-19), 47.12 (C, C-10), 46.67 (CH, C-5), 40.49 (C, C-4), 36.04 (CH₂, C-3), 35.46 (CH₂, C-1), 26.52 (CH, C-15), 23.73 (CH₃, C-21), 23.16 (CH₃, C-16), 19.81 (CH₃, C-17), 18.90 (CH₂, C-2), 17.92 (CH₃, C-20). IR (film): 2930, 2867, 1726, 1461, 1446, 1383, 1299, 1243, 1125, 1085, 1021, 987, 877 cm^{-1} . HRMS (FAB-TOF) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{23}\text{H}_{32}\text{O}_4$, 373.2379; found, 373.2370

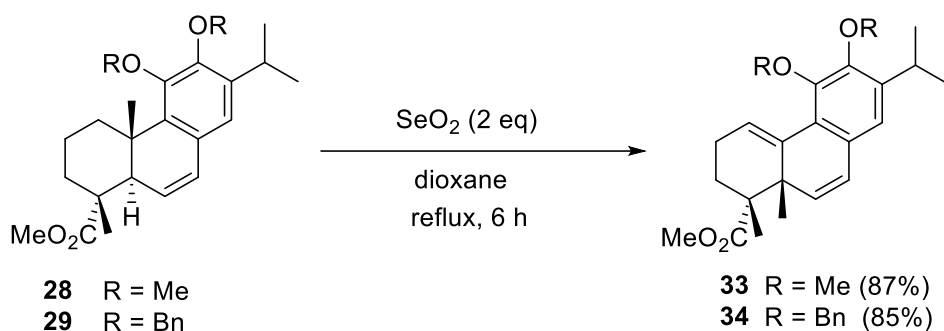
Methyl (1R,4aS,10aR)-5,6-bis(benzyloxy)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,10a-hexahydrophenanthrene-1-carboxylate (29)



Colorless oil, ^1H NMR (500 MHz, Chloroform- d) δ 7.45 – 7.41 (m, 2H, H-32, H-35), 7.39 – 7.34 (m, 4H, H-24, H-26, H-27, H-28), 7.34 – 7.30 (m, 4H, H-31, H-33, H-27, H-34), 6.75 (s, 1H, H-14), 6.48 (dd, $J = 9.4, 3.1$ Hz, 1H, H-22), 5.64 (dd, $J = 9.4, 3.1$ Hz, 1H, H-29), 5.11 (d, $J = 11.1$ Hz, 1H, H-6), 5.08 (d, $J = 11.1$ Hz, 1H, H-7), 5.03 (d, $J = 11.0$ Hz, 1H), 4.92 (d, $J = 11.0$ Hz, 1H), 3.69 (s, 3H, H-19), 3.34 (hept, $J = 6.9$ Hz, 1H, H-15), 3.10 (br, 1H, H-5), 3.06 (q, $J = 3.0$ Hz, 2H), 2.01 (d, $J = 4.1$ Hz, 2H), 1.92 – 1.57 (m, 2H), 1.42 (s, 3H, H-21), 1.24 (s, 3H, H-20), 1.20 (dd, $J = 27.7, 6.9$ Hz, 6H, H-16, H-17). ^{13}C NMR (126 MHz, Chloroform- d) δ 178.61 (C=O, C-18), 149.58 (C, C-11), 140.86 (C, C-12), 137.90 (C, C-13), 137.68 (C, C-9), 137.66 (C, C-8), 130.81 (C, C-23), 128.62 (CH, C-26), 128.60 (CH, C-33), 128.39 (2 \times CH, C-25, C-27), 128.35 (2 \times CH, C-31, C-35), 128.15 (2 \times CH, C-31, C-35), 127.92 (2 \times CH, C-24, C-28), 127.83 (CH, C-14), 127.66 (CH), 120.77 (CH), 75.09 (CH₂, C-22), 74.84

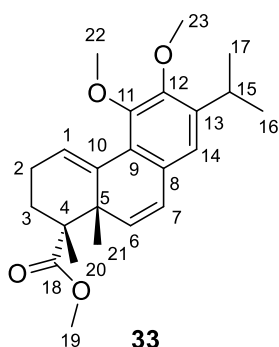
(CH₂, C-29), 52.06 (CH₃, C-19), 47.13, 46.75 (CH), 40.60, 36.27 (CH₂), 35.48 (CH₂), 26.44 (CH), 23.72 (CH₃, C-21), 23.29 (CH₃, C-16), 20.02 (CH₃, C-17), 18.78 (CH₃, C-20), 17.99 (CH₂). IR (film): 2959, 2867, 1725, 1454, 1422, 1363, 1296, 1243, 1142, 1126, 1083, 1007, 752, 732, 696 cm⁻¹. HRMS (FAB-TOF) m/z: [M + H]⁺ calcd for C₃₅H₄₀O₄, 525.3005; found, 525.3008

General procedure for the synthesis of compounds **33**, and **34**.



Two equivalents of SeO₂ were added to a solution of the mixture of compound **28** (120 mg, 0.322 mmol) or **29** (120 mg, 0.229 mmol) in dry 1,4-dioxane, and the mixture was stirred at reflux under an argon atmosphere for 6 hours. Following the same work-up procedure as in the general reference 2, the product **33** (103.8 mg, 87%) or **34** (101.8 mg, 85%) was obtained after column chromatography using a 10% EtOAc/hexane mixture.

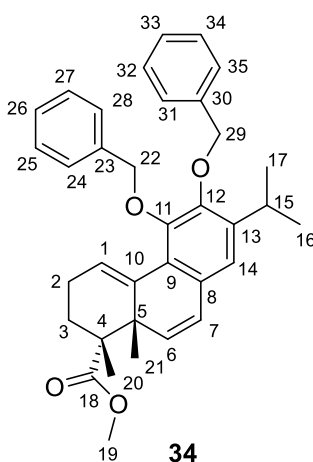
Methyl (1R,10aS)-7-isopropyl-5,6-dimethoxy-1,10a-dimethyl-1,2,3,10a-tetrahydrophenanthrene-1-carboxylate (**33**)



¹H NMR (400 MHz, Chloroform-*d*) δ 6.64 (s, 1H, H-14), 6.58 (br, 1H, H-1), 6.25 (d, *J* = 9.7 Hz, 1H, H-6), 5.97 (d, *J* = 9.7 Hz, 1H, H-7), 3.86 (s, 3H, H-22), 3.75 (s, 3H, H-23), 3.64 (s, 3H, H-19), 3.28 (hept, *J* = 6.9 Hz, 1H, H-15), 2.31 (ddt, *J* = 13.4, 5.2, 3.2 Hz, 2H, H-2), 2.07 – 1.89 (m, 1H, H-3), 1.59 (m, 1H, H-3), 1.37 (s, 3H, H-21), 1.24 (d, *J* = 6.9 Hz, 3H, H-16), 1.20 (d, *J* = 6.9 Hz, 3H, H-17), 1.17 (s, 3H, H-20). ¹³C NMR (101 MHz, Chloroform-*d*) δ

176.38 (C=O, C-18), 151.51 (C, C-11), 150.52 (C, C-12), 140.79 (C, C-13), 134.64 (C, C-9), 134.27 (CH, C-14), 129.28 (C, C-8), 127.08 (CH, C-1), 124.37 (C, C-10), 123.48 (CH, C-6), 119.64 (CH, C-7), 61.13 (CH₃, C-22), 59.70 (CH₃, C-23), 51.50 (CH₃, C-19), 47.45 (C, C-5), 41.30 (C, C-4), 29.91 (CH₂, C-2), 26.72 (CH, C-15), 24.27 (CH₂, C-2), 23.69 (CH₃, C-21), 23.23 (CH₃, C-20), 22.55 (CH₃, C-16), 20.83 (CH₃, C-17). IR (film): 2960, 1779, 1723, 1468, 1447, 1416, 1393, 1331, 1299, 1258, 1161, 1118, 1057, 999, 878, 763 cm⁻¹. HRMS (FAB-TOF) m/z: [M + H]⁺ calcd for C₂₃H₃₀O₄, 371.2222; found, 371.2223

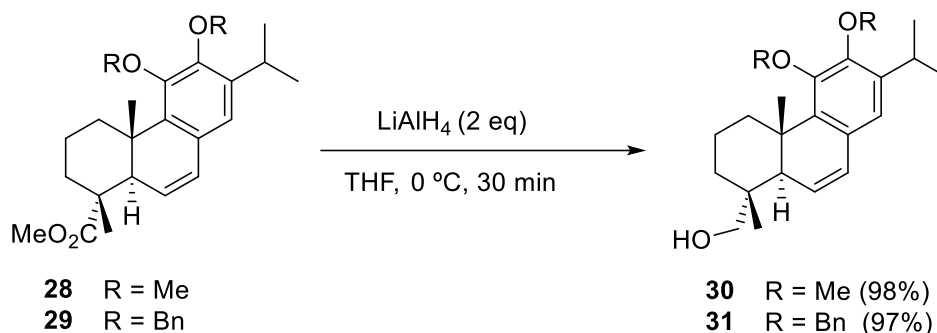
Methyl (1R,10aS)-5,6-bis(benzyloxy)-7-isopropyl-1,10a-dimethyl-1,2,3,10a-tetrahydrophenanthrene-1-carboxylate (34)



¹H NMR (500 MHz, Chloroform-*d*) δ 7.33 (d, *J* = 1.4 Hz, 2H, Har), 7.31 – 7.21 (m, 4H, Har), 7.19 (s, 2H, Har), 6.63 (dd, *J* = 5.1, 3.1 Hz, 1H, H-1), 6.60 (s, 1H, H-14), 6.18 (d, *J* = 9.7 Hz, 1H, H-6), 5.90 (d, *J* = 9.7 Hz, 1H, H-7), 5.21 (d, *J* = 11.0 Hz, 1H, H-22), 4.85 (d, *J* = 10.6 Hz, 1H, H-29), 4.75 (d, *J* = 10.6 Hz, 1H, H-29), 4.70 (d, *J* = 11.0 Hz, 1H, H-22), 3.55 (s, 3H, H-19), 3.24 (hept, *J* = 6.9 Hz, 1H, H-15), 2.31 – 2.20 (m, 1H), 2.11 (dd, *J* = 19.0, 4.4 Hz, 1H), 1.92 – 1.83 (m, 2H), 1.28 (s, 3H, H-21), 1.14 (d, *J* = 6.9 Hz, 3H, H-16), 1.05 (d, *J* = 8.1 Hz, 3H, H-17), 1.04 (s, 3H, H-20). ¹³C NMR (126 MHz, Chloroform-*d*) δ 175.30 (C=O, C-18), 149.44 (C, C-11), 148.36 (C, C-12), 140.24 (C, C-13), 136.97 (C, C-9), 136.91 (C, C-8), 133.47 (CH, C-14), 133.38 (C, C-30), 128.53 (C, C-23), 127.50 (2 × CH, C-25, C-27), 127.35 (2 × CH, C-32, C-34), 127.24 (2 × CH, C-24, C-28), 127.22 (2 × CH, C-26, C-33), C-31, C-35, 127.12 (CH, C-6), 126.81 (CH, C-7), 126.79 (CH, C-1), 124.02 (C, C-10), 122.33 (CH), 118.86 (CH, C-1), 74.40 (CH₂, C-22), 73.89 (CH₂, C-29), 50.51 (CH₃, C-19), 46.42 (C), 40.29 (C), 28.95 (CH₂), 25.56 (CH₃, C-21), 23.21 (CH₂), 22.52 (CH₃, C-20), 22.51 (CH₃, C-16), 21.39 (CH, C-15), 19.81 (CH₃, C-17). IR (film): 2960, 1720, 1454, 1426, 1360, 1328,

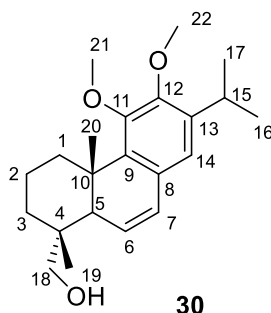
1294, 1258, 1160, 1117, 1079, 1028, 972, 801, 733, 696 cm^{-1} . HRMS (FAB-TOF) m/z : $[M + H]^+$ calcd for $\text{C}_{35}\text{H}_{38}\text{O}_4$, 523.2848; found, 523.2847

General procedure for the synthesis of compounds **30**, and **31**.



Dissolve the compound **28** (120 mg, 0.322 mmol) or **29** (120 mg, 0.229 mmol) in dry THF (10 ml) and cool to 0°C. Two equivalents of LiAlH_4 were added gradually, and the mixture was stirred for 30 minutes. After confirming by TLC that no starting material remained, the reaction mixture was slowly poured over ice, and ethyl ether was added and stirred for ten minutes. Afterward, the solution was cooled again to 0°C, and concentrated HCl was added until the pH became acidic, stirring for an additional fifteen minutes. After this time, the phases were separated, and the organic phase was washed with water (3 x 5 ml) and brine (2 x 6 ml) before being dried over Na_2SO_4 . Filter and evaporate the solvent to obtain product of **30** (108.7 mg, 98%) or **31** (110.3 mg, 97%) as an oily substance.

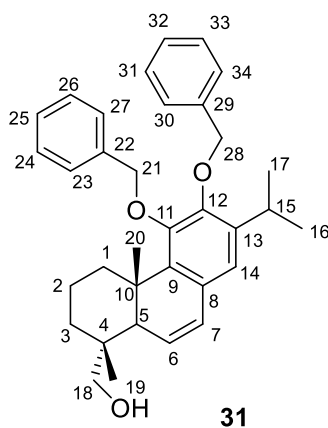
((1R,4aS,10aR)-7-isopropyl-5,6-dimethoxy-1,4a-dimethyl-1,2,3,4,10a-hexahydrophenanthren-1-yl) methanol (**30**)



^1H NMR (500 MHz, CHCl_3 - d) δ 6.68 (s, 1H, H-14), 6.47 (dd, $J = 9.6, 3.1$ Hz, 1H, H-7), 5.87 (dd, $J = 9.6, 3.1$ Hz, 1H, H-6), 3.82 (s, 3H, H-22), 3.81 (s, 3H, H-21), 3.51 (d, $J = 11.1$ Hz, 1H, H-18), 3.26 (d, $J = 11.1$ Hz, 1H, H-18), 3.24 (hept, $J = 6.9$ Hz, 1H, H-15), 3.09 – 2.66 (m, 2H), 2.45 (t, $J = 3.1$ Hz, 1H, 1.85 (s, 3H, H-20), 1.89 – 1.46 (m, 4H), 1.24 (d, $J = 6.9$ Hz,

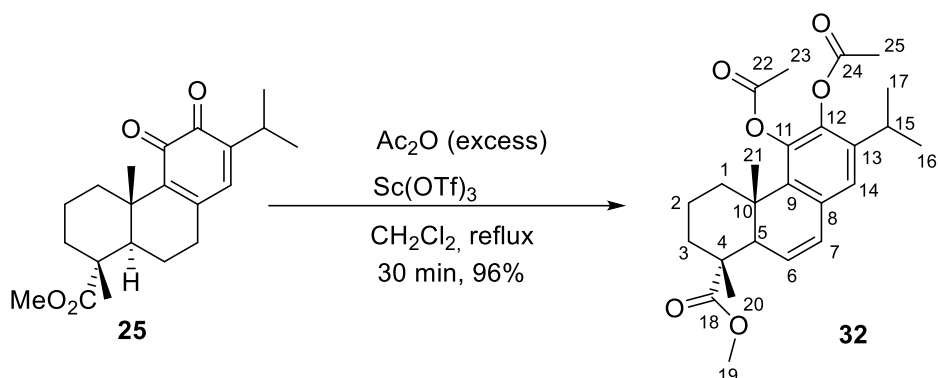
3H, H-17), 1.18 (d, $J = 6.9$ Hz, 3H, H-16), 1.01 (s, 3H, H-19). ^{13}C NMR (126 MHz, Chloroform- d) δ 150.85 (C, C-11), 150.78 (C, C-12), 140.12 (C, C-13), 137.76 (C, C-9), 130.33 (C, C-8), 128.75 (CH, C-14), 127.18 (CH, C-6), 120.21 (CH, C-7), 71.69 (CH₂), 60.39 (O-CH₃, C-21), 60.12 (O-CH₃, C-22), 45.28 (CH, C-5), 40.86 (C), 37.60 (C), 36.26 (CH₂), 34.18 (CH₂), 26.51 (CH, C-15), 23.75 (CH₃, C-19), 23.17 (CH₃, C-17), 19.73 (CH₃, C-16), 18.74 (CH₂), 18.25 (CH₃, C-20). IR (film): 3396; 2958; 2925; 2865, 1726, 1461, 1445, 1378, 1297, 1227, 1065, 1020, 986, 876, 630 cm^{-1} . HRMS (FAB-TOF) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{32}\text{O}_3$, 345.2430; found, 345.2423

((1R,4aS,10aR)-5,6-bis(benzyloxy)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,10a-hexahydrophenanthren-1-yl) methanol (31)



^1H NMR (500 MHz, Chloroform- d) δ 7.45 – 7.41 (m, 2H, H-30, H-34), 7.38 – 7.33 (m, 4H), 7.32 – 7.30 (m, 4H), 6.75 (s, 1H, H-14), 6.52 (dd, $J = 9.6, 3.1$ Hz, 2H, H-6), 5.92 (dd, $J = 9.6, 2.9$ Hz, 2H, H-7), 5.08 (s, 2H, H-21), 5.03 (d, $J = 11.0$ Hz, 1H, H-28), 4.90 (d, $J = 11.0$ Hz, 1H, H-28), 3.52 (s, 1H), 3.34 (hept, $J = 6.9$ Hz, 1H, H-15), 3.28 (d, $J = 11.2$ Hz, 1H, H-18), 3.08 (dt, $J = 13.3, 3.7$ Hz, 1H, H-18), 2.51 (t, $J = 3.0$ Hz, 1H), 1.94 – 1.85 (m, 1H), 1.71 (m, 1H), 1.61 (s, 1H), 1.52 (td, $J = 13.1, 4.1$ Hz, 1H), 1.44 – 1.35 (m, 1H), 1.24 (s, 3H, H-20), 1.22 (d, $J = 6.9$ Hz, 3H, H-17), 1.16 (d, $J = 6.9$ Hz, 3H, H-16), 1.02 (s, 3H, H-19). ^{13}C NMR (125 MHz, Chloroform- d) δ 149.62 (C), 140.70 (C), 138.24 (C), 137.96 (C), 137.72 (C), 130.85 (C), 128.85 (C), 128.37 (2 \times CH), 128.33 (2 \times CH), 128.15 (2 \times CH), 127.94 (2 \times CH), 127.80 (CH), 127.62 (CH), 127.43 (CH), 120.64 (CH), 75.07 (O-CH₂), 74.84 (O-CH₂, C-28), 71.69 (O-CH₂, C-21), 45.32 (CH), 40.95 (C), 37.64 (C), 36.52 (CH₂), 34.18 (CH₂), 26.43 (CH, C-15), 23.73 (CH₃), 23.30 (CH₃), 19.93 (CH₃), 18.62 (CH₂), 18.32 (CH₃). IR (film): 1371, 3033, 2960, 2925, 2866, 1497, 1454, 1421, 1363, 1294, 1217, 1058, 1008, 750, 696 cm^{-1} . HRMS (FAB-TOF) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{34}\text{H}_{40}\text{O}_3$, 497.3056; found, 497.3053

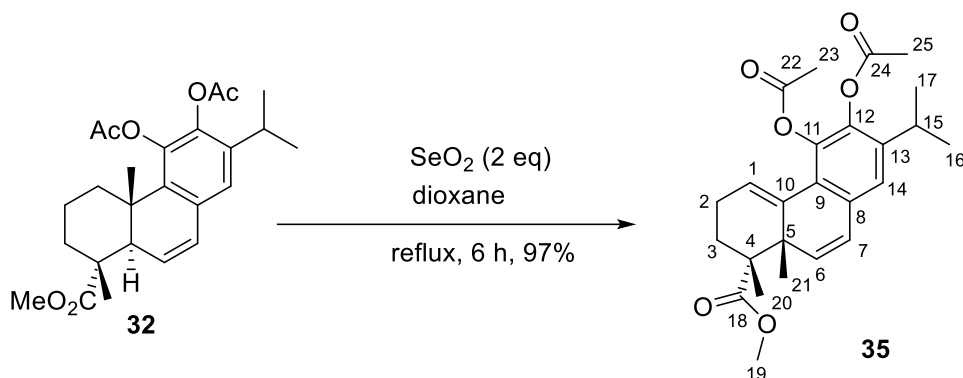
Treatment of orthoquinone **25 with Ac₂O and cat. Sc(OTf)₃.**



Compound 32: ¹H NMR (500 MHz, Chloroform-*d*) δ 6.81 (s, 1H, H-16), 6.41 (dd, $J = 9.5$, 3.1 Hz, 1H, H-7), 5.59 (dd, $J = 9.5$, 2.8 Hz, 1H, H-6), 3.58 (s, 3H, H-19), 2.81 (hept, $J = 6.9$ Hz, 1H, H-15), 2.22 (s, 3H, H-25), 2.21 (s, 3H, H-23), 1.71 (td, $J = 8.7$, 3.1 Hz, 2H), 1.66 (d, $J = 3.1$ Hz, 1H), 1.65 – 1.59 (m, 2H), 1.58 – 1.47 (m, 2H), 1.29 (s, 3H, H-21), 1.13 (d, $J = 6.9$ Hz, 3H, H-17), 1.09 (d, $J = 6.9$ Hz, 3H, H-16), 1.08 (s, 3H, H-20). ¹³C NMR (125 MHz, Chloroform-*d*) δ 178.23 (C=O, C-18), 168.96 (C=O, C-22), 168.53 (C=O, C-24), 139.64 (C, C-9), 139.36 (C, C-13), 139.21 (C, C-11), 136.17 (C, C-12), 133.05 (C, C-8), 130.07 (CH, C-14), 128.12 (CH, C-7), 122.86 (CH, C-6), 52.11 (CH, C-5), 46.86 (C, C-4), 45.91 (CH₃), 40.21 (C, C-10), 35.02 (CH₂, C-1), 27.36 (2 \times CH₃, C-16, C-17), 23.09 (CH₃, C-21), 22.64 (CH, C-15), 21.02 (CH₃, C-25), 20.43 (CH₃, C-23), 18.67 (2 \times CH₂, C-2, C-21), 17.89 (CH₃). IR (film): 2964, 1772, 1725, 1370, 1248, 1207, 1178, 1141, 1123, 1013, 882 cm⁻¹. HRMS (FAB-TOF) m/z : [M + H]⁺ calcd for C₂₅H₃₂O₆, 429.2277; found, 429.2268

Sc(OTf)₃ (10 mg) was introduced into a solution containing quinone **25** (130 mg, 0.377 mmol) in anhydrous CH₂Cl₂ (5 mL) and acetic anhydride (1 mL, 10.6 mmol). The mixture underwent reflux for 30 minutes, during which TLC indicated the absence of any remaining starting material. Subsequently, the reaction was allowed to cool to room temperature, CH₂Cl₂ (15 mL) was introduced, and the organic phase underwent washing with H₂O (3 \times 10 mL). After drying over anhydrous Na₂SO₄ and evaporation, a crude product was obtained. Column chromatography on silica gel with a 20% EtOAc/hexane mixture yielded product **32** (155 mg, 96%).

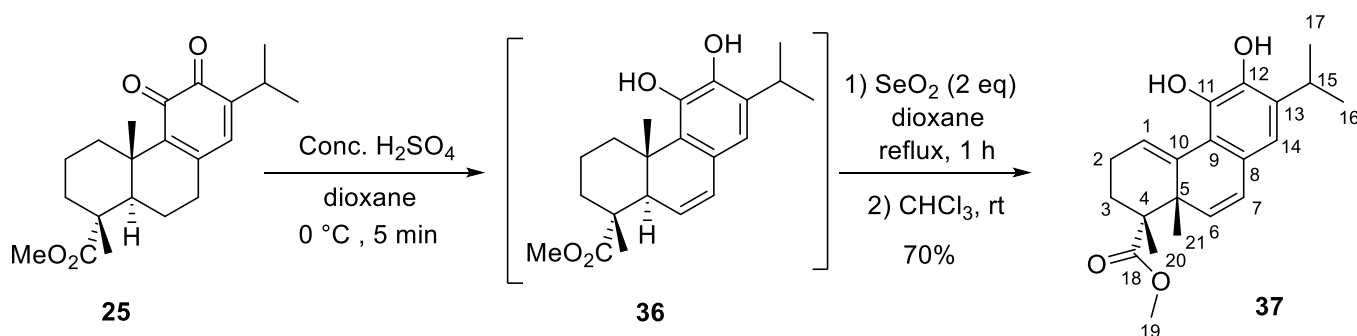
Synthesis of **35**.



The compound **35** was synthesized from compound **32** (100 mg, 0.233 mmol) through the action of SeO_2 (51.7 mg, 0.446 mmol) following the same procedure as the synthesis of compounds **33** and **34**, with a significant yield (96.4 mg, 97%).

Compound 35: ^1H NMR (500 MHz, Chloroform-*d*) δ 6.75 (s, 1H, H-14), 6.19 (d, $J = 9.7$ Hz, 1H, H-7), 6.15 (s, 1H, H-1), 5.94 (d, $J = 9.7$ Hz, 1H, H-6), 3.53 (s, 3H, H-19), 2.85 (hept, $J = 6.9$ Hz, 1H, H-15), 2.23 (s, 3H, H-25), 2.22 – 2.18 (m, 1H), 2.13 (s, 3H, H-23), 2.11 – 1.94 (m, 2H), 1.86 – 1.78 (m, 2H), 1.71 – 1.53 (m, 1H), 1.25 (s, 3H, H-20), 1.19 (d, $J = 1.4$ Hz, 1H), 1.15 (d, $J = 6.9$ Hz, 3H, H-17), 1.09 (d, $J = 6.9$ Hz, 3H, H-16), 1.03 (s, 3H, H-21). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 176.23 (C=O, C-18), 168.63 (C=O, C-22), 168.02 (C=O, C-24), 140.11 (C, C-9), 139.91 (C, C-12), 139.76 (C, C-11), 136.02 (CH, C-6), 134.78 (C, C-10), 131.58 (C, C-13), 126.89 (CH, C-7), 125.19 (C, C-8), 122.66 (CH, C-1), 121.62 (CH, C-14), 51.56 (CH₃, C-19), 47.23 (C, C-4), 41.50 (C, C-5), 29.74 (CH₂, C-3), 27.48 (CH, C-15), 24.35 (CH₂, C-2), 23.03 (CH₃, C-16), 22.71 (CH₃, C-17), 22.16 (CH₃, C-21), 20.88 (CH₃, C-25), 20.75 (CH₃, C-23), 20.44 (CH₃, C-20). IR (film): 2965, 1770, 1736, 1430, 1368, 1203, 1183, 1117, 1034, 880, 796, 744 cm^{-1} . HRMS (FAB-TOF) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{25}\text{H}_{31}\text{O}_6$, 427.2121; found, 427.2119

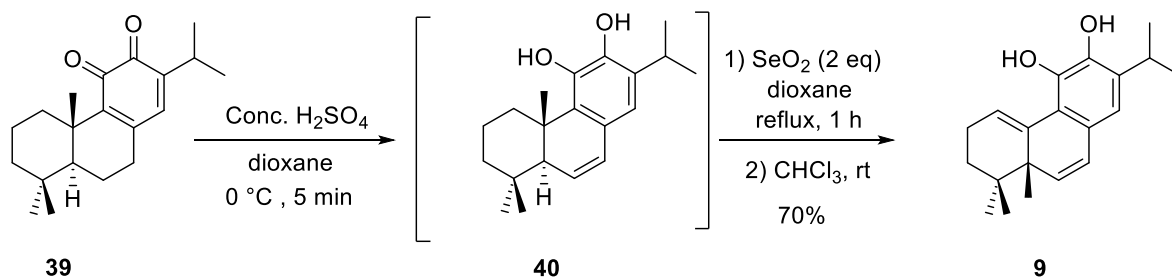
Synthesis of derivative of Prattinin A (**37**)



The synthesis of the intermediate **36** (unstable) from quinone **25** (120 mg, 0.348 mmol) was achieved through the action of sulfuric acid in dioxane, quantitatively, following the same protocol described in our previous work (ref. 2). This intermediate was immediately transformed in the subsequent reaction by the action of SeO_2 (77.3 mg, 0.697 mmol) in dry dioxane at reflux for 2 hours. The reaction resulted in the complete transformation of the product, and the reaction mixture was treated with saline water and ethyl acetate. After decantation and drying with Na_2SO_4 , filtration and solvent concentration yielded a crude product. The crude product was dissolved in CHCl_3 and stirred for 2 hours at room temperature. Solvent concentration and separation by column chromatography filled with silica gel using a 15% AcOEt /hexane mixture allowed the isolation of product **37** (83.4 mg, 70%) in its pure state.

Derivative of Pratinin A 37: ^1H NMR (400 MHz, Chloroform-*d*) δ 1.10 (s, 3H, H-21), 1.21 (dd, $J = 13.4, 7.0$ Hz, 6H, H-16, H-17), 1.33 (s, 3H, H-20), 1.98 – 1.87 (m, 2H), 2.39 – 2.19 (m, 2H), 3.19 (hept, $J = 6.9$ Hz, 1H, H-15), 3.59 (s, 3H, H-19), 5.79 (d, $J = 9.7$ Hz, 1H, H-7), 6.12 (t, $J = 3.9$ Hz, 1H, H-1), 6.20 (d, $J = 9.7$ Hz, 1H, H-6), 6.44 (s, 1H, H-14). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 20.74 (CH_3 , C-16), 22.18 (CH_3 , C-17), 22.29 (CH_3 , C-21), 22.55 (CH_3 , C-20), 24.06 (CH_2 , C-3), 26.99 (CH, C-15), 29.88 (CH_2 , C-2), 41.68 (C, C-4), 47.10 (C, C-5), 51.49 (CH_3 , C-19), 116.17 (CH, C-14), 116.42 (C, C-9), 123.79 (CH, C-1), 123.86 (CH, C-7), 125.14 (C, C-8), 132.01 (CH, C-6), 133.13 (C, C-13), 138.28 (C, C-10), 140.27 (C, C-11), 141.37 (C, C-12), 176.04 (C, C-18). IR (film): 3463, 2957, 2926, 2870, 1722, 1439, 1326, 1341, 1264, 1221, 1190, 1164, 1119, 1026, 760, 746 cm^{-1} . HRMS (ESI) m/z : calcd for $\text{C}_{21}\text{H}_{27}\text{O}_4$ ($\text{M}+\text{H}^+$) 343.1909, found: 343.1908.

Synthesis of Prattinin A (9)



The synthesis of Prattinin A (**9**)⁵ from quinone **39** (150 mg, 0.50 mmol), with a good yield (112 mg, 75%), was carried out using the same synthesis protocol as its analog **37** described above.

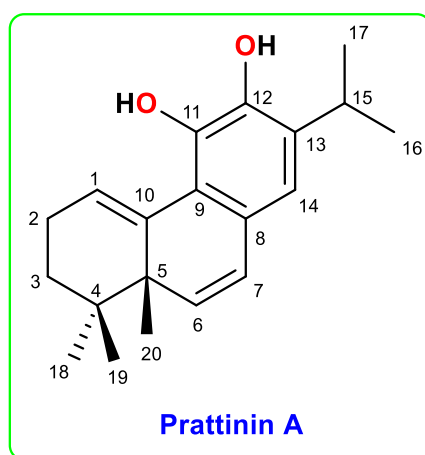


Table S2. ^1H NMR data for the synthetic and natural Prattinin A (9)

Position	Natural Prattinin A (9) (Ref. 6, 500 MHz, CDCl_3)	Synthetic Prattinin A (9) (500 MHz, CDCl_3)
1	6.08 (dd, 6.3, 2.9)	6.11 – 6.09 (m, 1H)
2 α	3.34 (dddd, 19.5, 13.5, 6.3, 2.9)	2.39 – 2.17 (m, 1H)
2 β	2.20 (br dt, 19.5, 6.3)	2.21 (dt, $J = 19.1, 5.0$ Hz, 1H)
3 α	1.31 (br dd, 13.5, 6.3)	1.31 (dd, $J = 13.3, 6.4$ Hz, 1H)
3 β	1.88 (td, 13.5, 6.3)	1.88 (td, $J = 12.6, 6.3$ Hz, 1H)
4	-	-
5	-	-
6	6.22 (d, 9.5)	6.23 (d, $J = 9.7$ Hz, 1H)
7	5.49 (d, 9.5)	5.81 (d, $J = 9.7$ Hz, 1H)
8	-	-
9	-	-
10	-	-
11	-	-
12	-	-
13	-	-

14	6.45, s	6.45 (s, 1H)
15	3.23 (septet, 6.9)	3.23 (sept, $J = 6.9$ Hz, 1H)
16	1.22 (d, 6.9)	1.22 (d, $J = 6.9$ Hz, 3H)
17	1.25 (d, 6.9)	1.25 (d, $J = 7.0$ Hz, 3H)
18	0.95 (s)	0.96 (s, 3H)
19	1.03 (s)	1.04 (s, 3H)
20	1.06 (s)	1.06 (s, 3H)
OH-11	5.72 (br s)	5.75 (s, 1H)
OH-12	5.53 (br s)	5.56 (s, 1H)

Table S3. ^{13}C NMR data for the synthetic and natural Prattinin A (9)

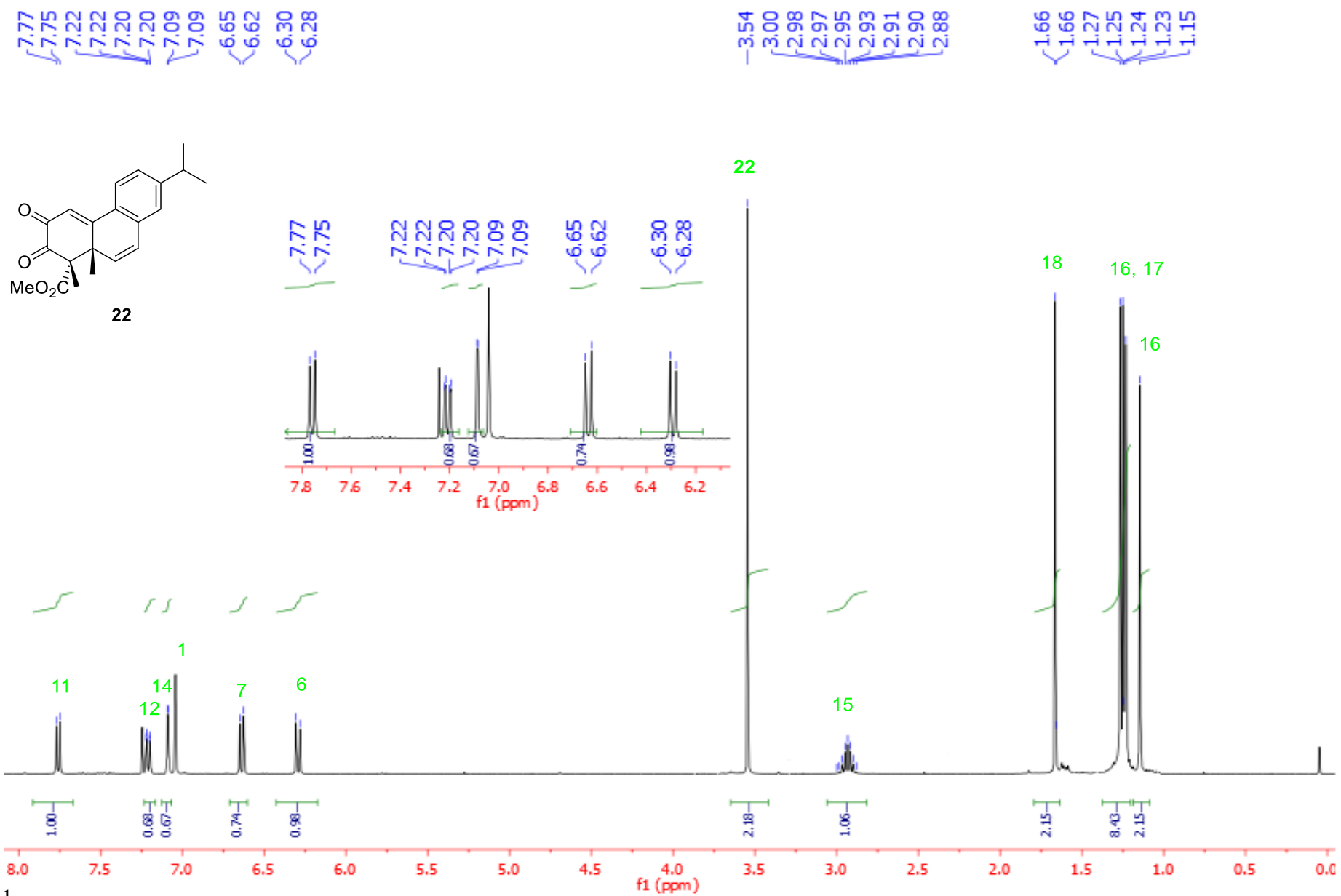
Position	Natural Prattinin A (9) Ref 6, 125 MHz, CDCl_3)	ynthetic Prattinin A (9) (125 MHz, CDCl_3)
1	124.6	124.58
2	23.6	23.54
3	32.3	32.32
4	33.0	32.96
5	43.1	43.07
6	132.1	132.05
7	124.8	124.80
8	125.1	125.08
9	116.5	116.56
10	138.6	138.52
11	140.2	140.23
12	141.5	141.52
13	133.1	133.10
14	115.8	115.79
15	27.0	27.00
16	22.2	22.22
17	22.6	22.59
18	24.7	24.71
19	24.9	24.91
20	21.8	21.80

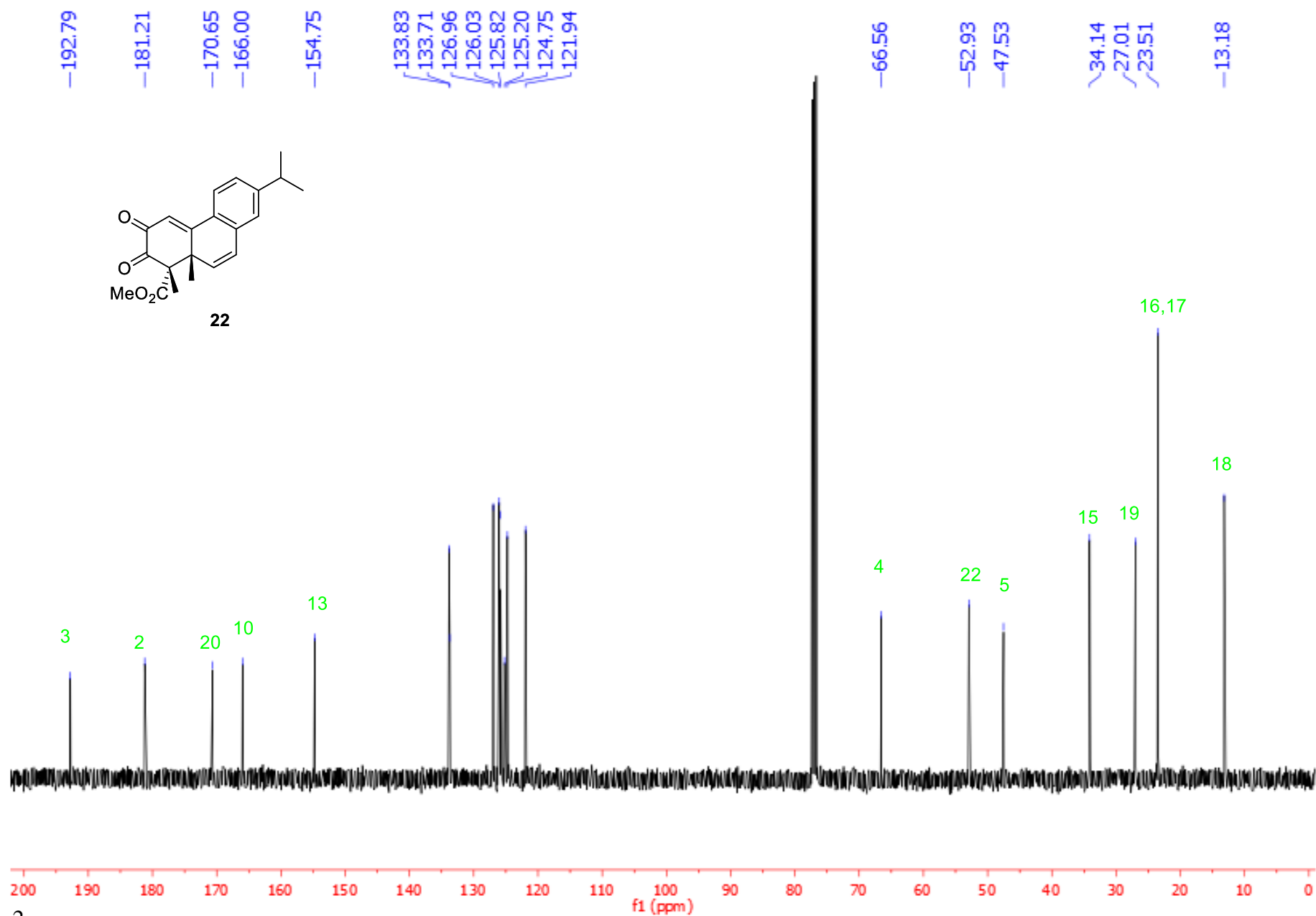
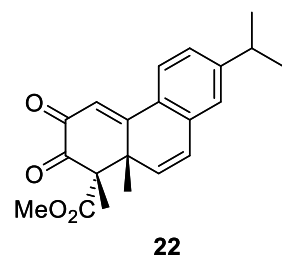
Note: The assignment of the molecules is based on the NMR analyses we conducted, as well as the NMR data of molecules similar to those we synthesized, cited in the bibliography, including those presented below:

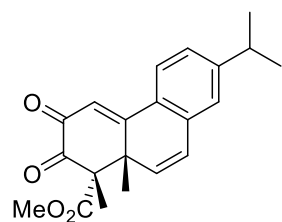
- [1] Ait El Had, M.; Guardia, J.J.; Ramos, J.M.; Taourirte, M.; Chahboun, R.; Alvarez-Manzaneda, E. Bioinspired Synthesis of Pygmaeocins and Related Rearranged Abietane Diterpenes: Synthesis of Viridoquinone. *Org. Lett.* **2018**, 20, 5666–5670.
- [2] Machumi, F.; Samoylenko, V.; Yenesew, A.; Derese, S.; Midiwo, J.O.; Wiggers, F.T.; Ilias, M. Antimicrobial and Antiparasitic Abietane Diterpenoids from the Roots of *Clerodendrum eriophyllum*. *Nat. Prod. Commun.* **2010**, 5, 853–858.
- [3] González, M.A. Synthetic Derivatives of Aromatic Abietane Diterpenoids and Their Biological Activities. *Eur. J. Med. Chem.* **2014**, 87, 834–842.
- [4] Kawabe, H.; Suzuki, R.; Hirota, H.; Matsuzaki, K.; Gong, X.; Ohsaki, A. A New Diterpenoid with a Rearranged Skeleton from *Salvia prattii*. *Nat. Prod. Commun.* **2017**, 12, 1177–1179.

References :

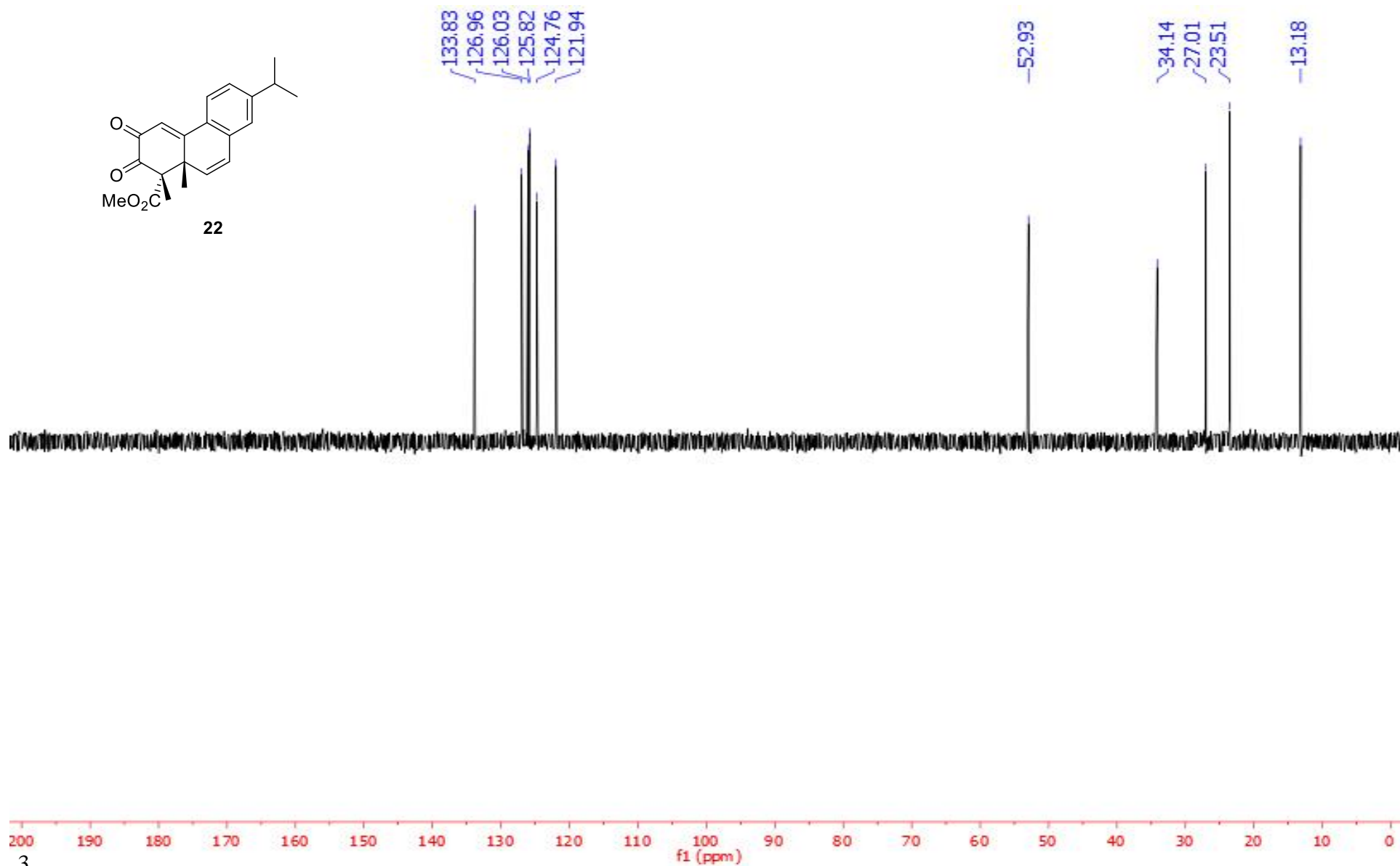
1. Tanaka, N.; Yamada, K.; Shimomoto, Y.; Tsuji, D.; Itoh, K.; Kawazoe, K.; Kashiwada, Y. Lophachinins A–E, Abietane Diterpenes from a Mongolian Traditional Herbal Medicine *Lophanthus chinensis*. *Fitoterapia* **2020**, *146*, 104702.
2. Ait El Had, M.; Guardia, J.J.; Ramos, J.M.; Taourirte, M.; Chahboun, R.; Alvarez-Manzaneda, E. Bioinspired Synthesis of Pygmaecins and Related Rearranged Abietane Diterpenes: Synthesis of Viridoquinone. *Org. Lett.* **2018**, *20*, 5666–5670.
3. Wu, W.M.; Liu, Y.; Chen, X.; Jin, A.; Zhou, M.; Tian, T.; Ruan, H.L. Diterpenoids from the Branch and Leaf of *Abies fargesii*. *Fitoterapia* **2016**, *110*, 123–128.
4. González-Cardenete, M.A.; Hamulic, D.; Miquel-Leal, F.J.; González-Zapata, N.; Jimenez-Jarava, O.J.; Brand, Y.M.; Marín, M.L. Antiviral Profiling of C-18-or C-19-Functionalized Semisynthetic Abietane Diterpenoids. *J. Nat. Prod.* **2022**, *85*, 2044–2051.
5. Domingo, V.; Prieto, C.; Silva, L.; Rodilla, J.M.; Quilez del Moral, J.F.; Barrero, A.F. Iodine, a Mild Reagent for the Aromatization of Terpenoids. *J. Nat. Prod.* **2016**, *79*, 831–837.
6. Kawabe, H.; Suzuki, R.; Hirota, H.; Matsuzaki, K.; Gong, X.; Ohsaki, A. A New Diterpenoid with a Rearranged Skeleton from *Salvia prattii*. *Nat. Prod. Commun.* **2017**, *12*, 1177–1179.

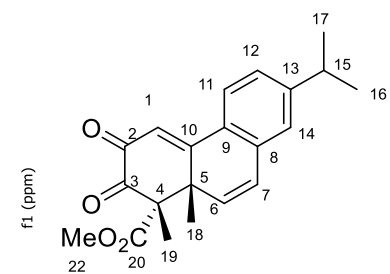
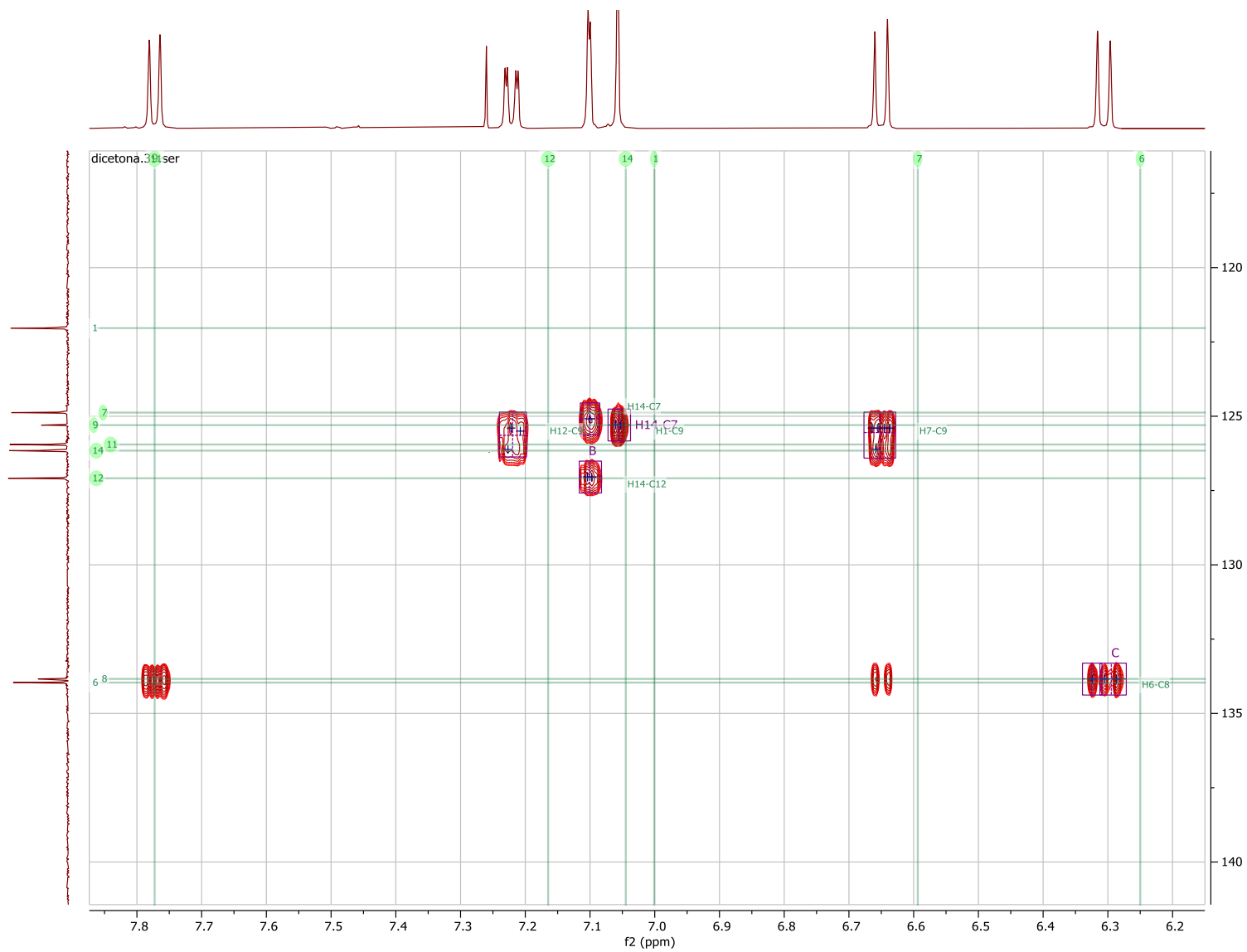


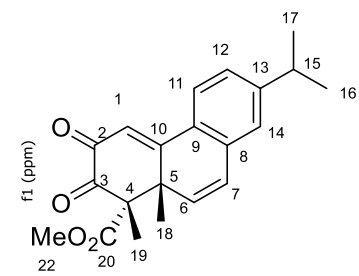
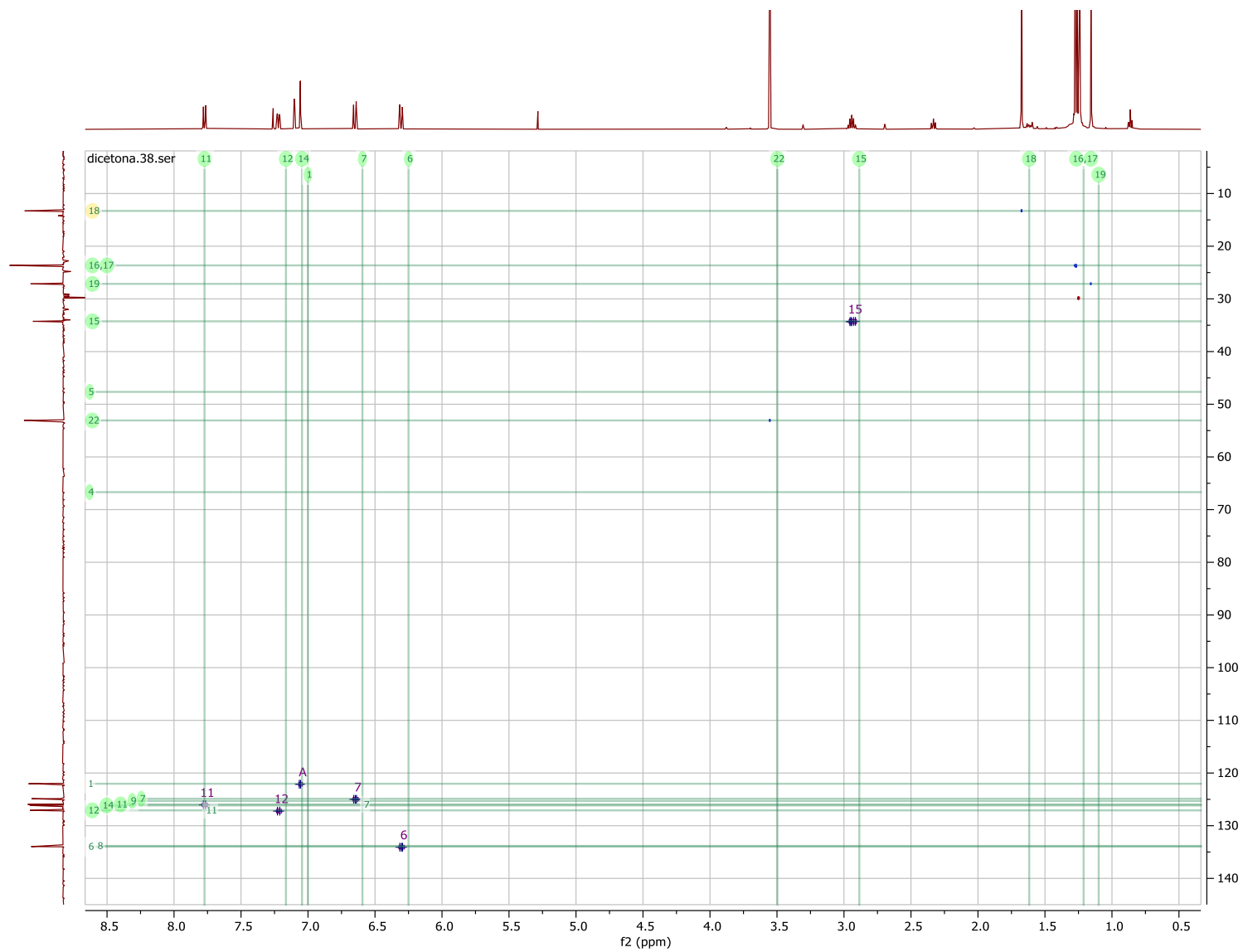


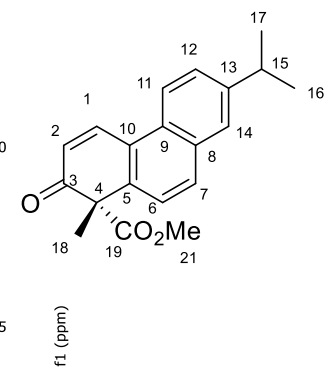
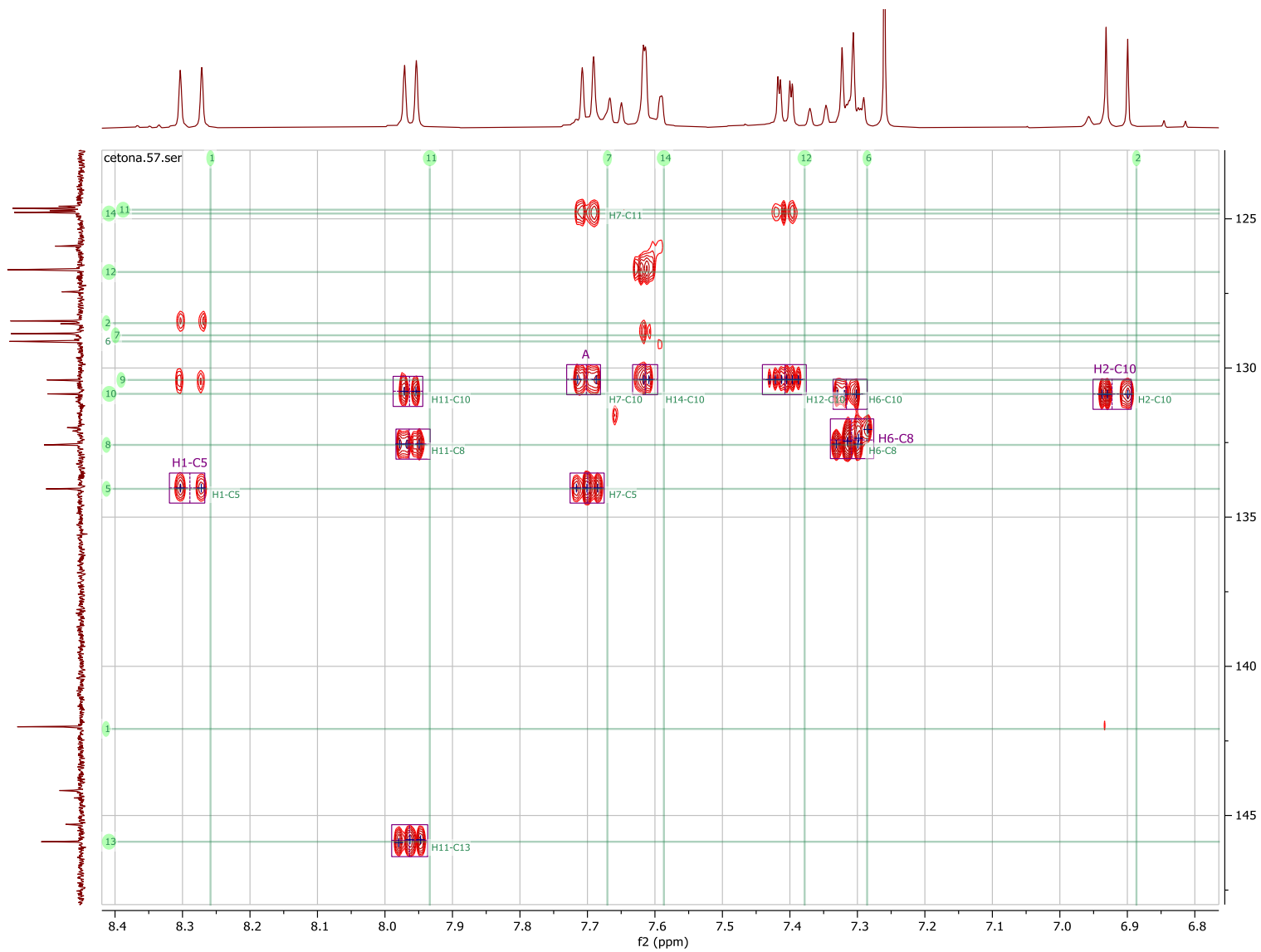


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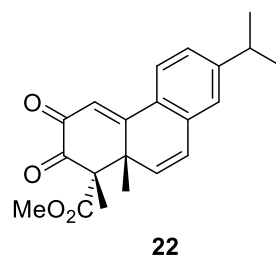






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340.1624

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361.1408

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251.1426

209.0957

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83.0125

489.3578

456.0861

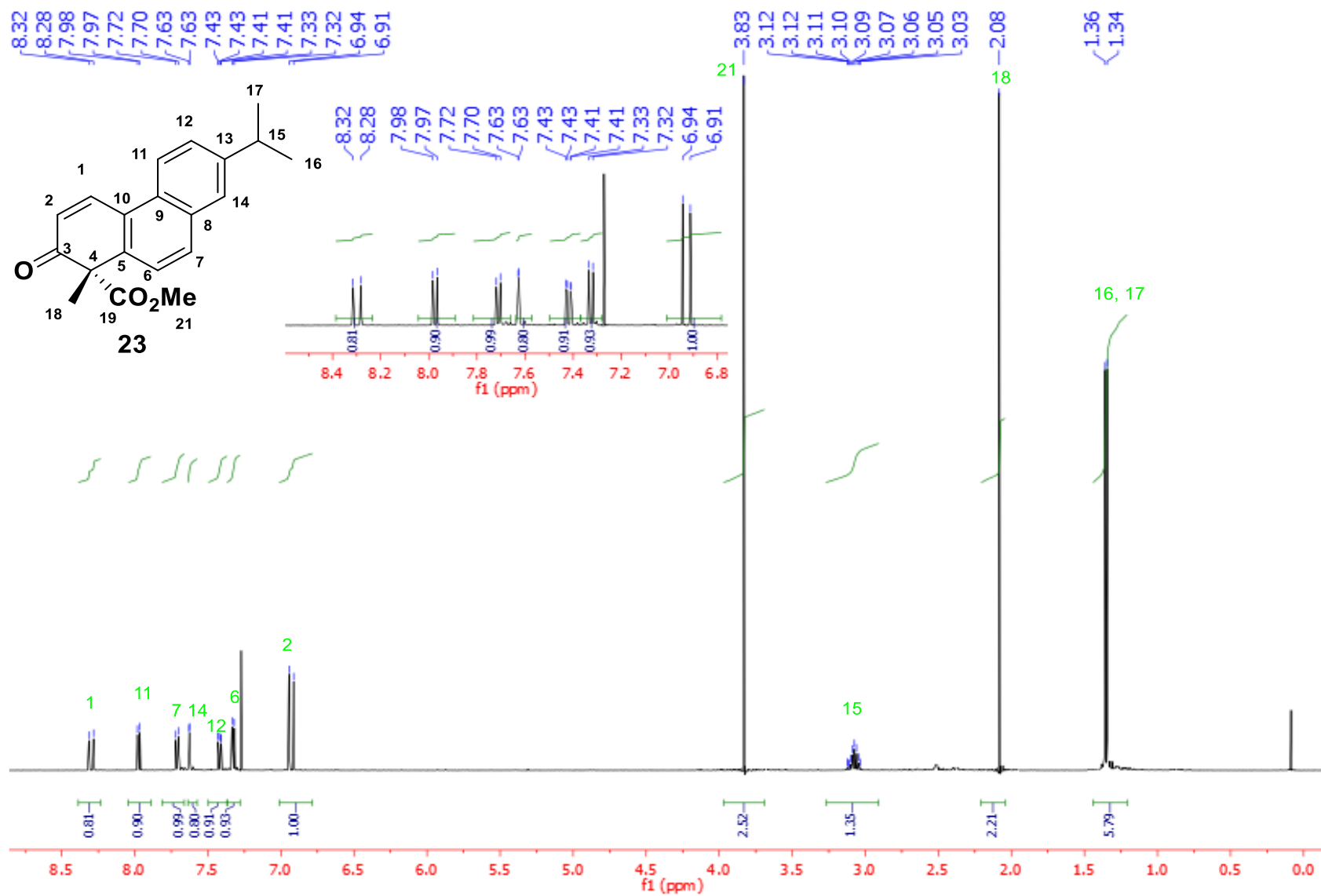
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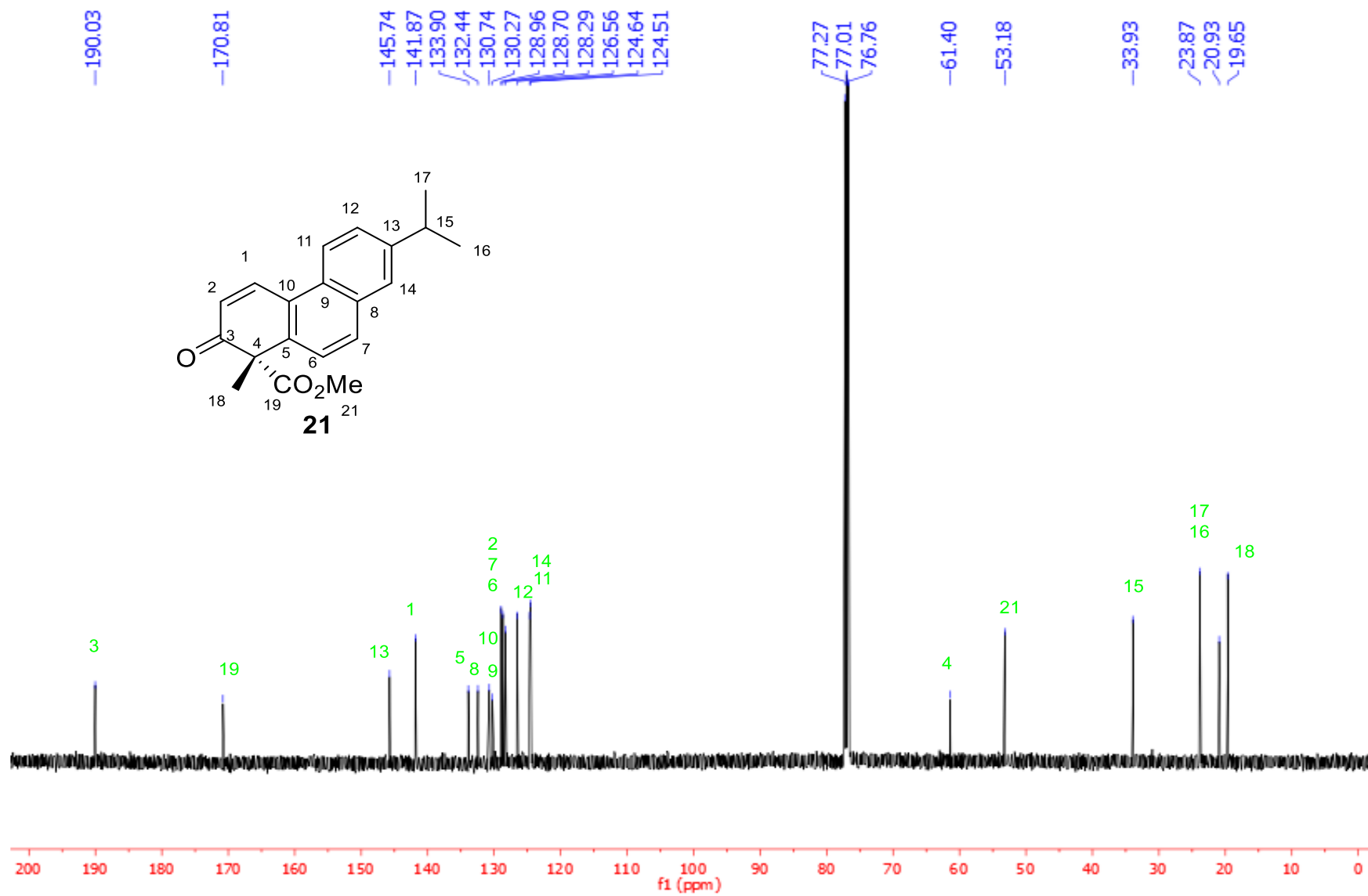
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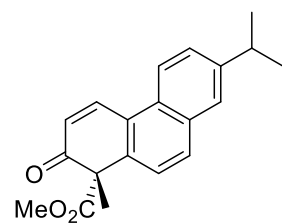
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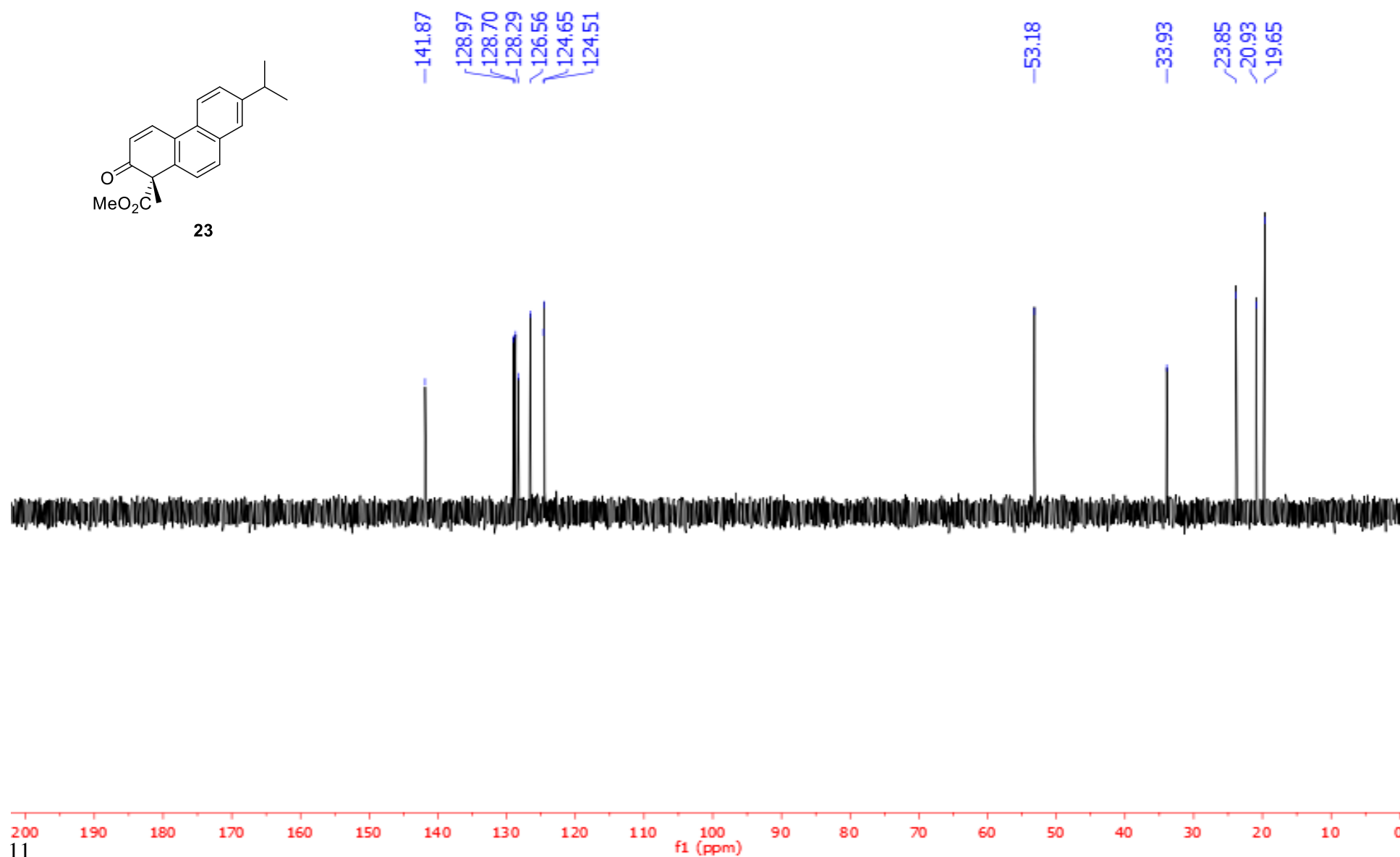
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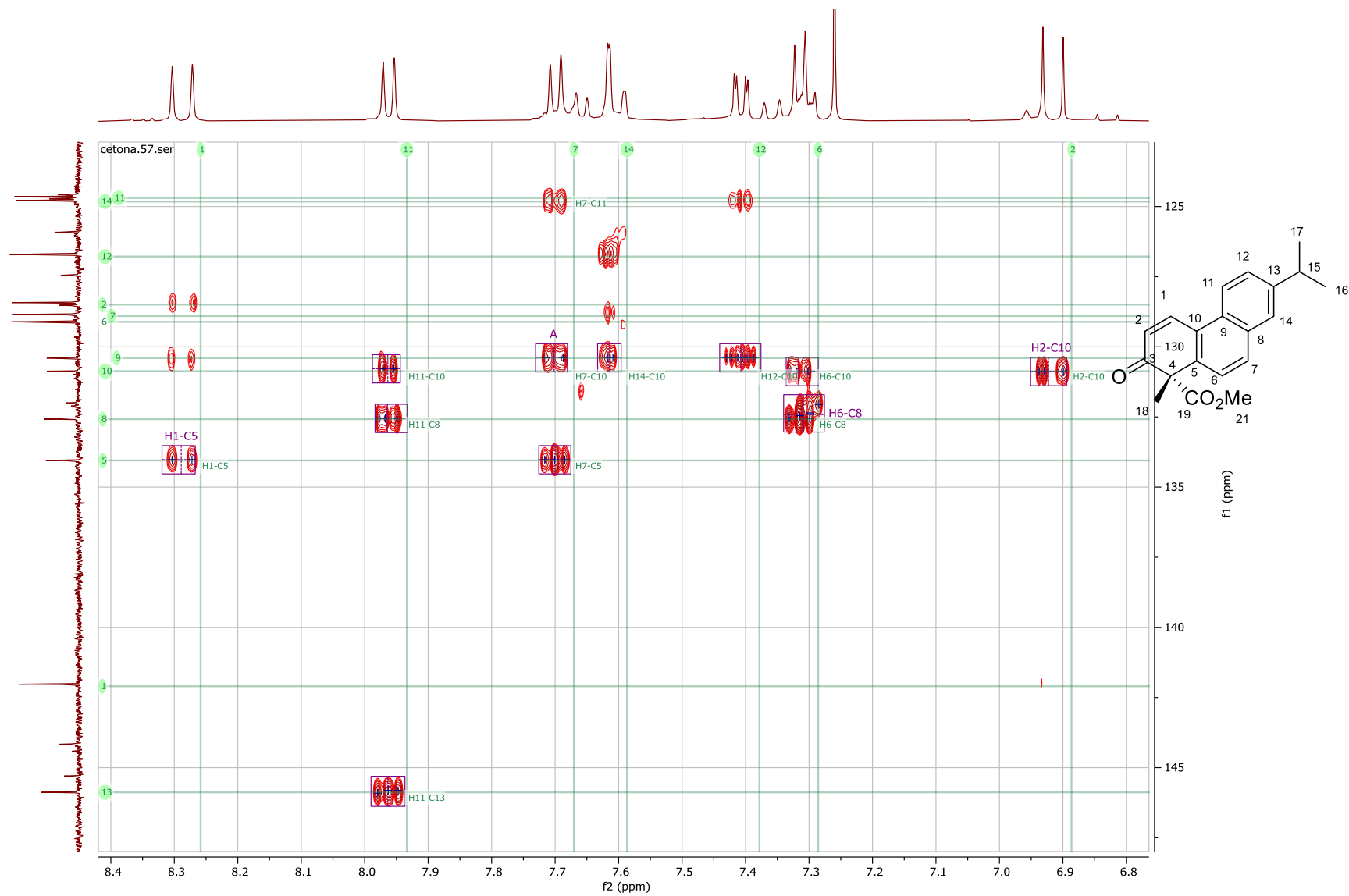


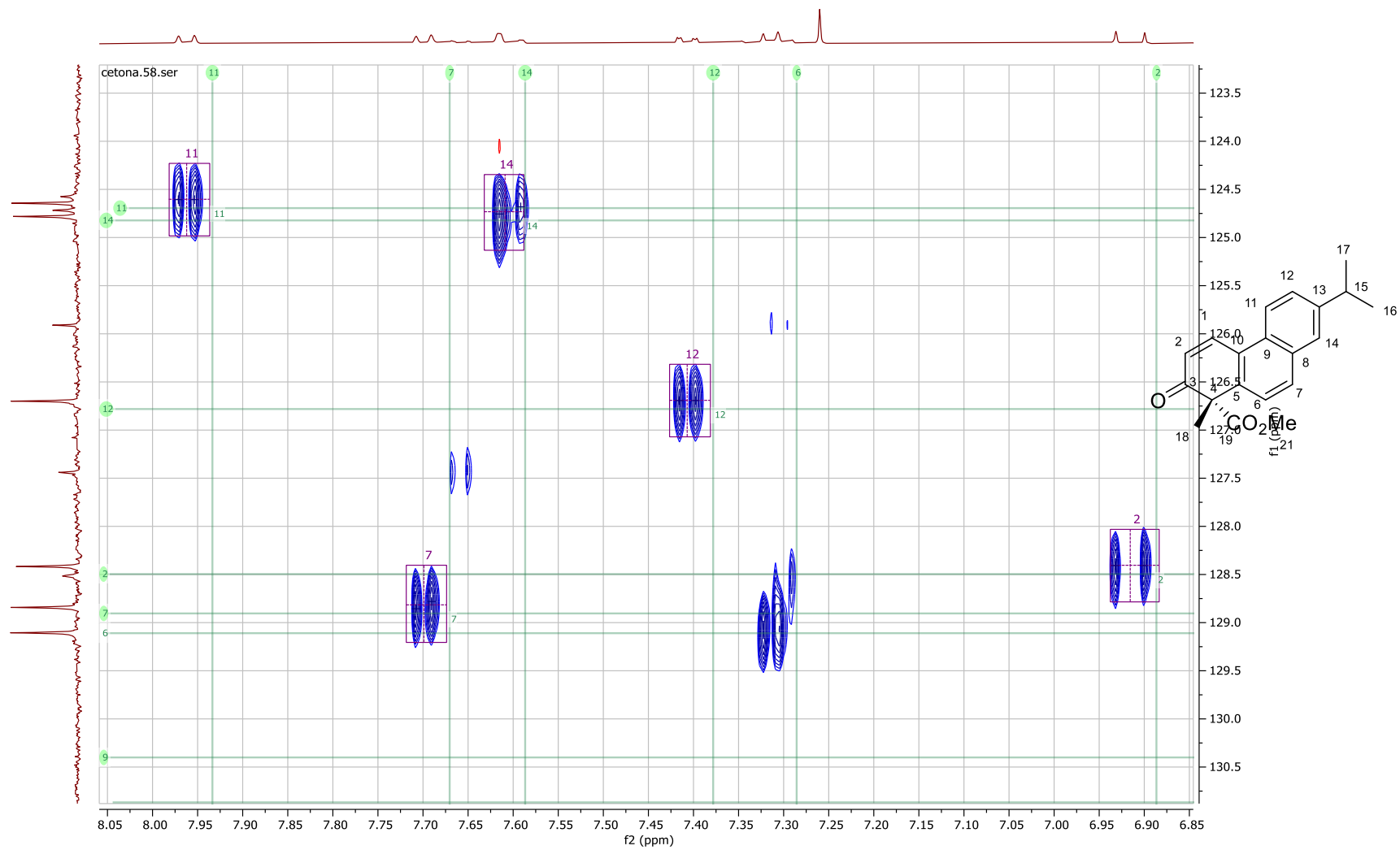


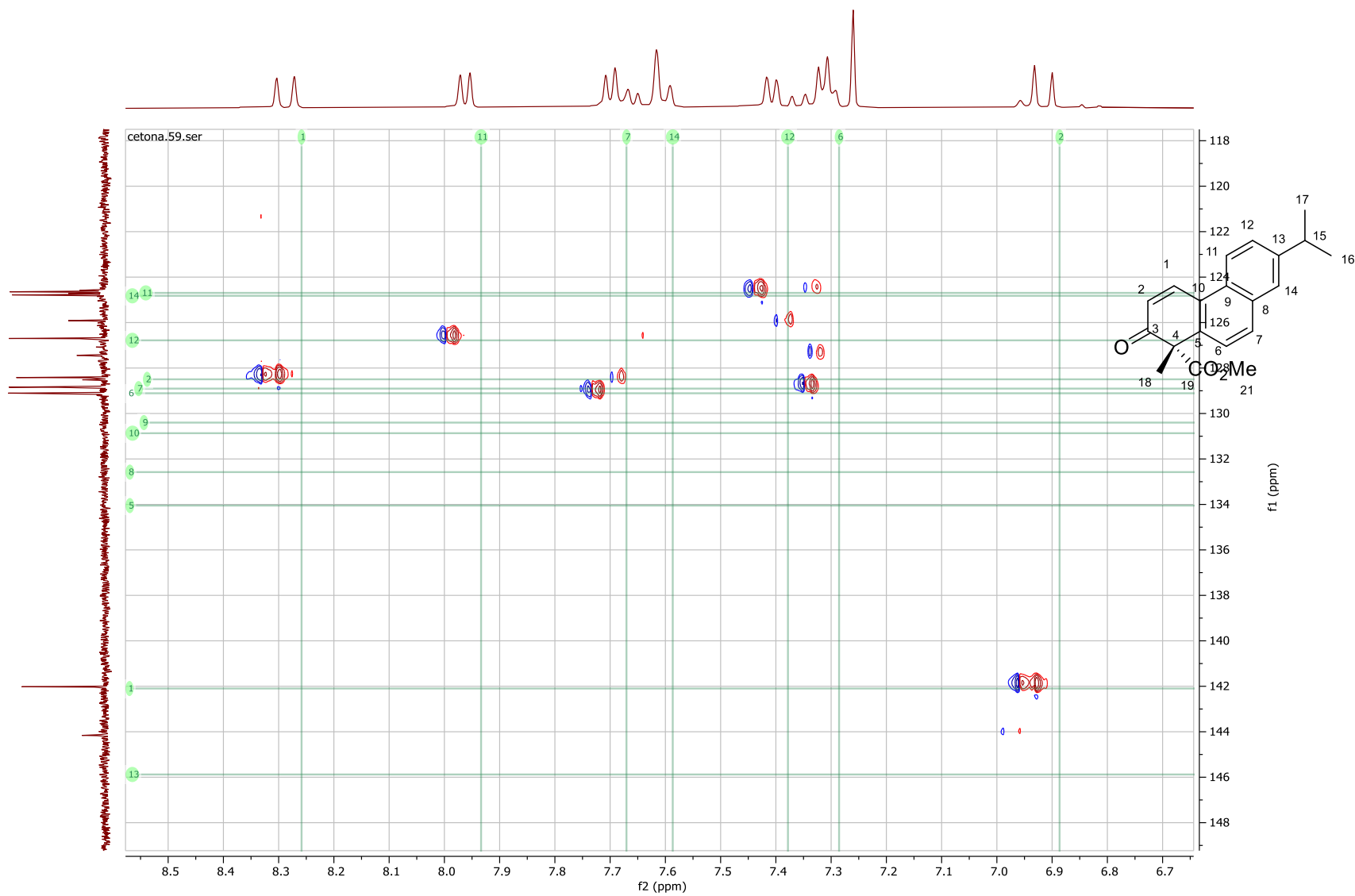


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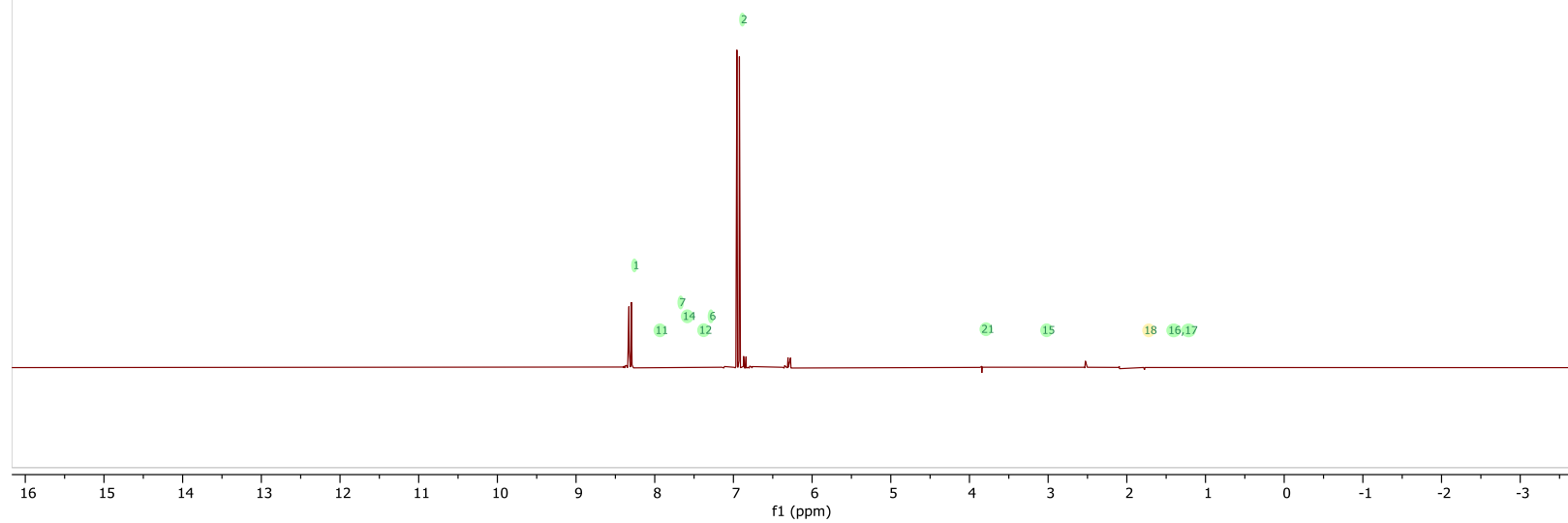
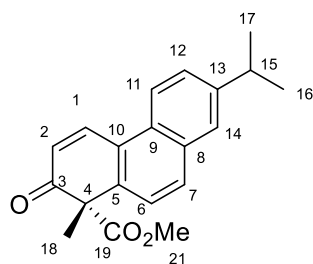






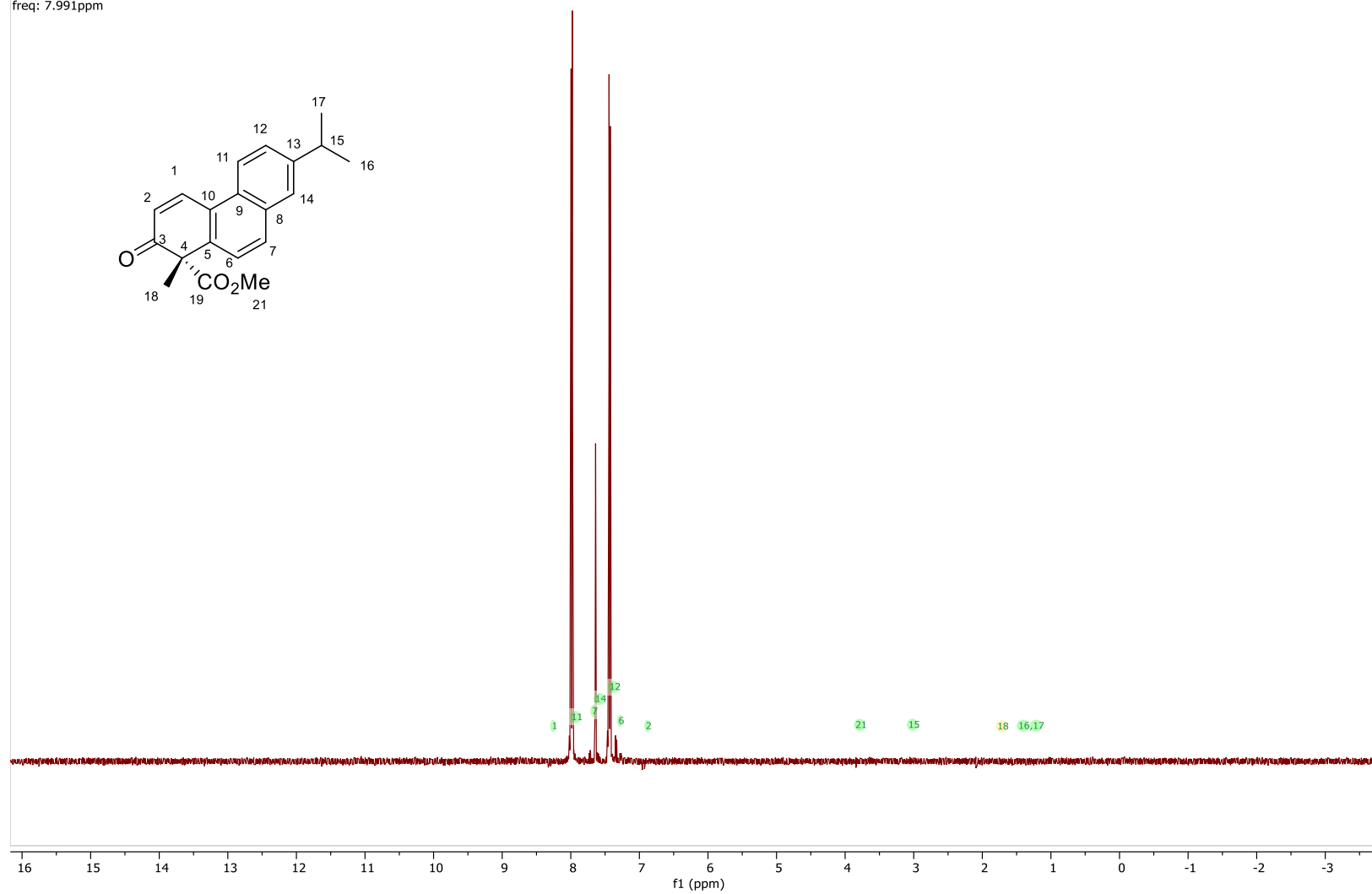
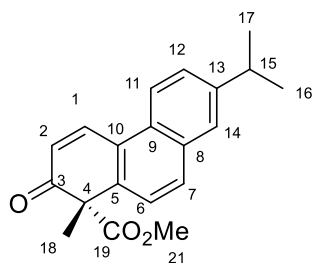
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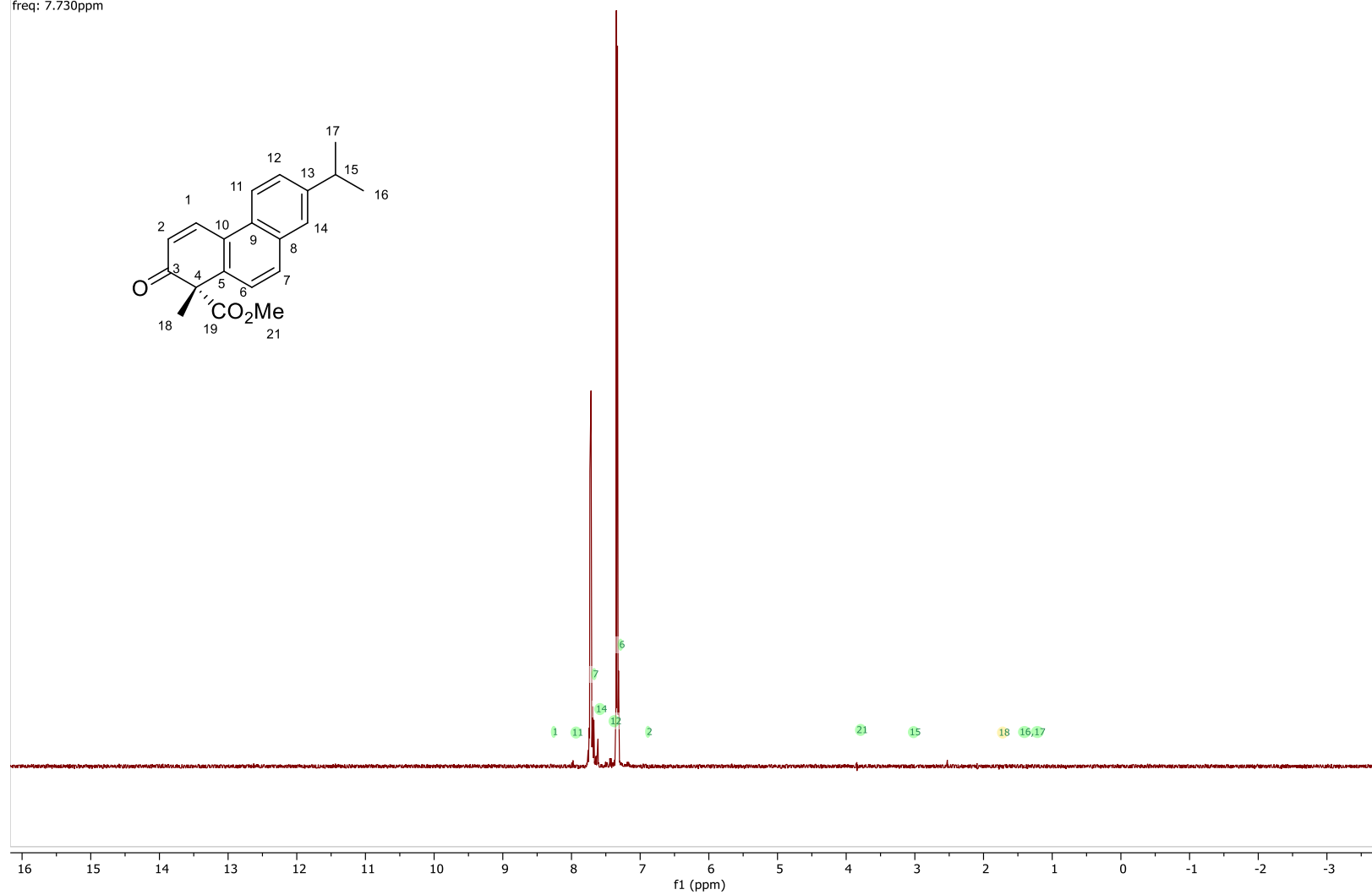
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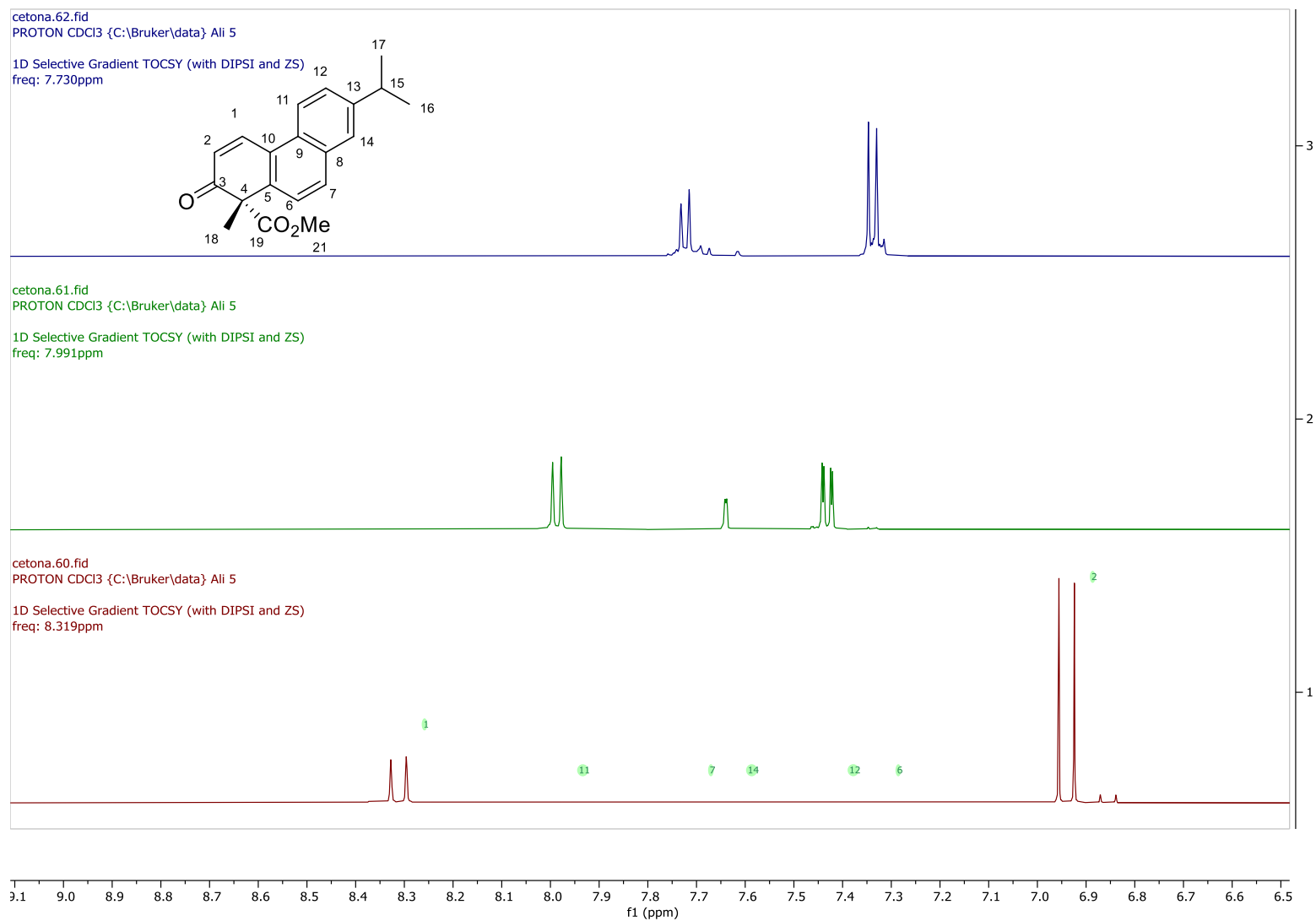
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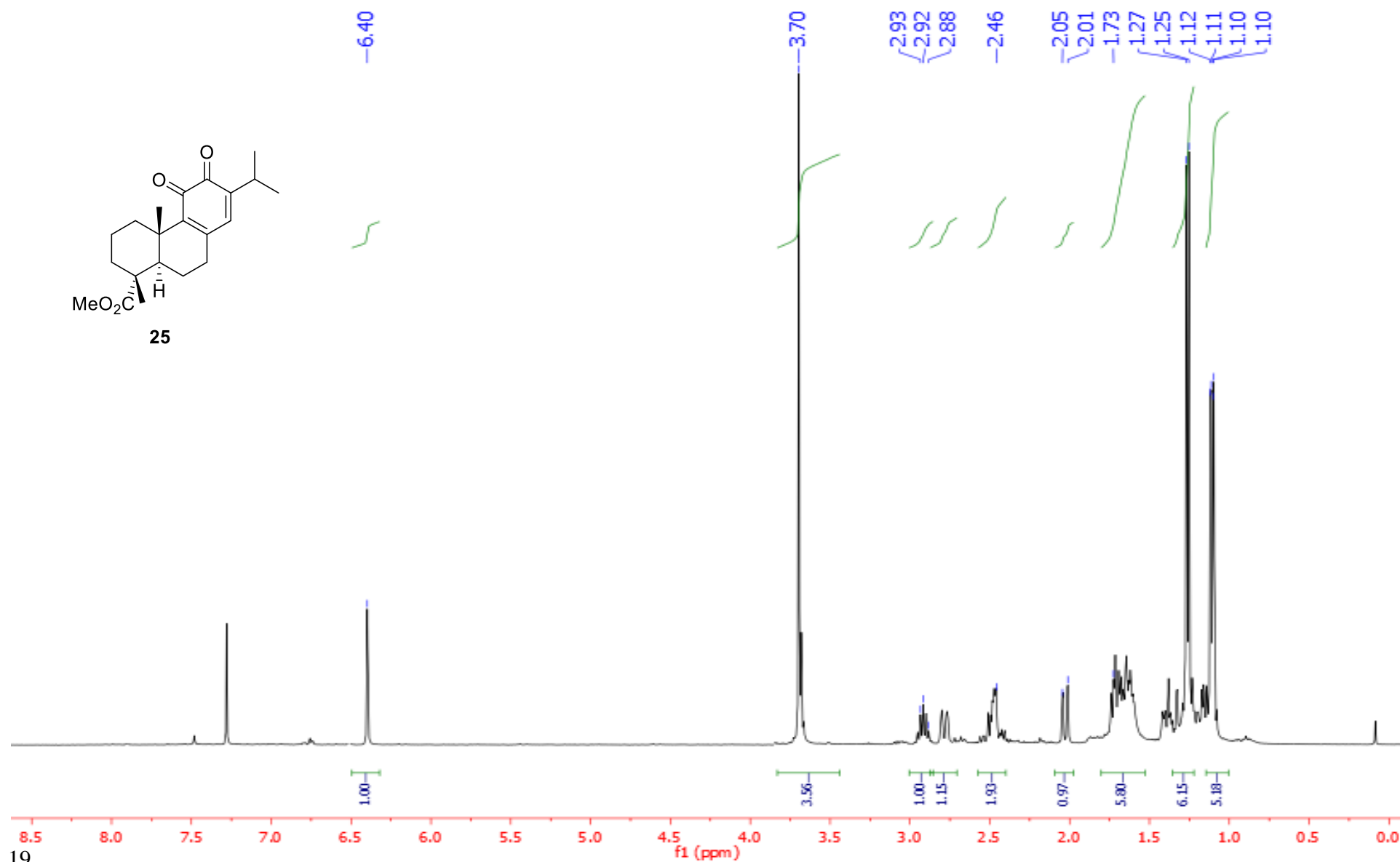
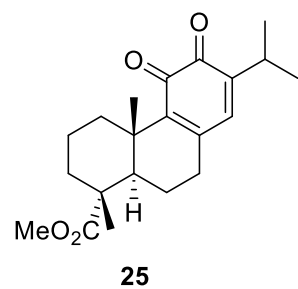


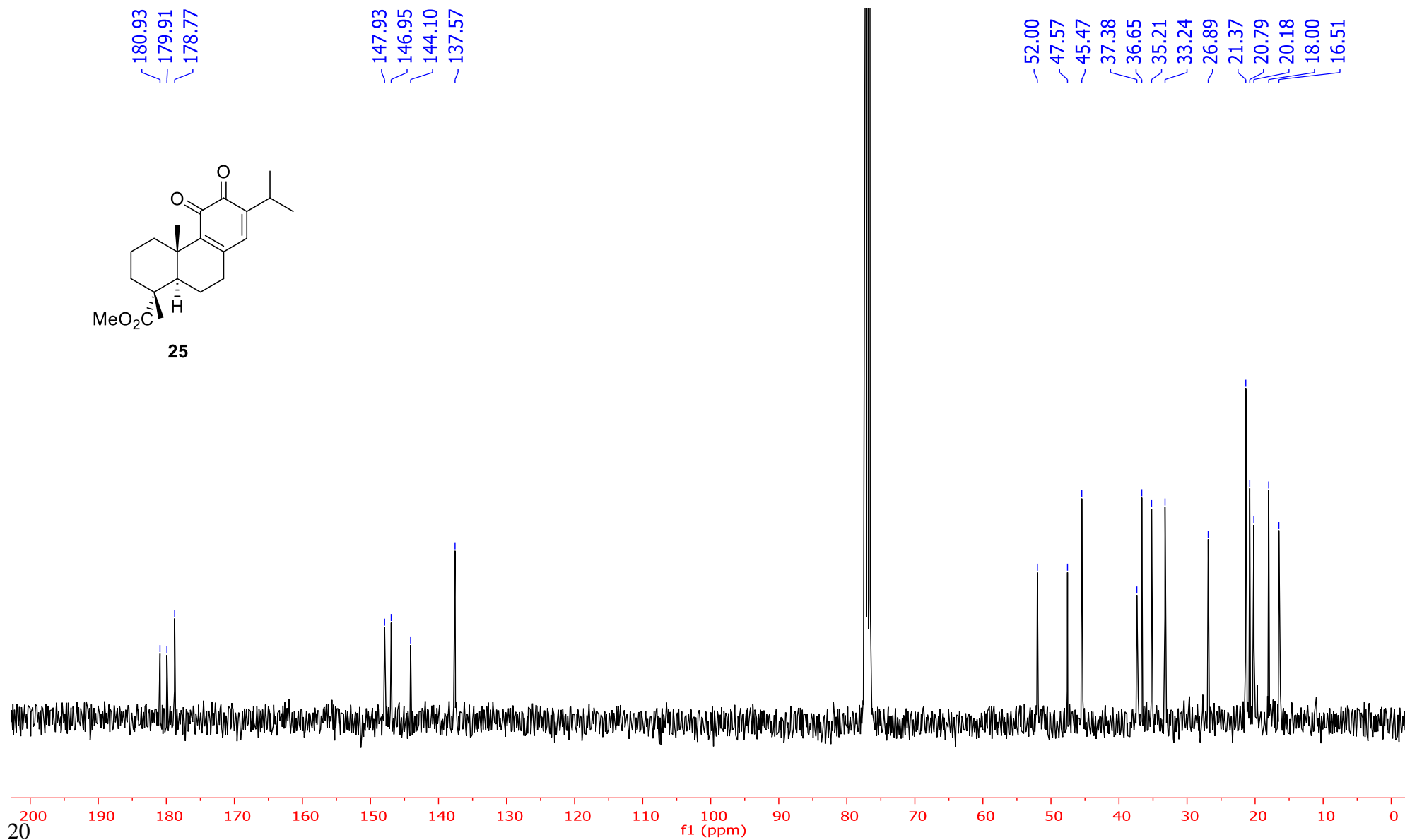
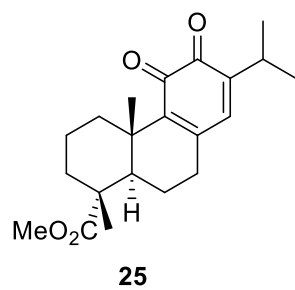
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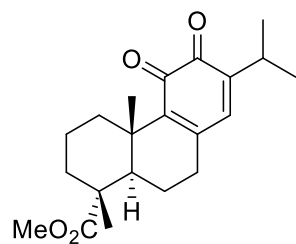
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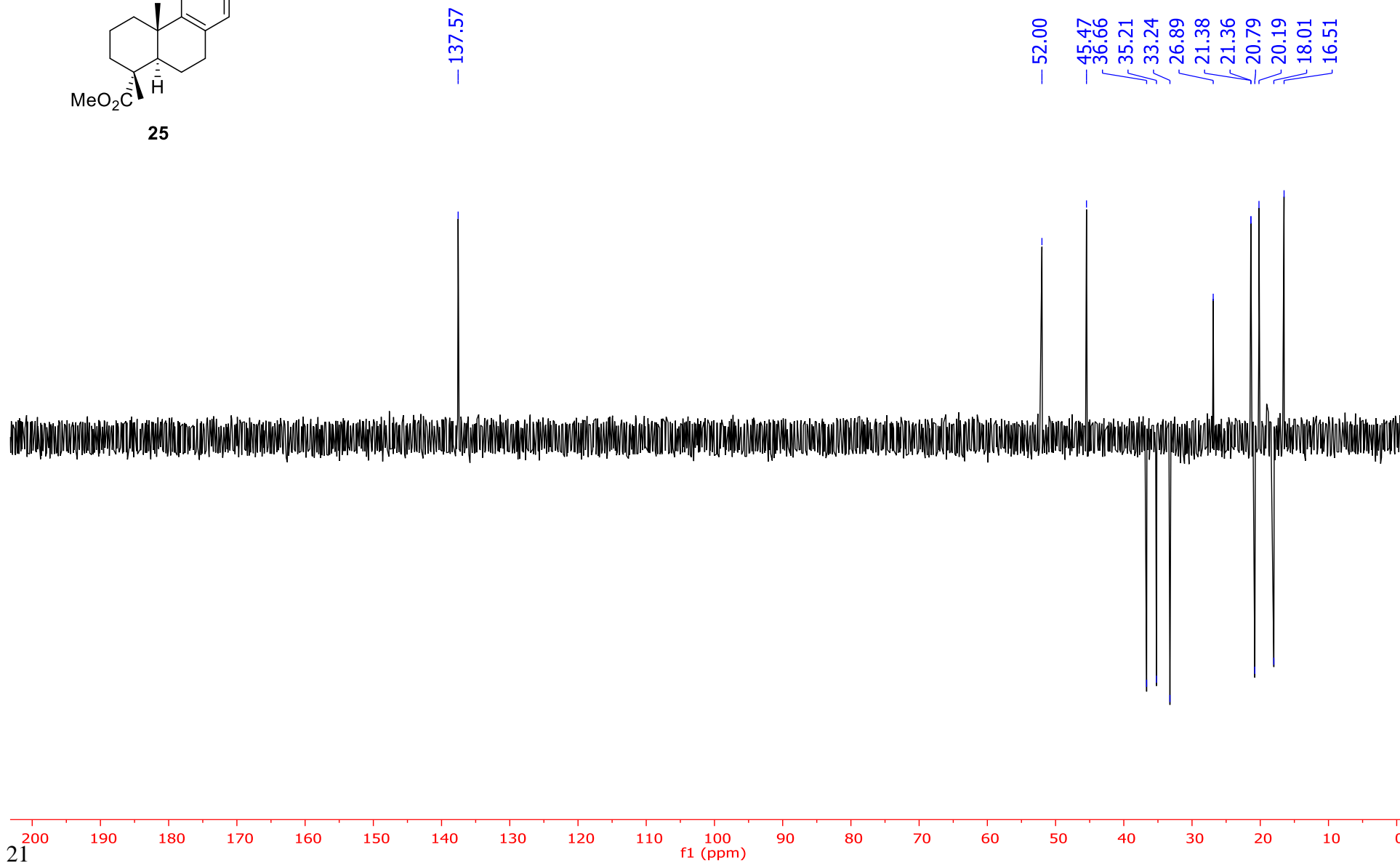


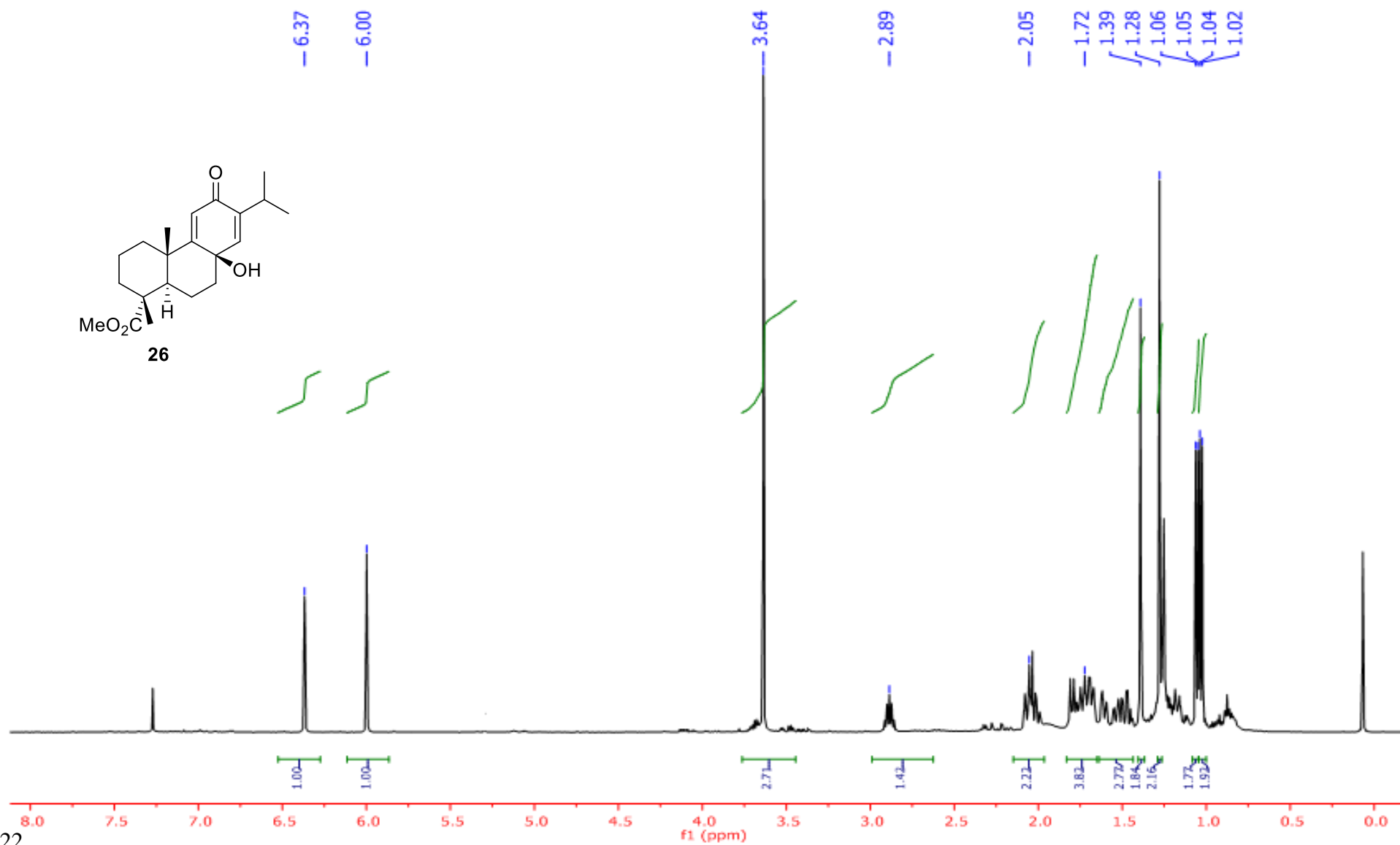


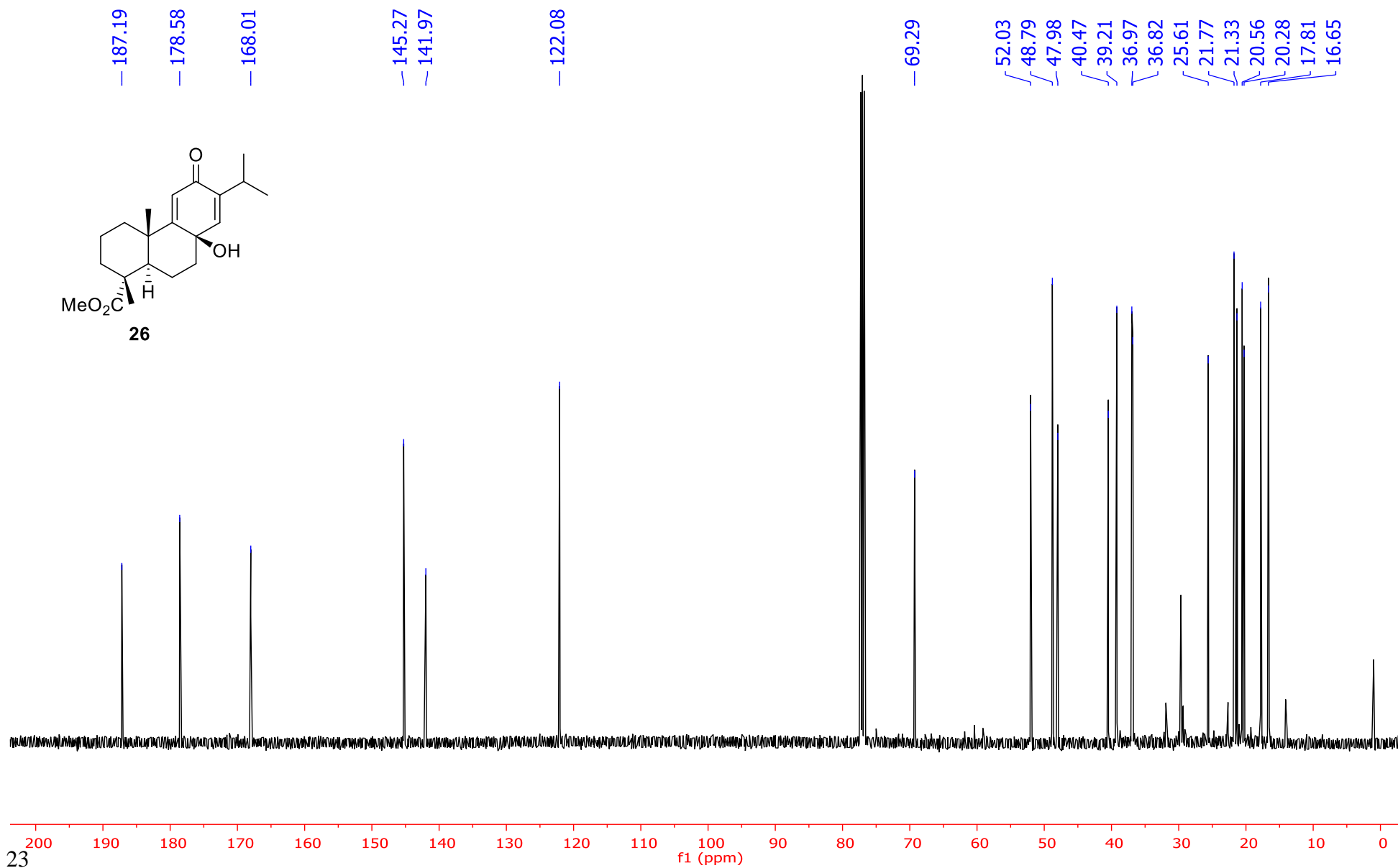
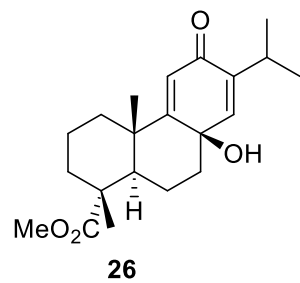


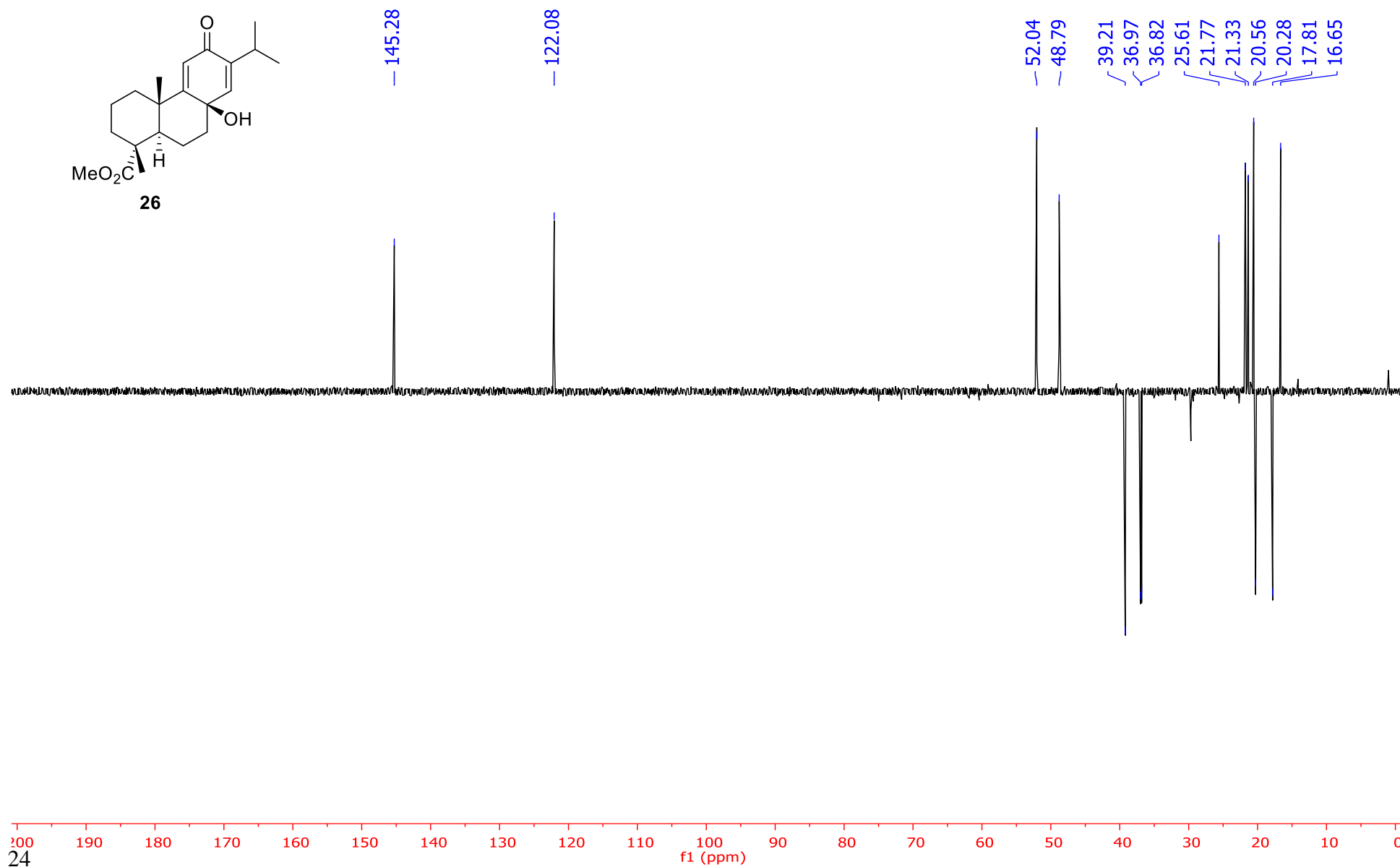
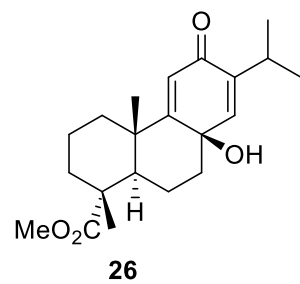


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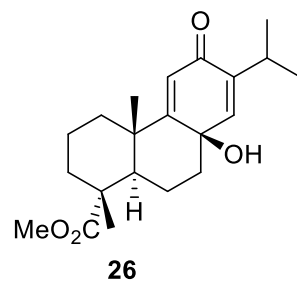




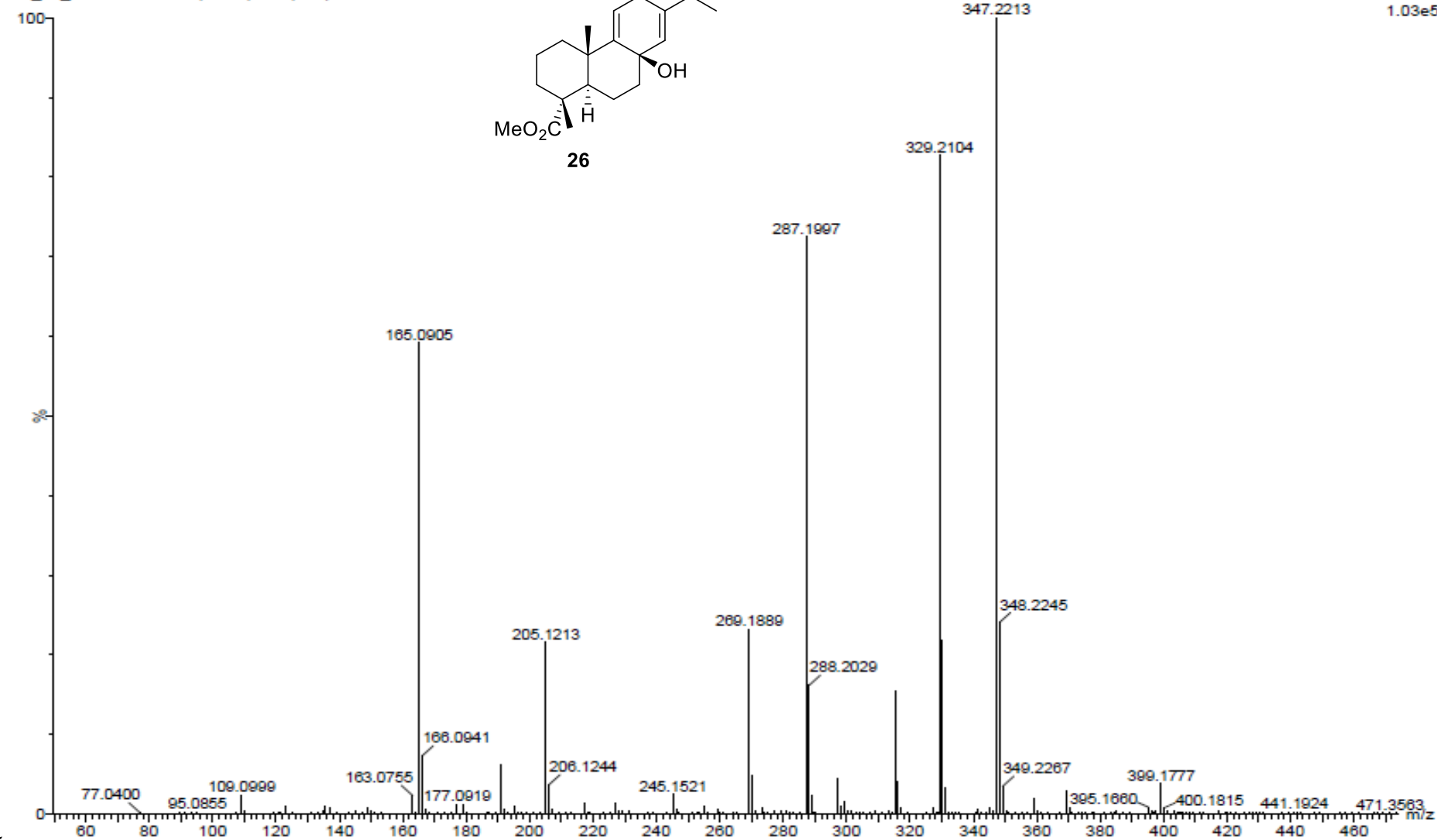


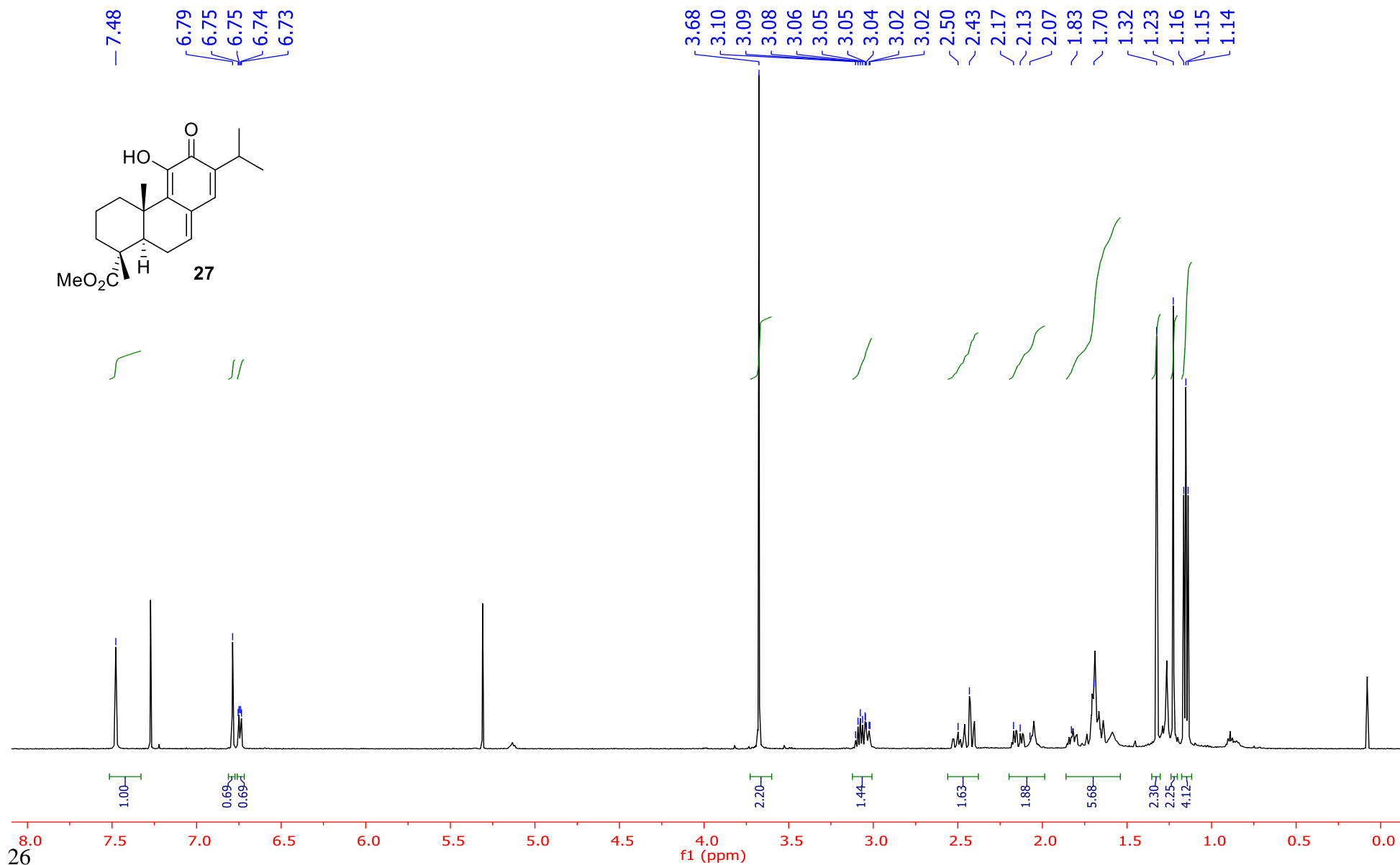


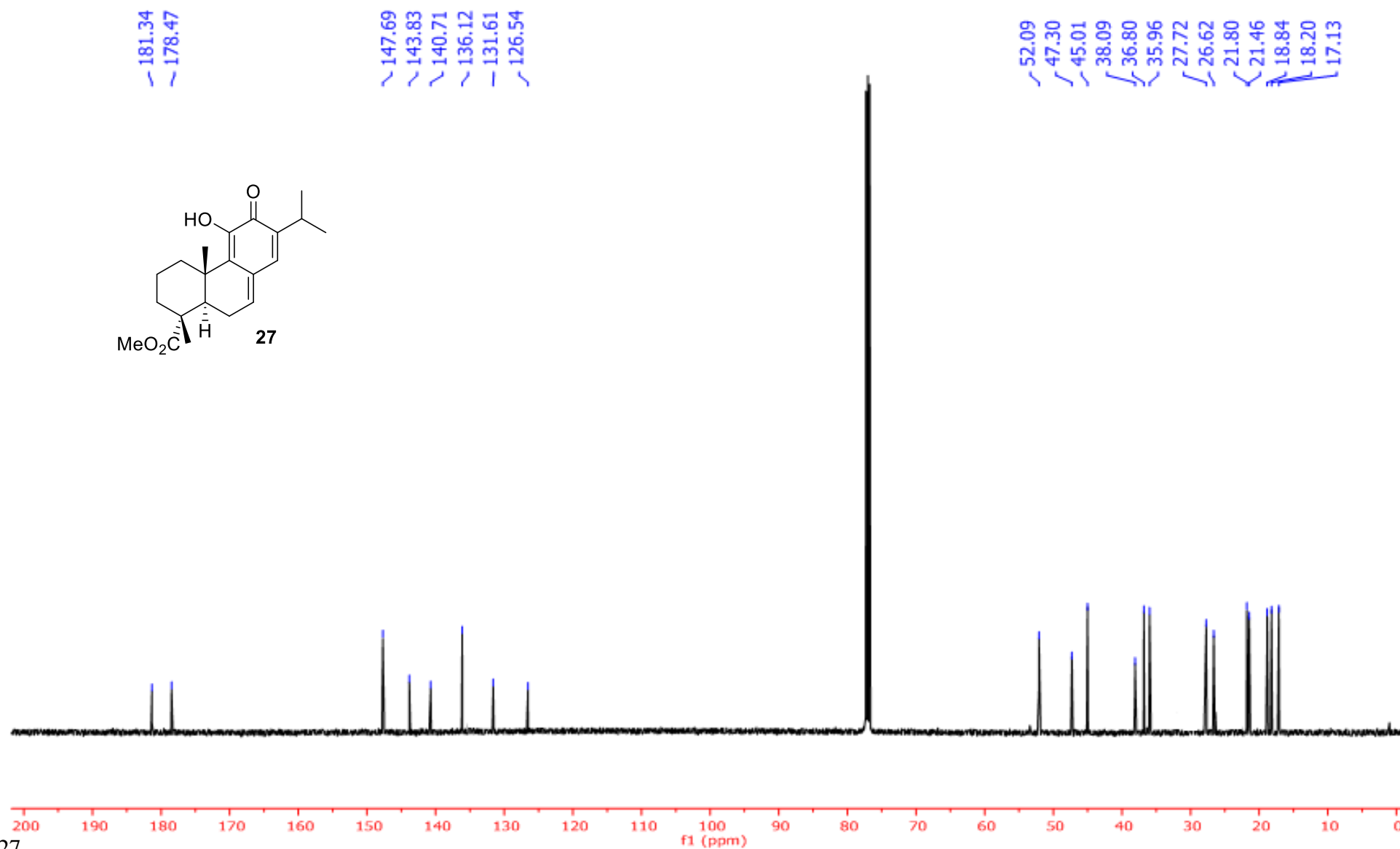
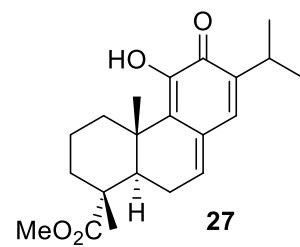
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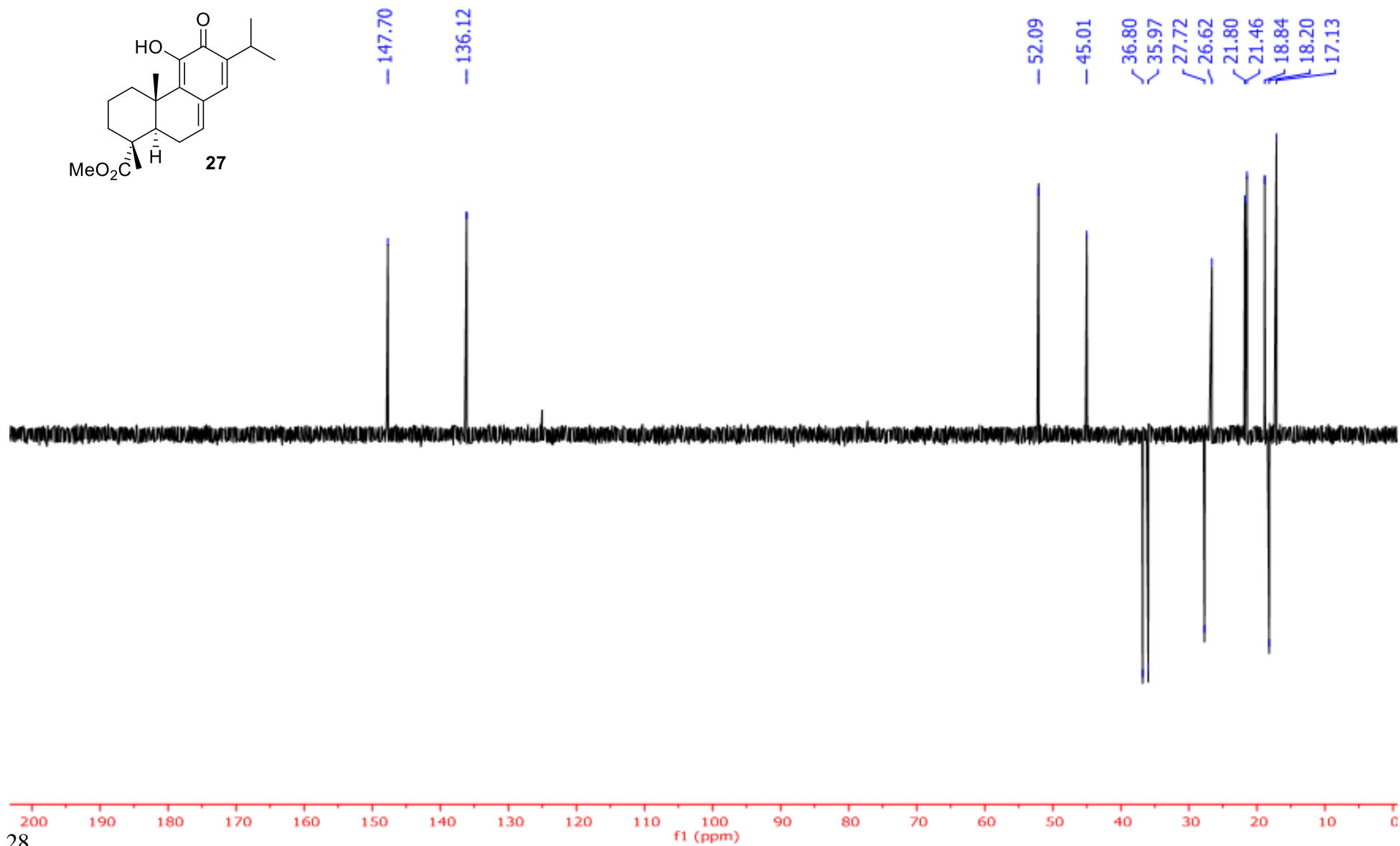
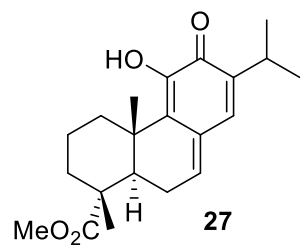


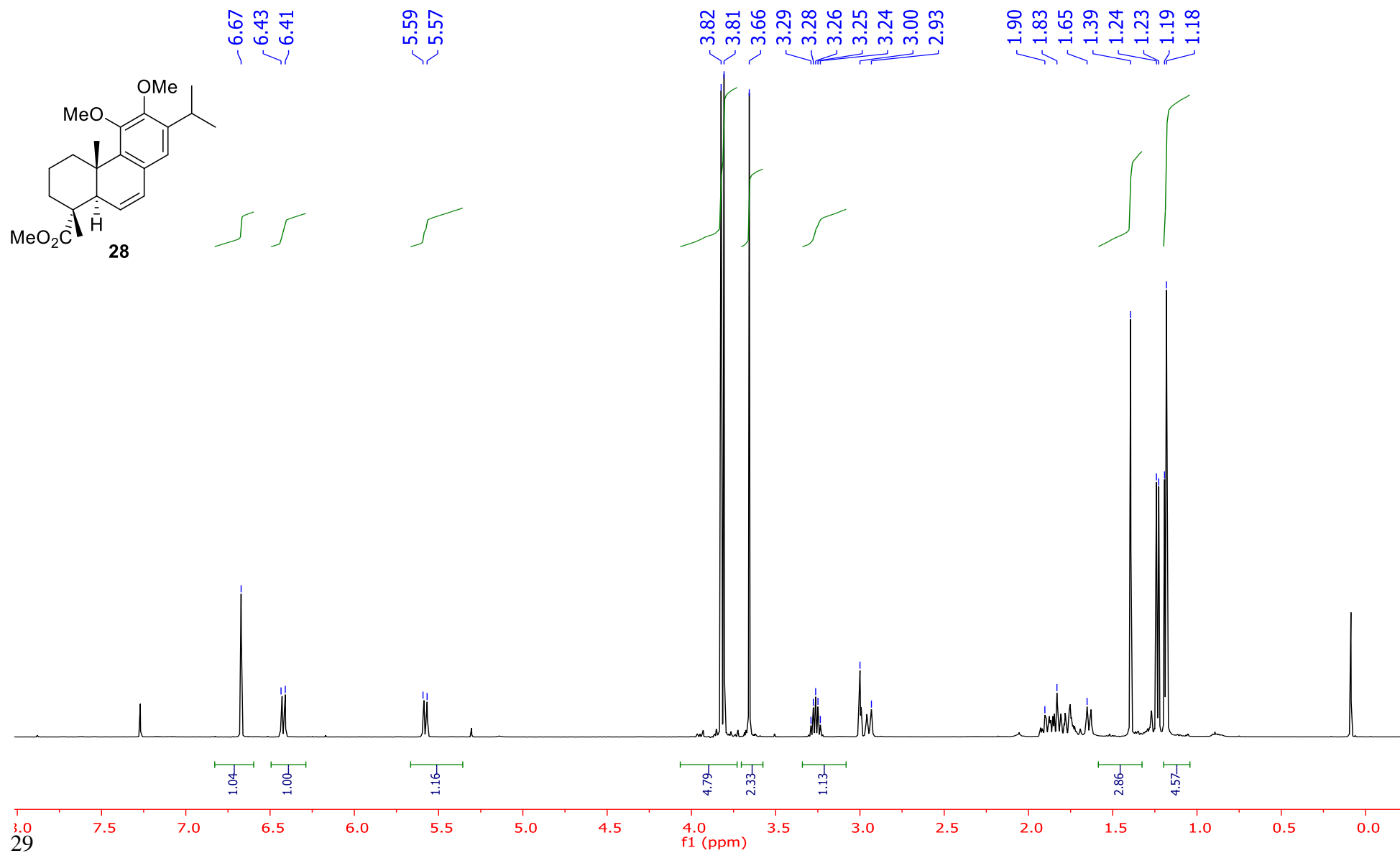
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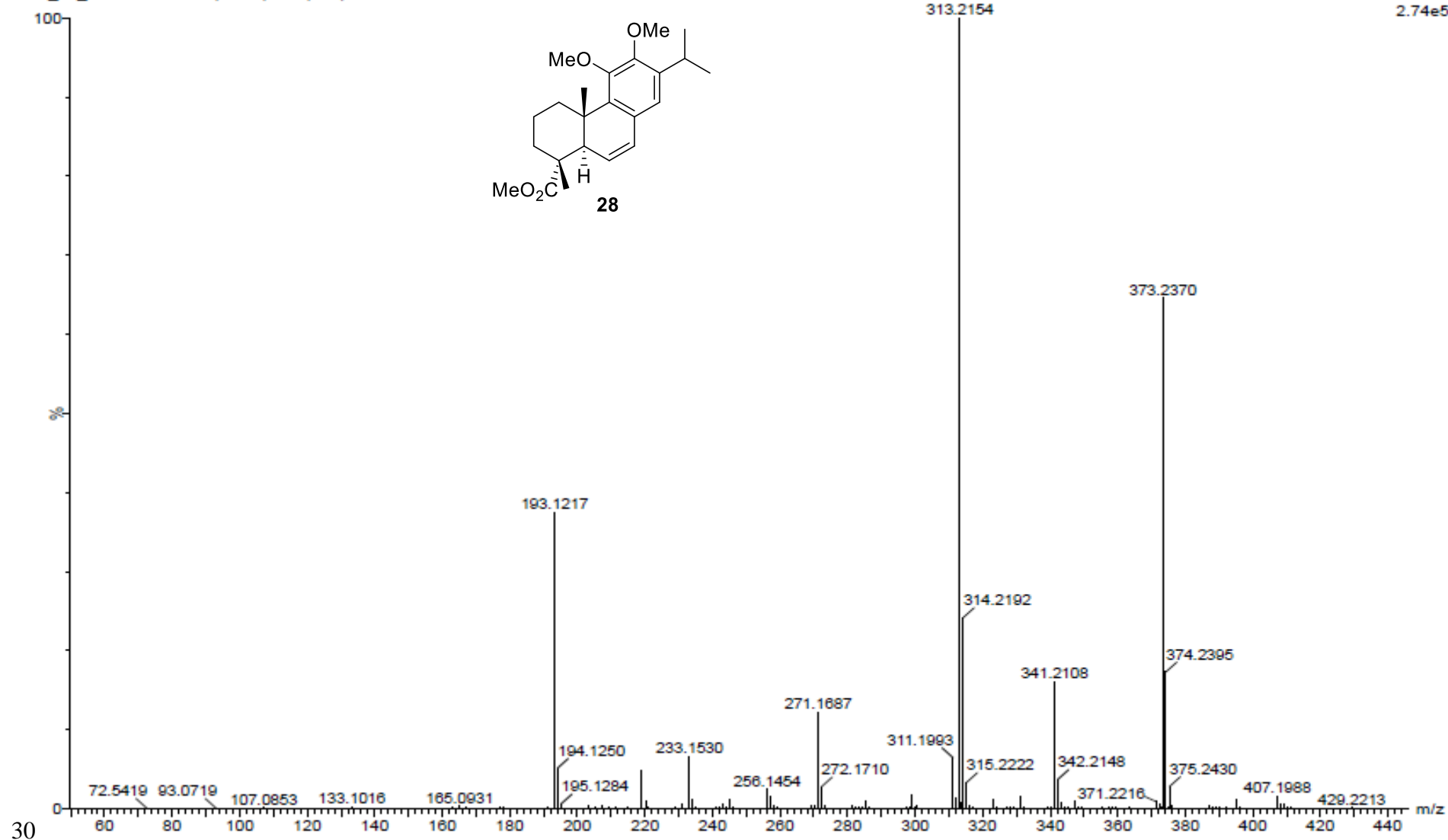
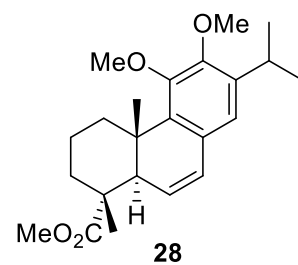


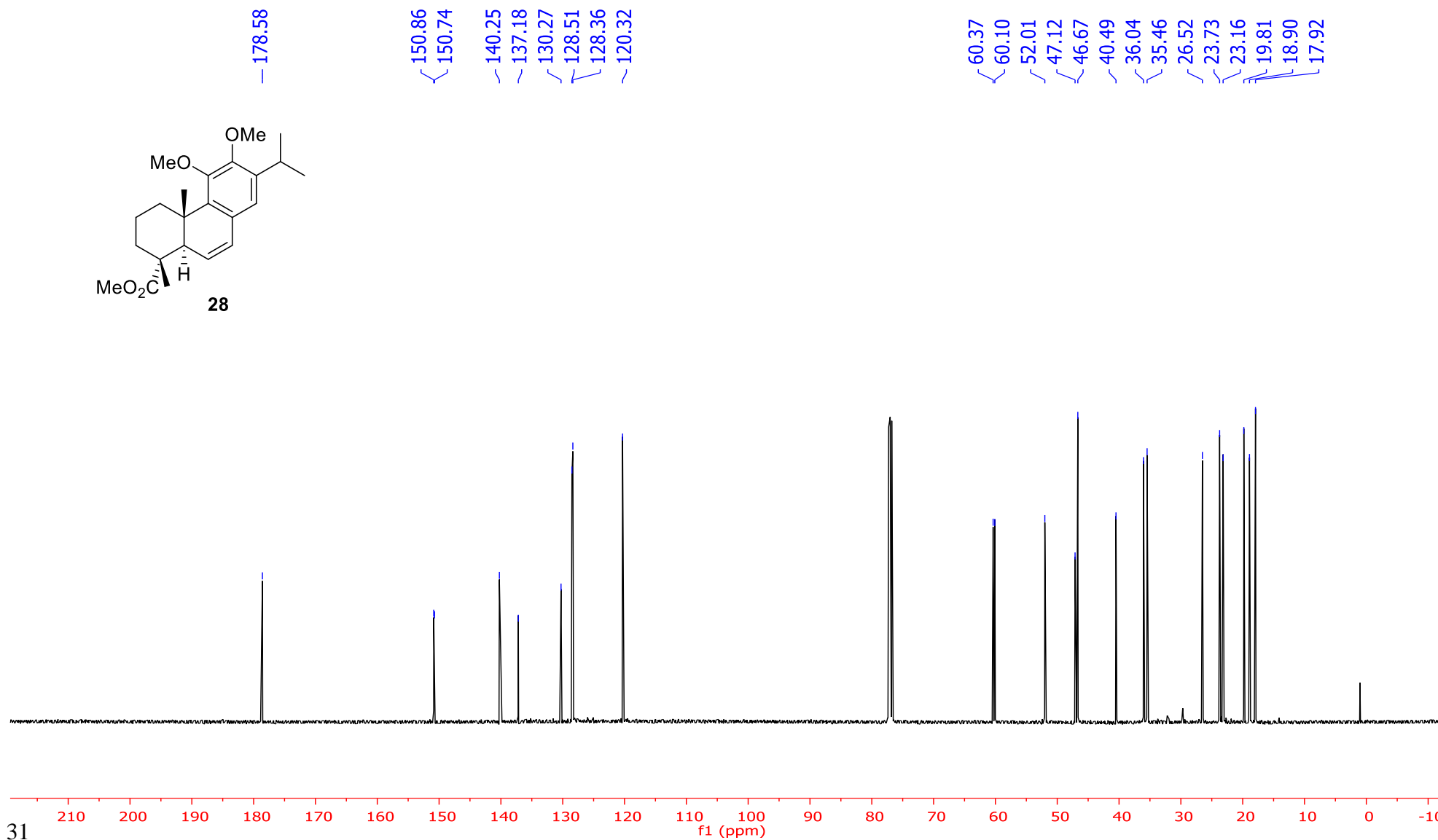
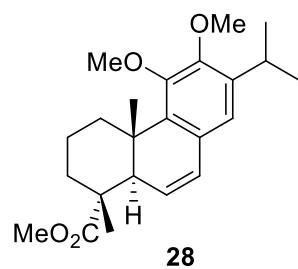


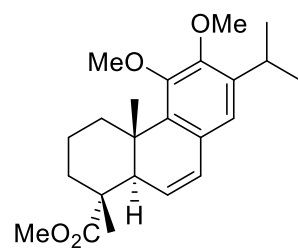


23_10_16 AMG 2 847 (6.468) Cm (847)

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28

128.51
128.36

120.32

60.37
60.10

52.01

46.67

36.04
35.46

26.51

23.73

23.16

19.81

18.90

17.92

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150

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120

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100

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40

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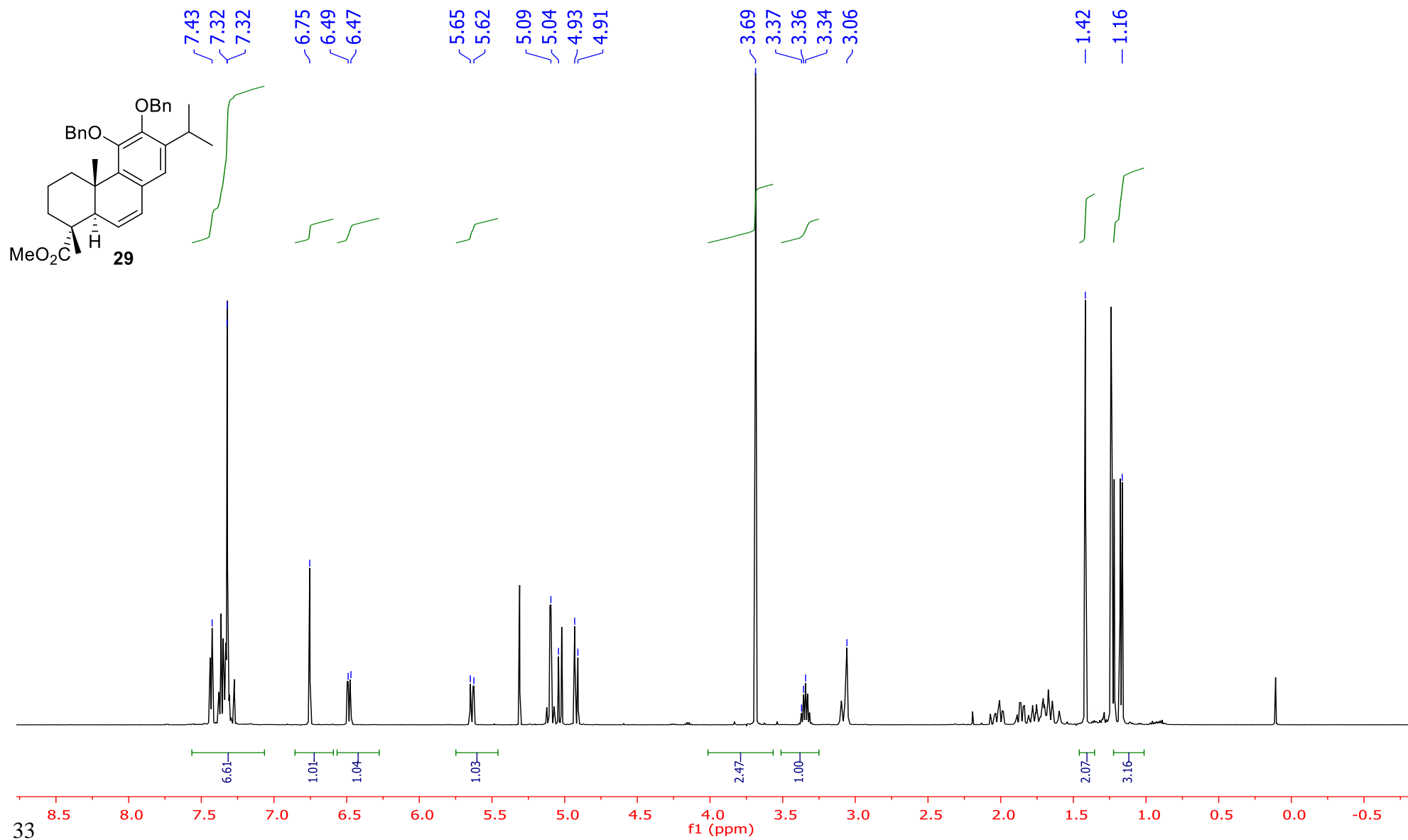
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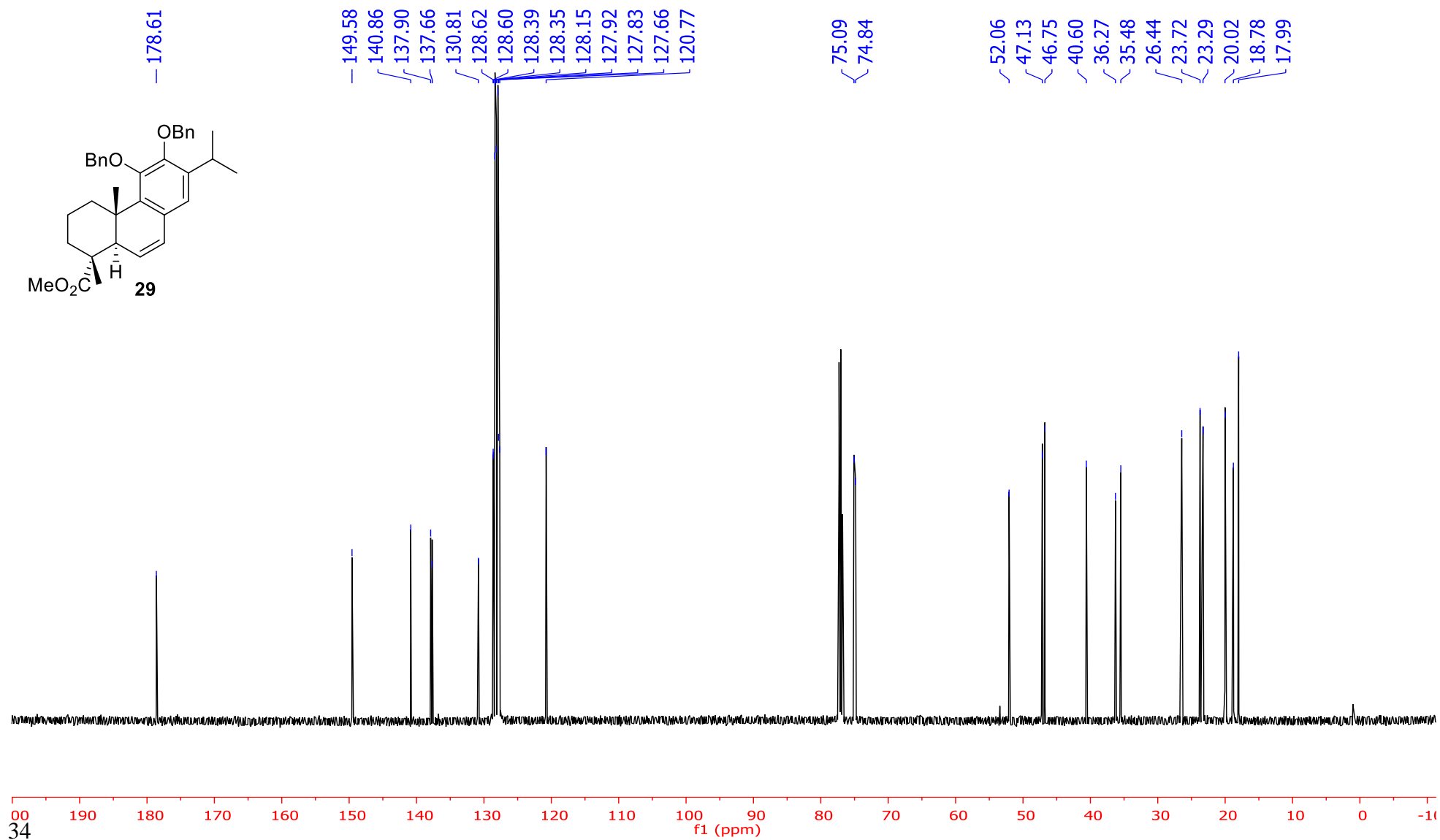
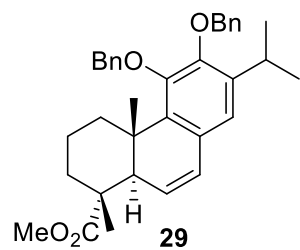
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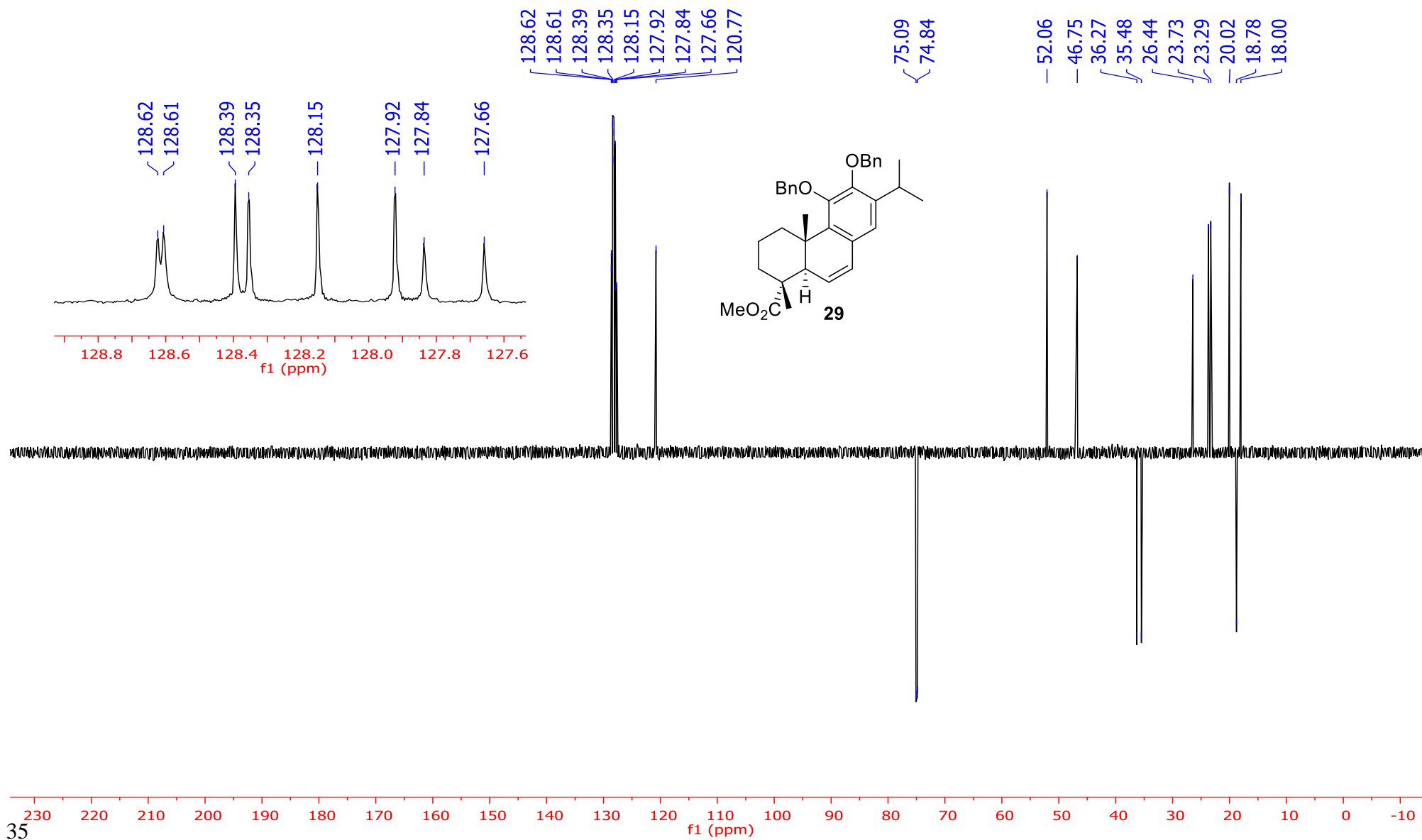
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f1 (ppm)

S53

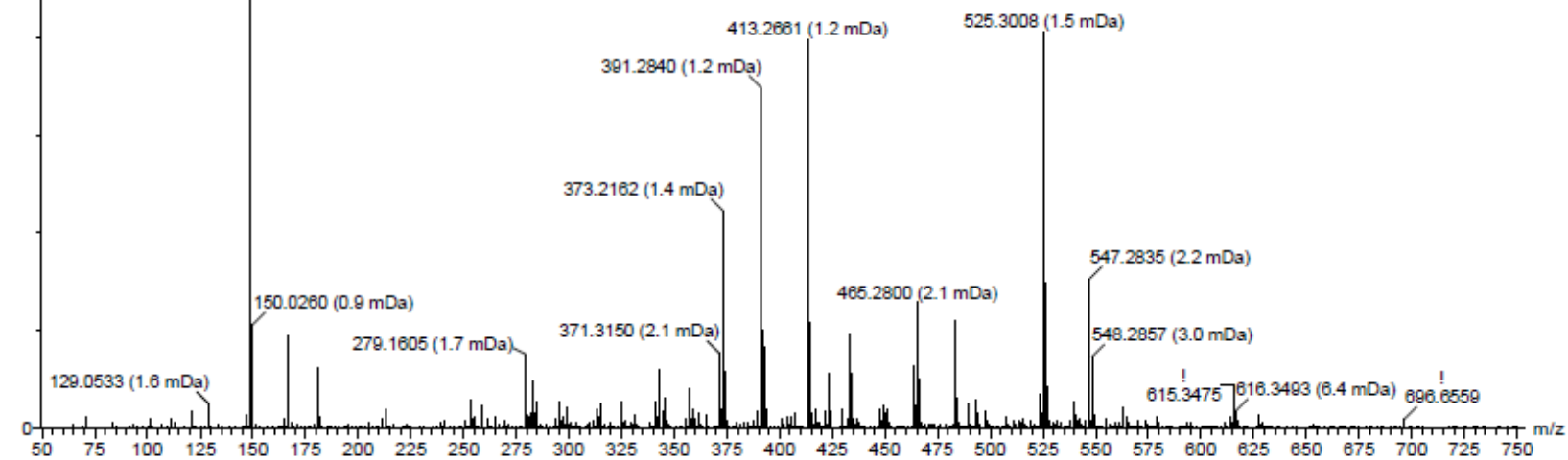
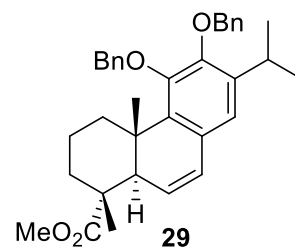


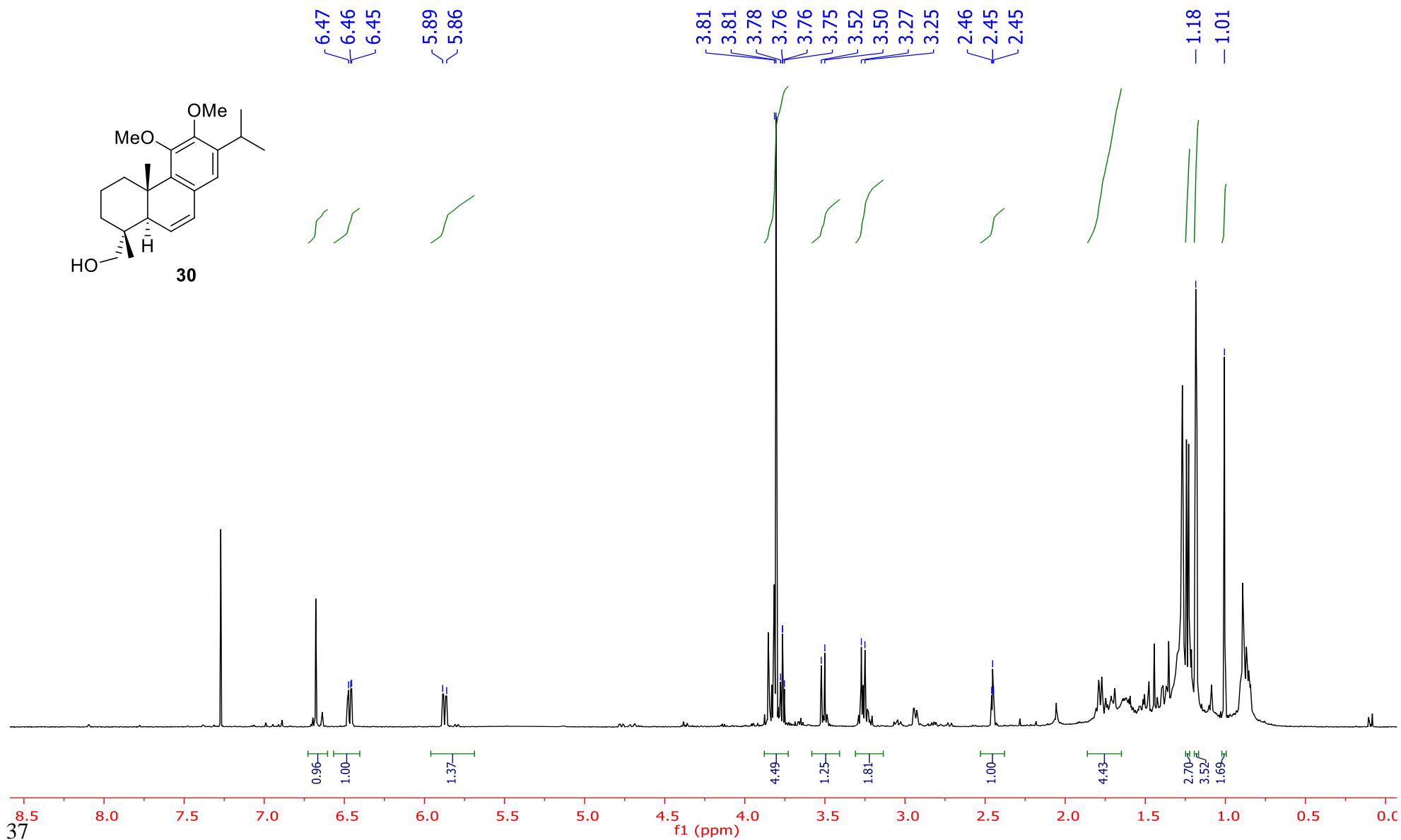
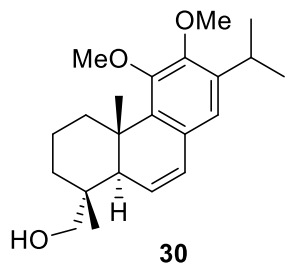


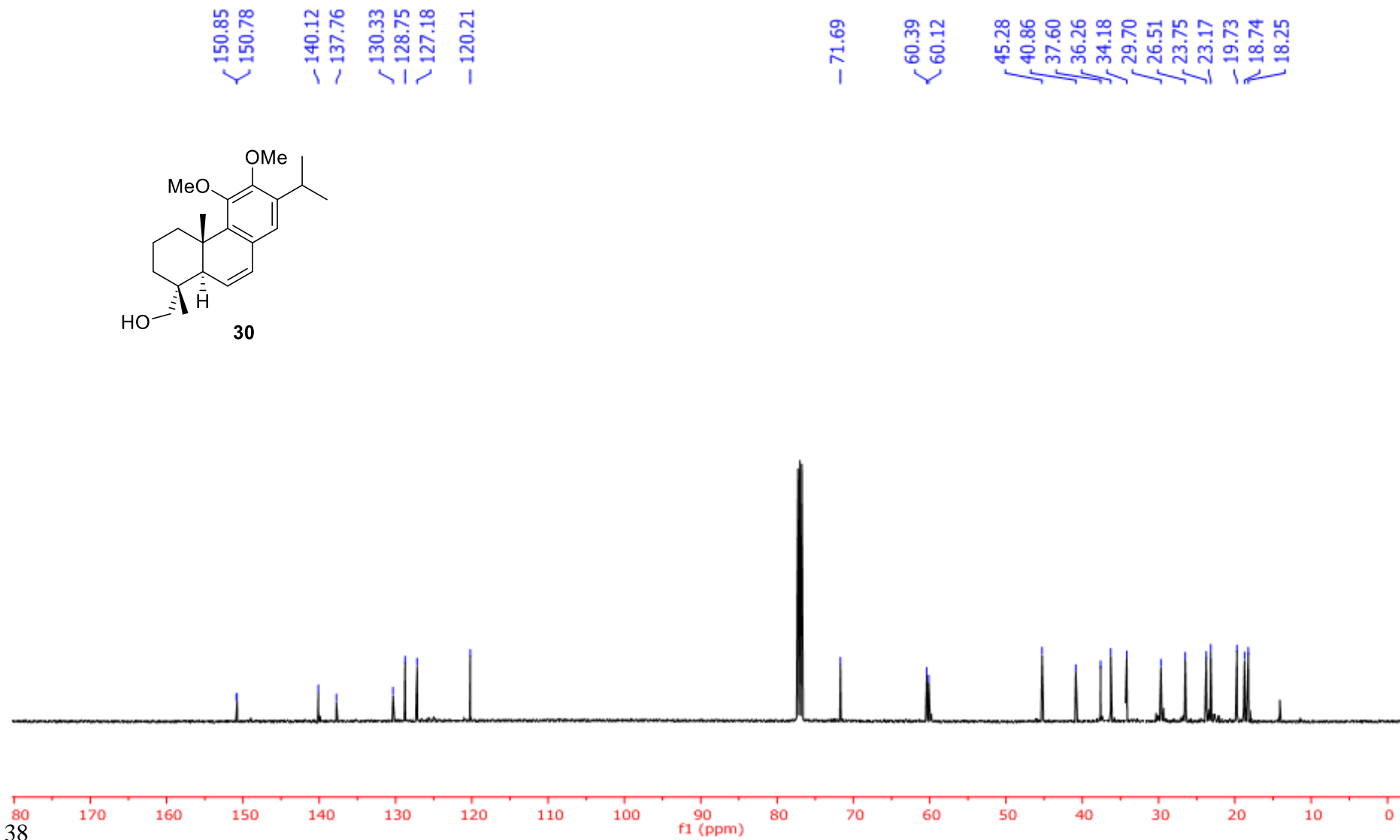
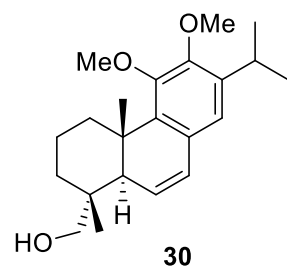


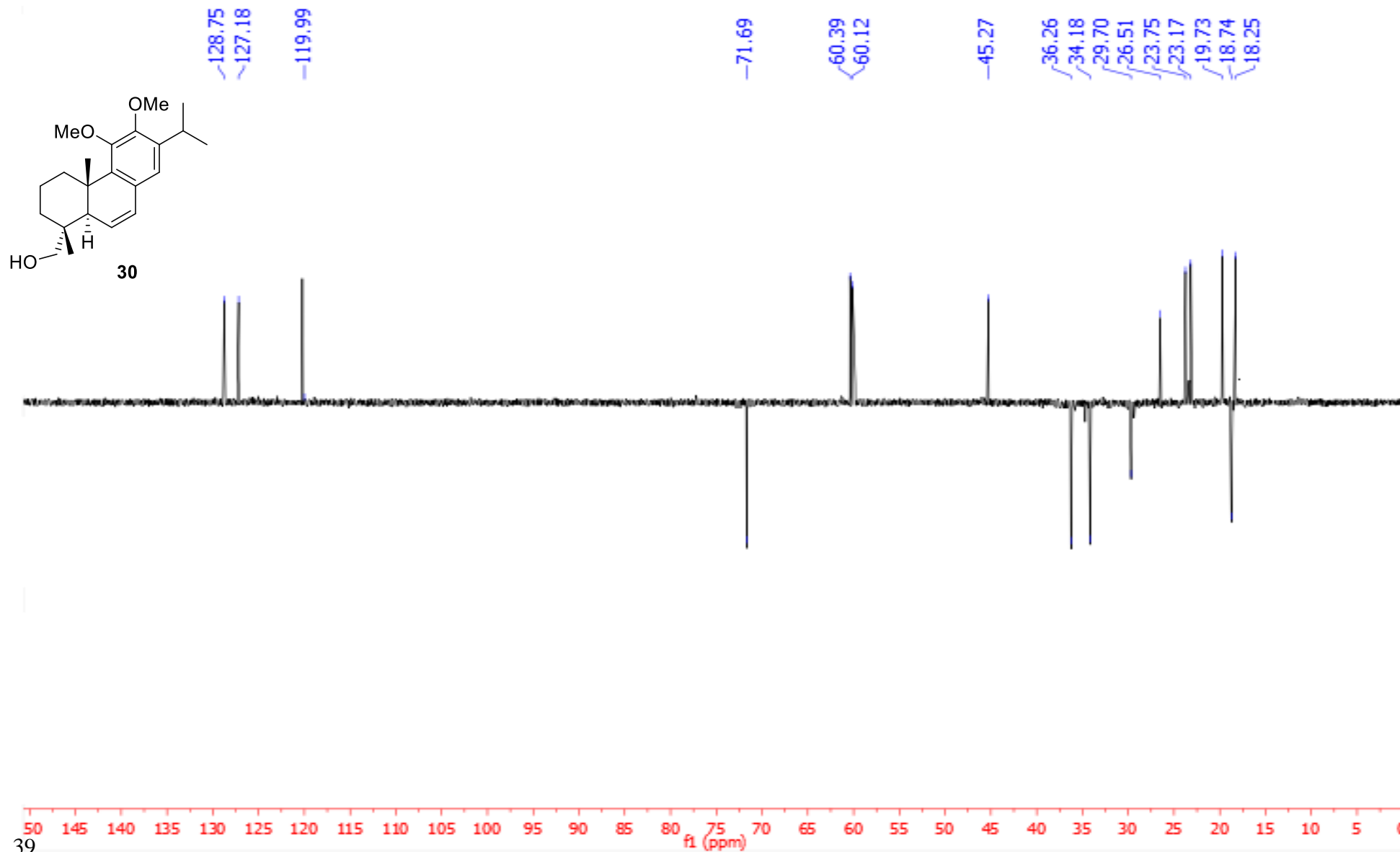
23_10_16 AMG 3 984 (7.355)
149.0228 (0.4 mDa)

1: TOF MS ES+
5.05e4

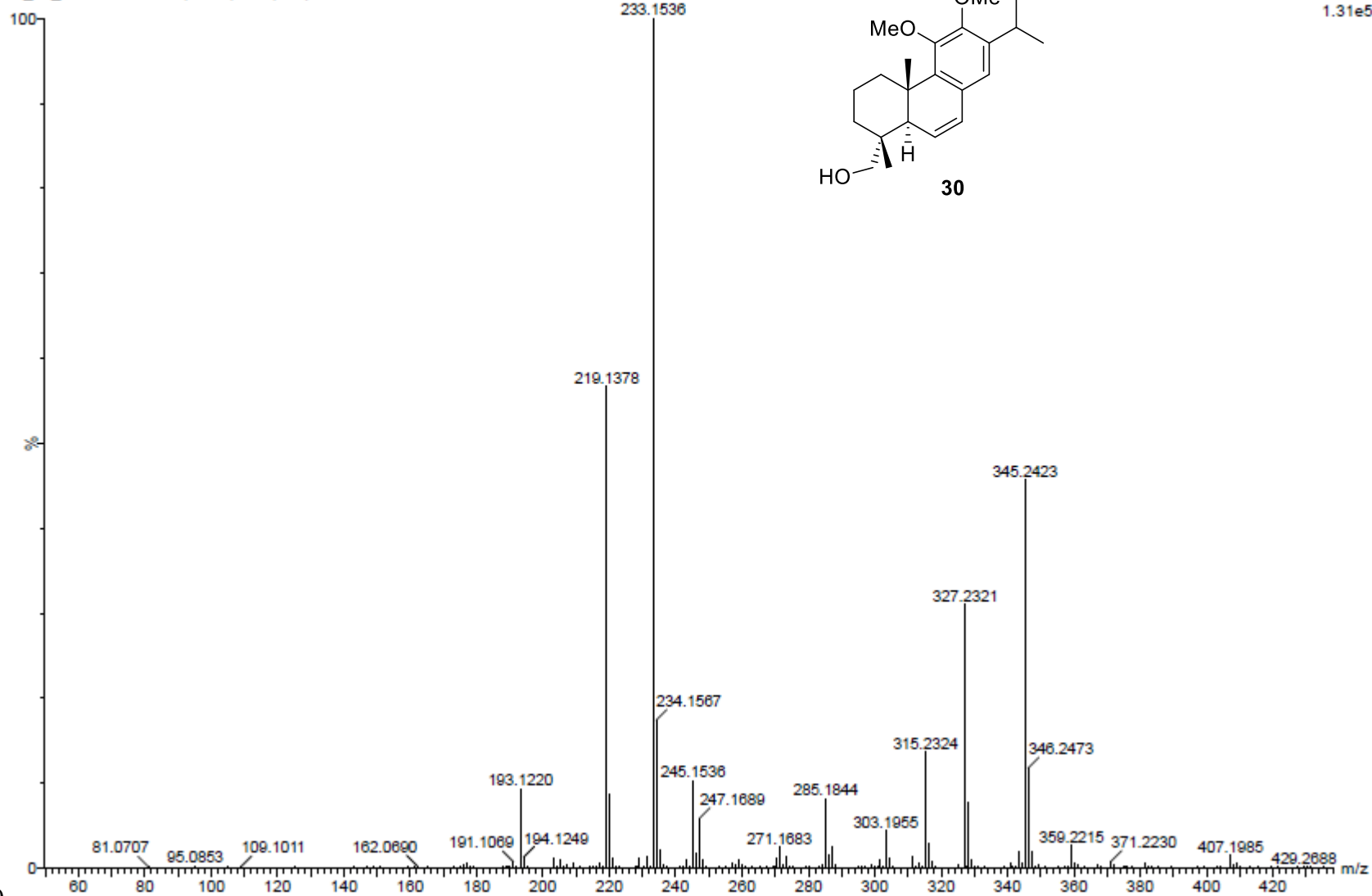




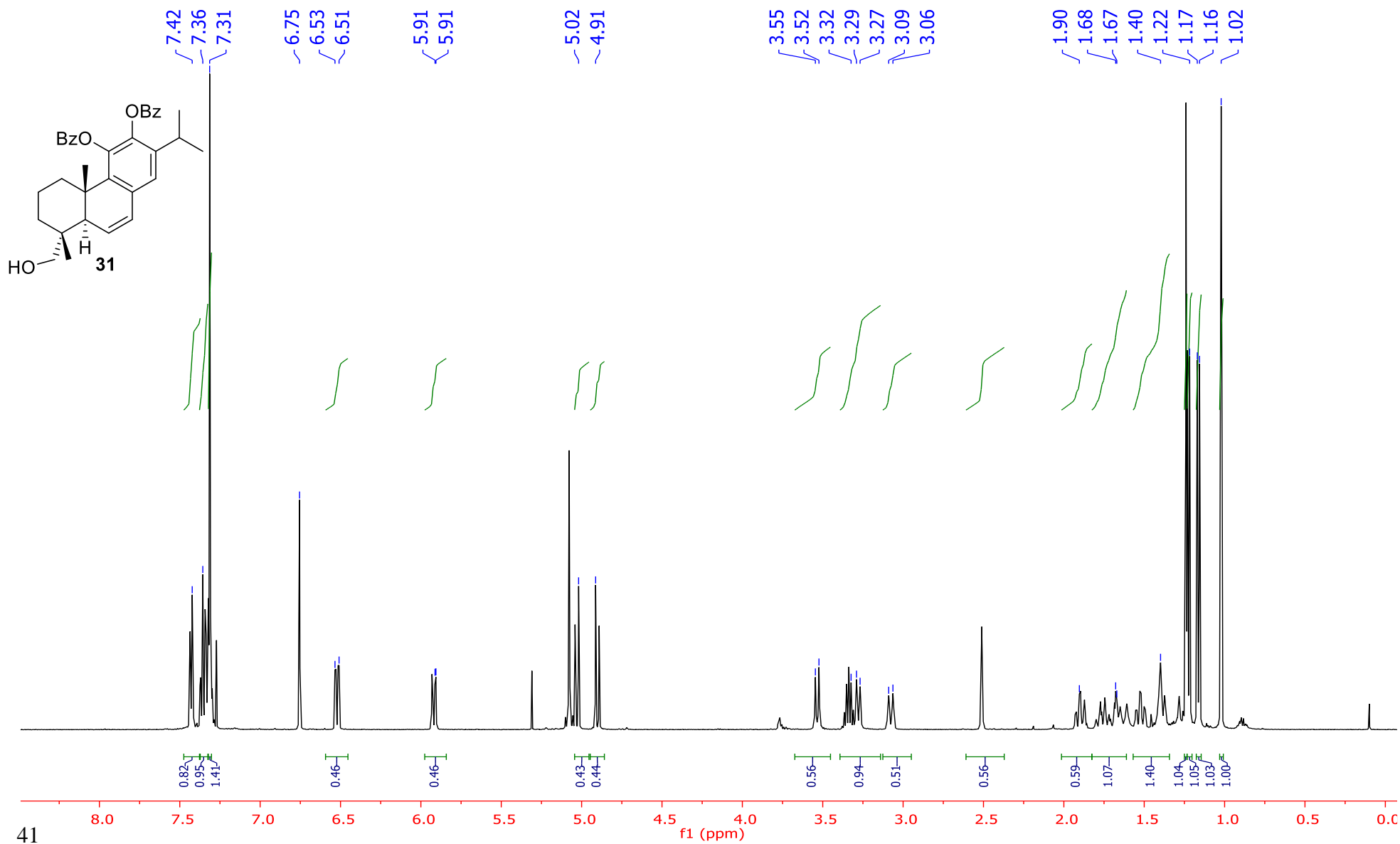


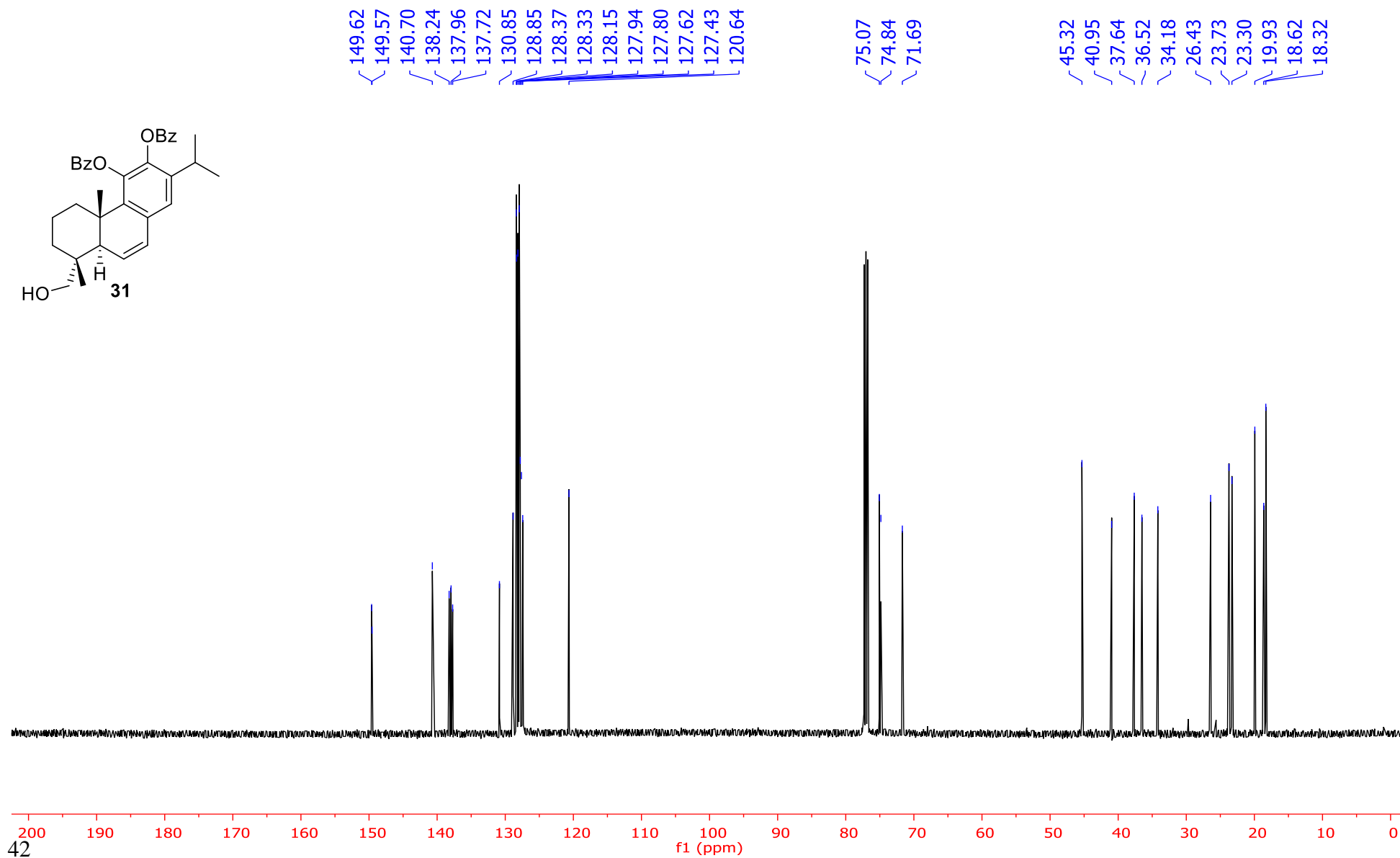
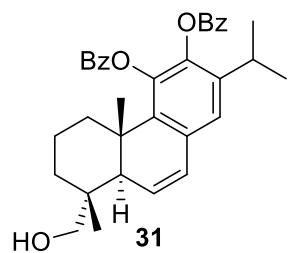


23_10_16 AMG 4 743 (5.672) Cm (743)



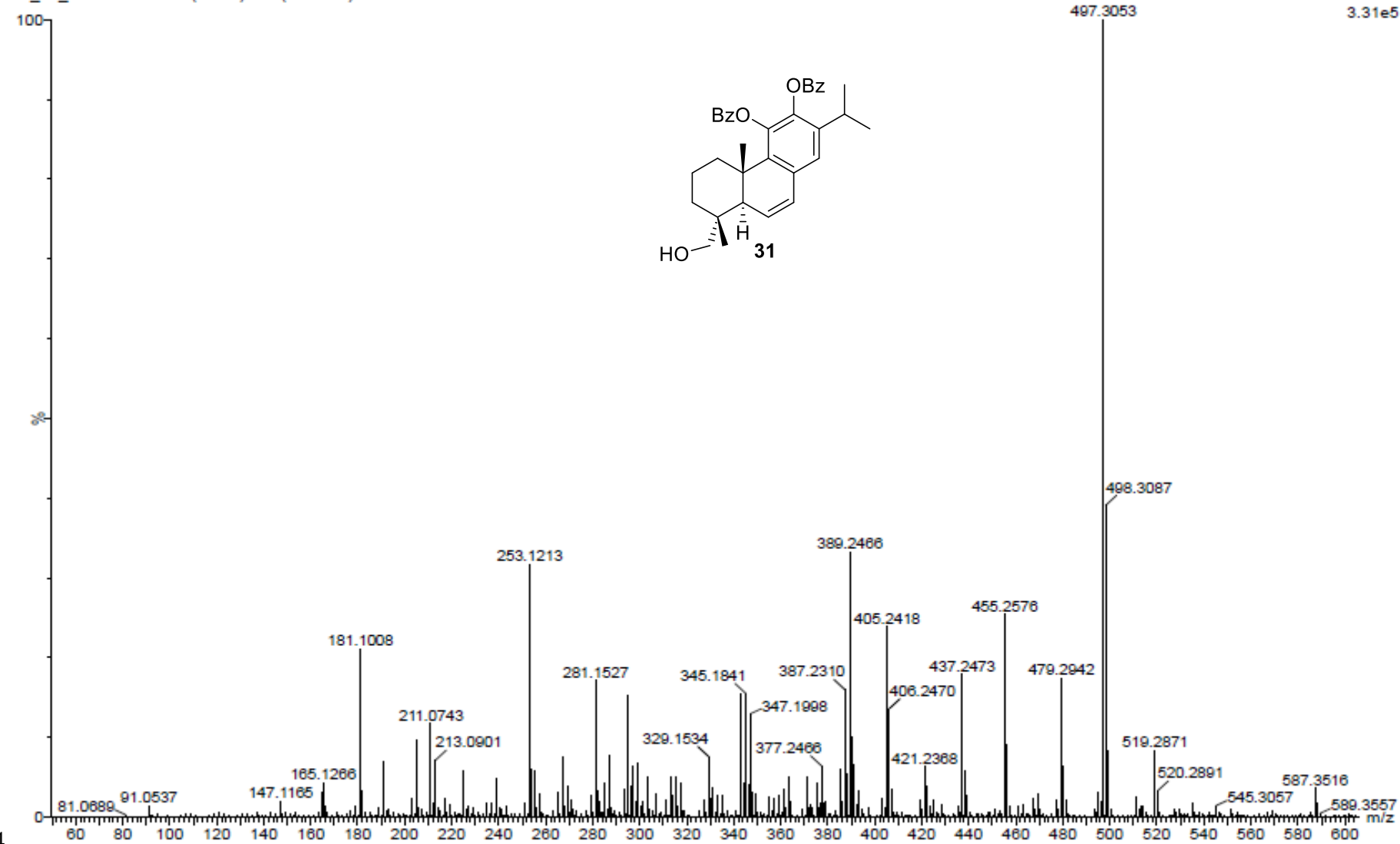
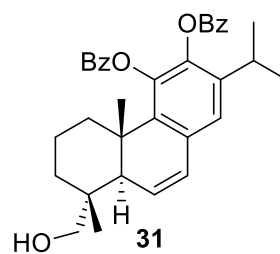
1: TOF MS ES+
1.31e5

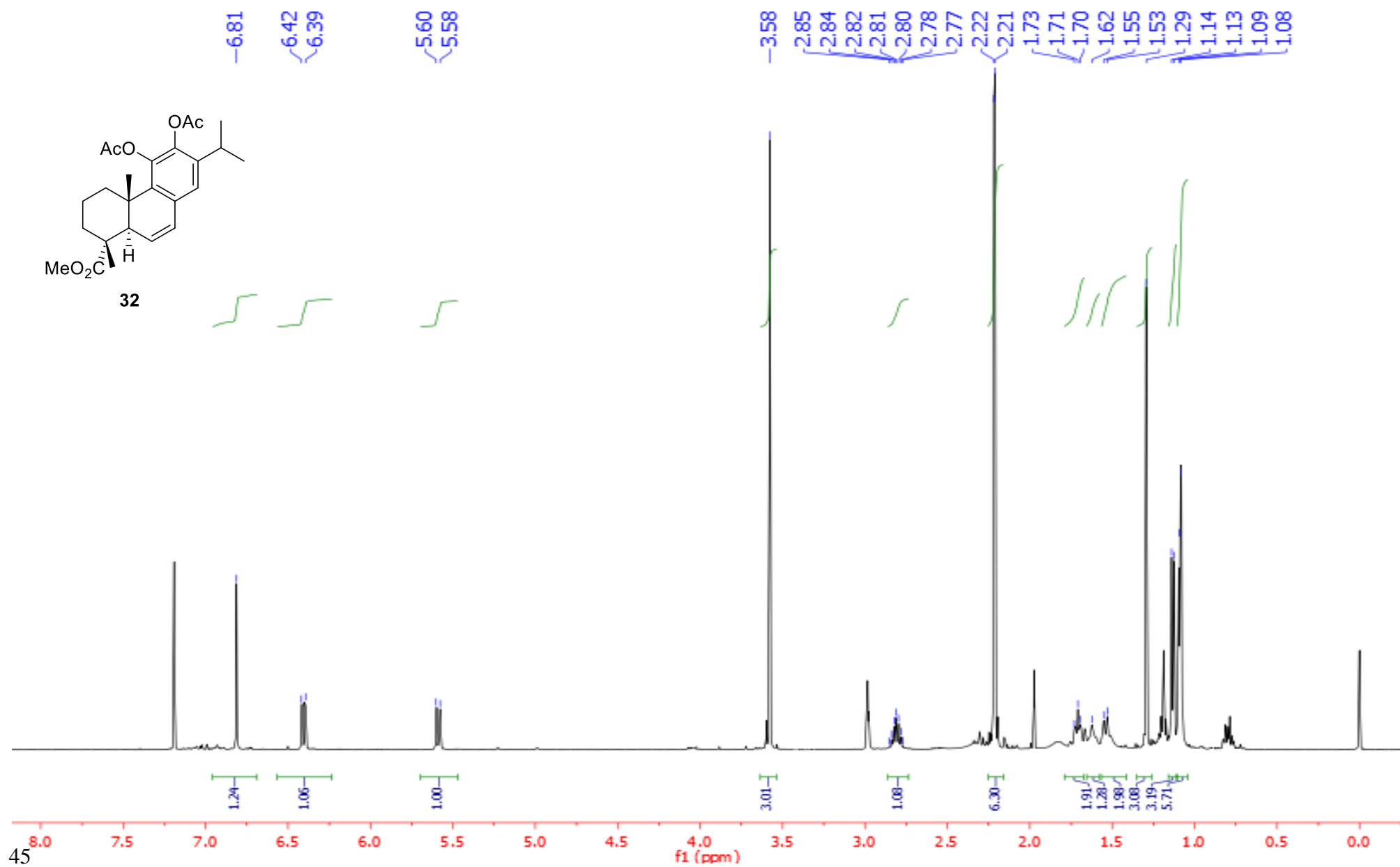


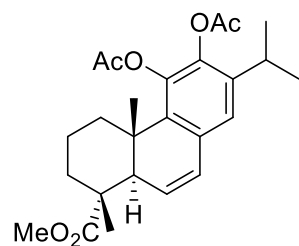


23_10_16 AMG 5 894 (6.826) Cm (893:901)

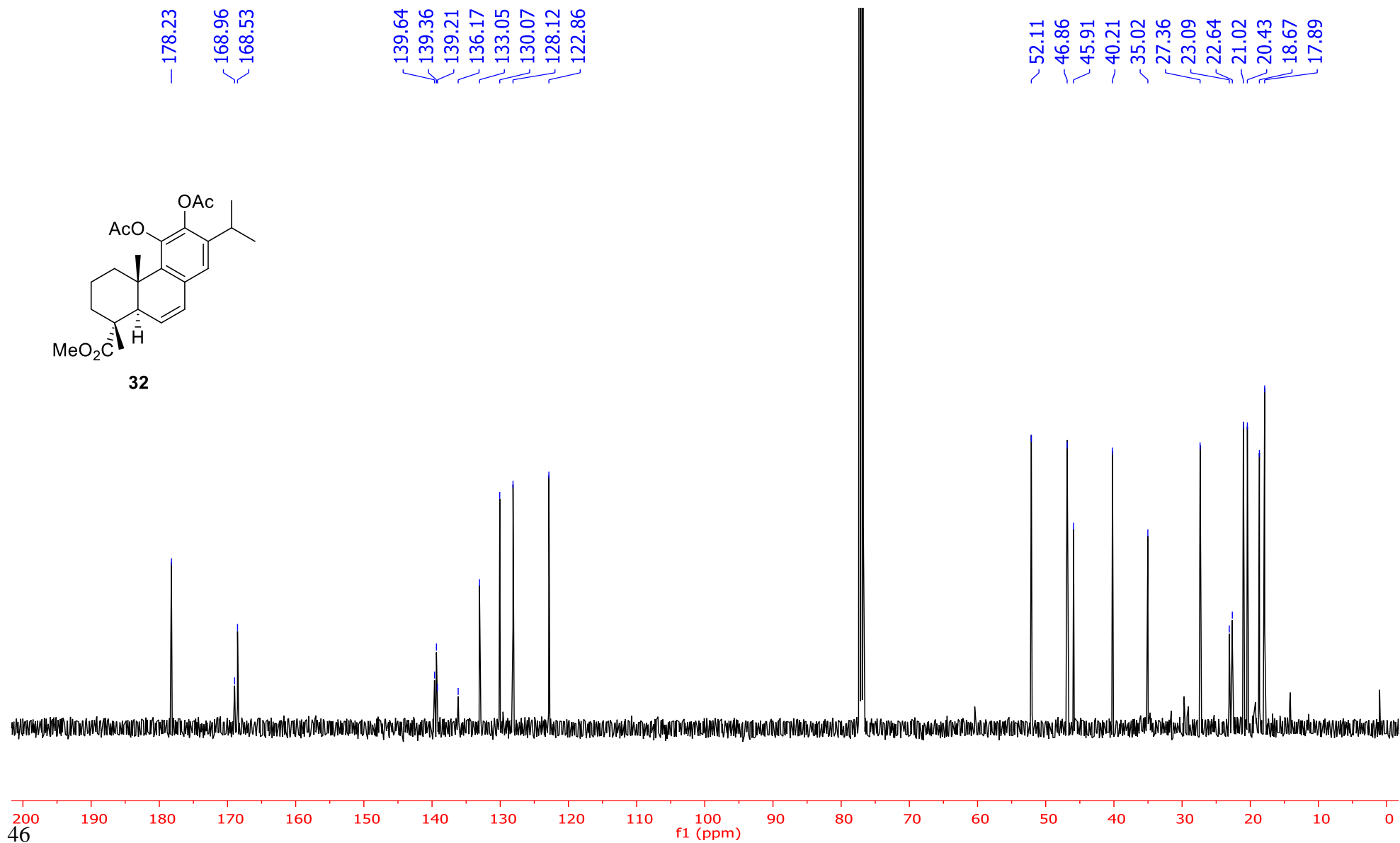
1: TOF MS ES+
3.31e5

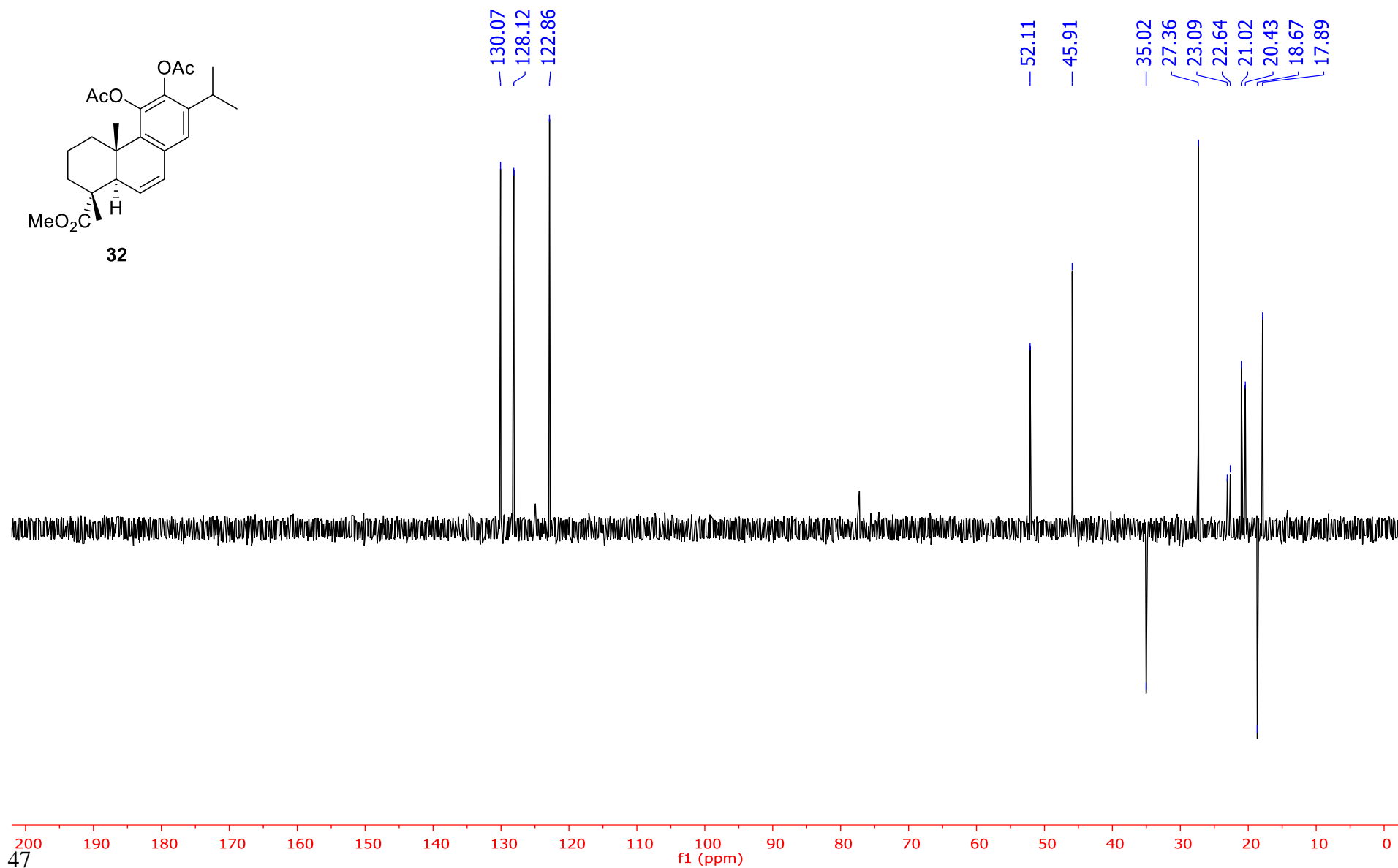
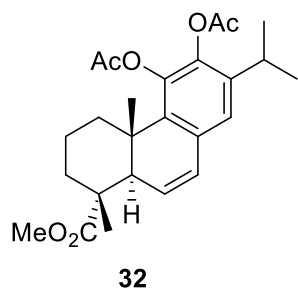


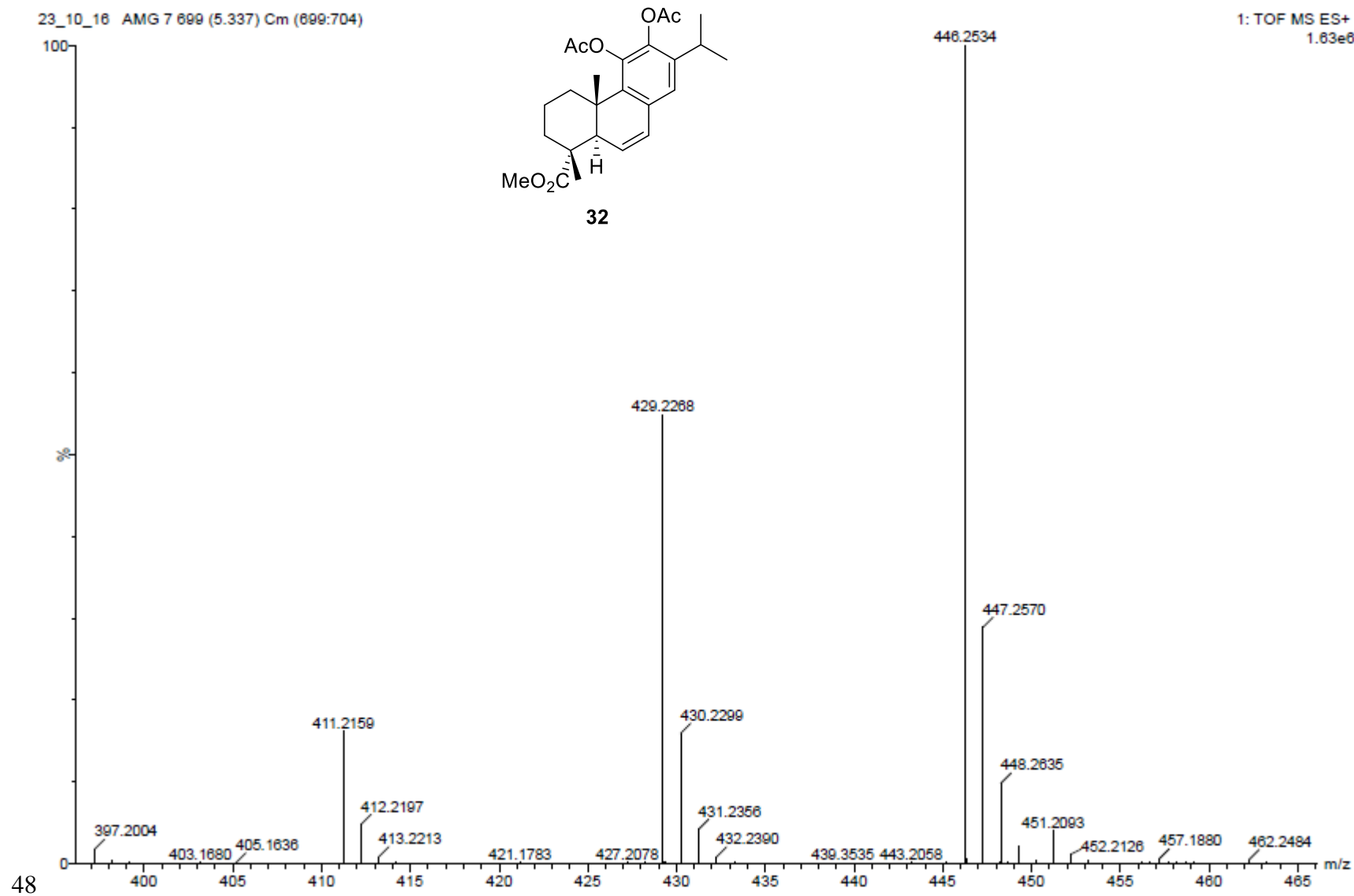


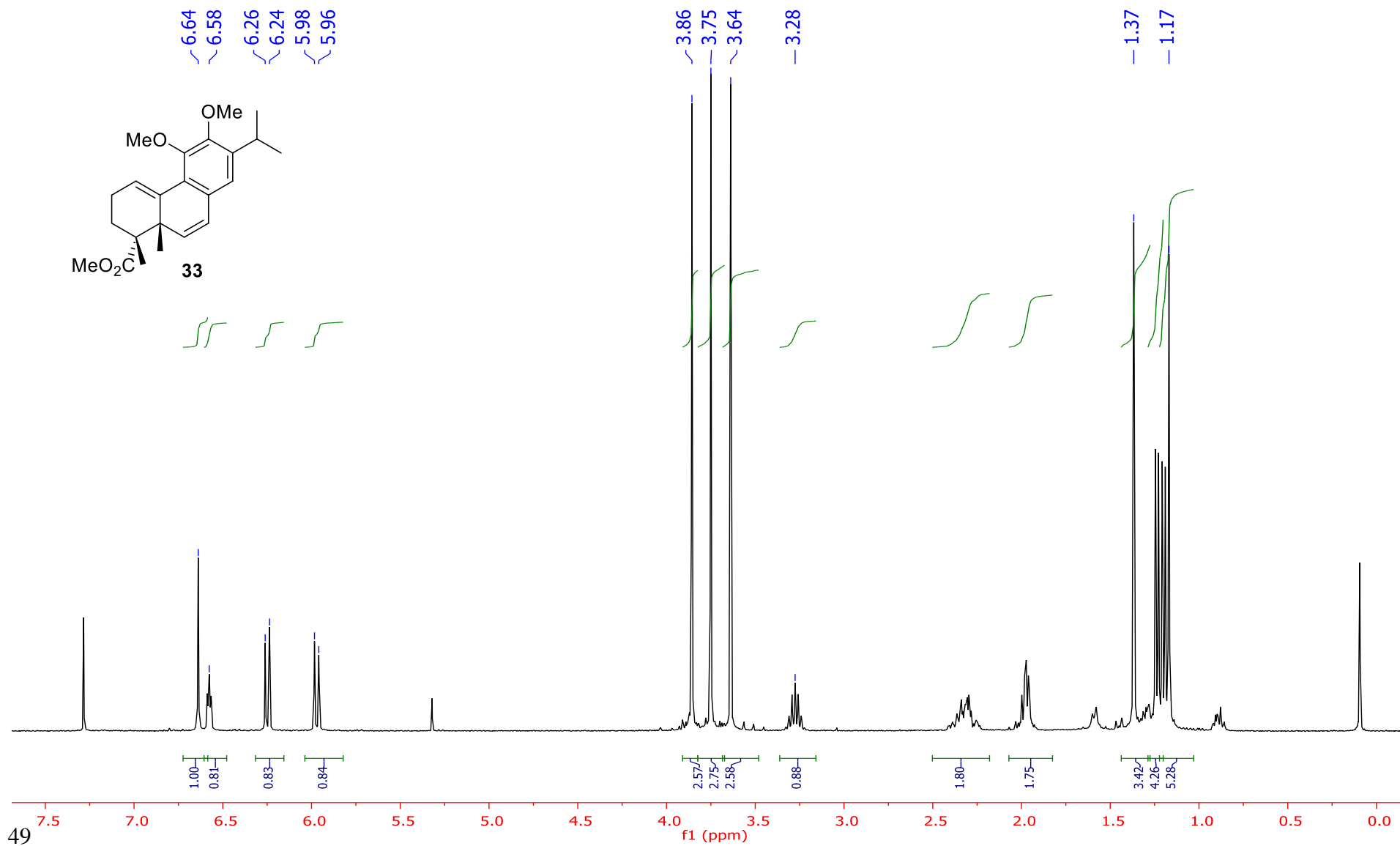


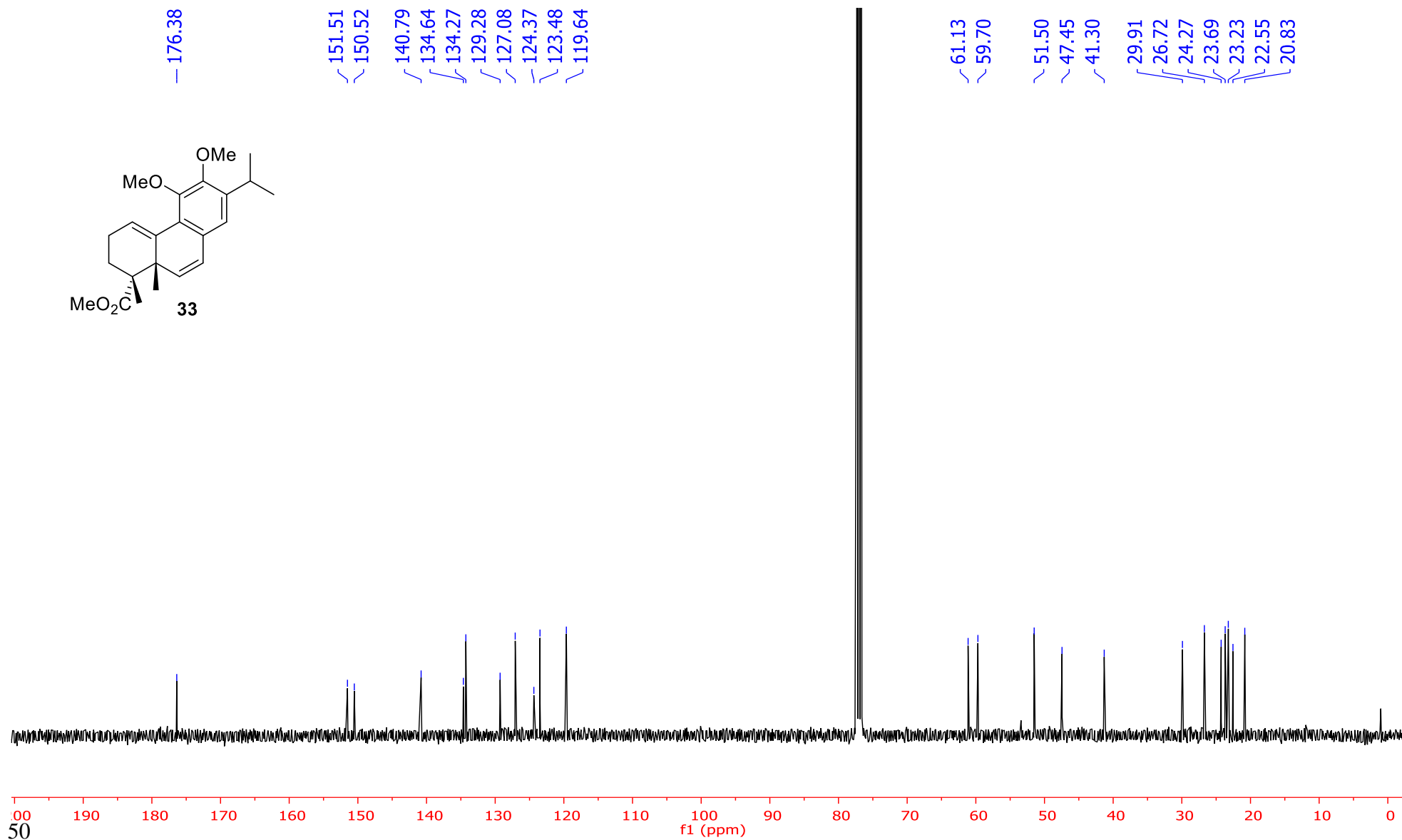
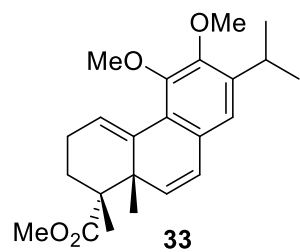
32

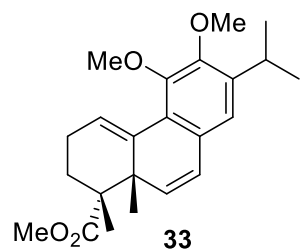








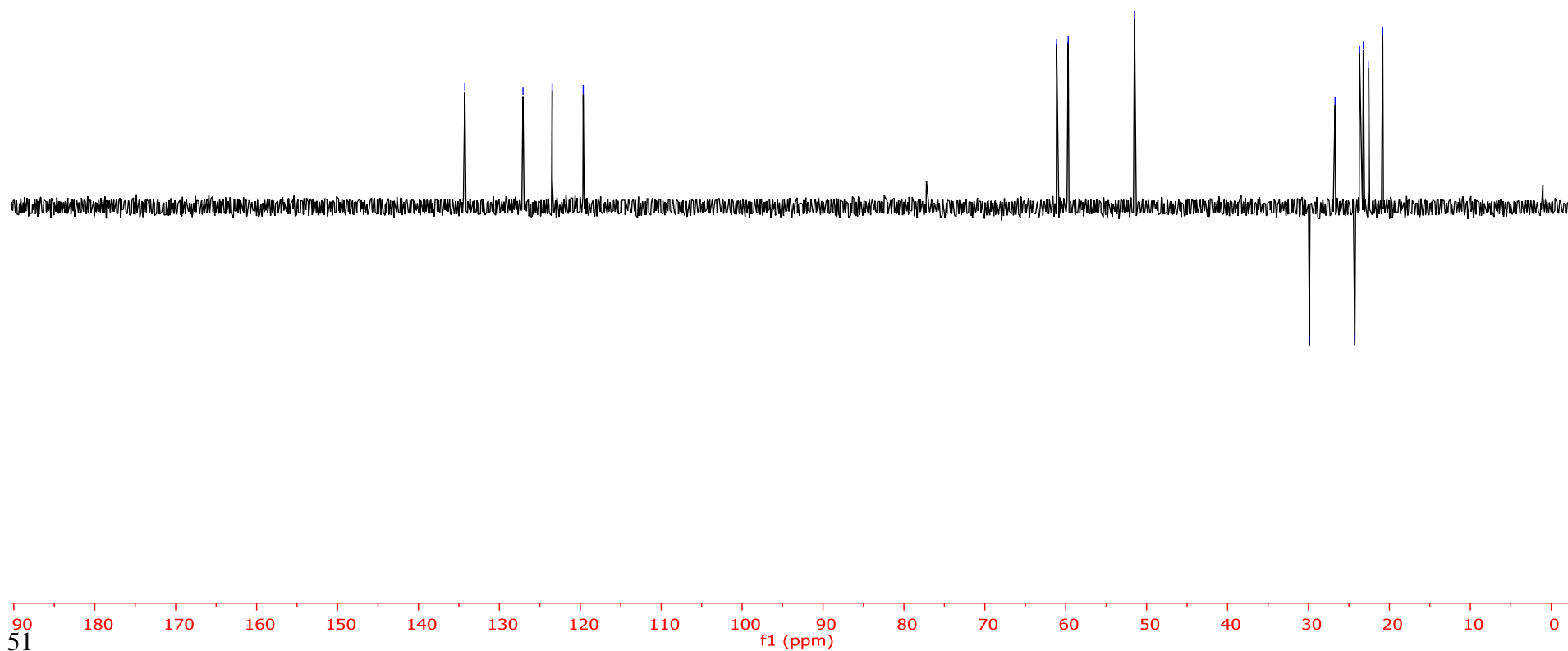




— 134.27
 — 127.08
 — 123.48
 — 119.64

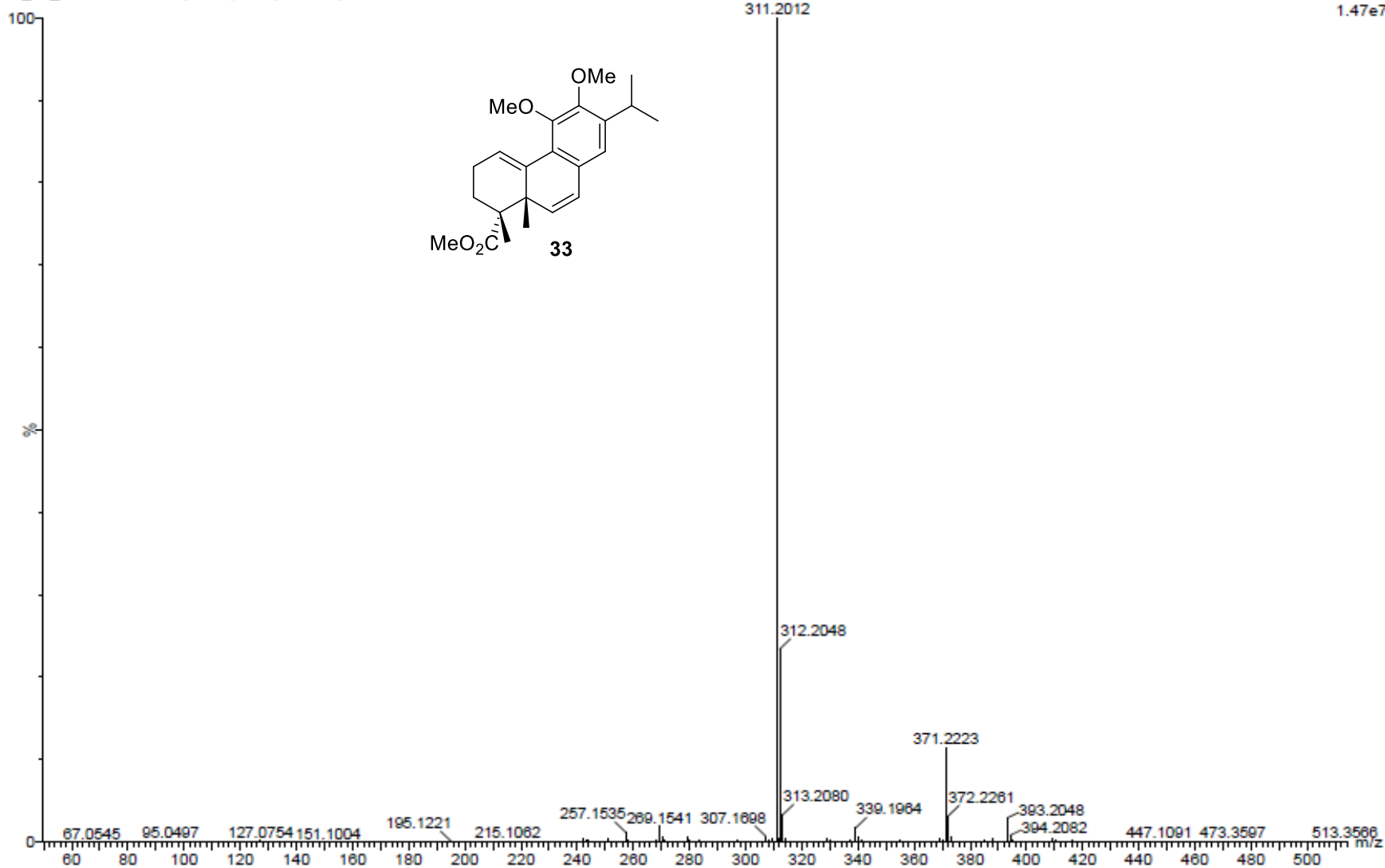
~ 61.13
 ~ 59.70
 — 51.50

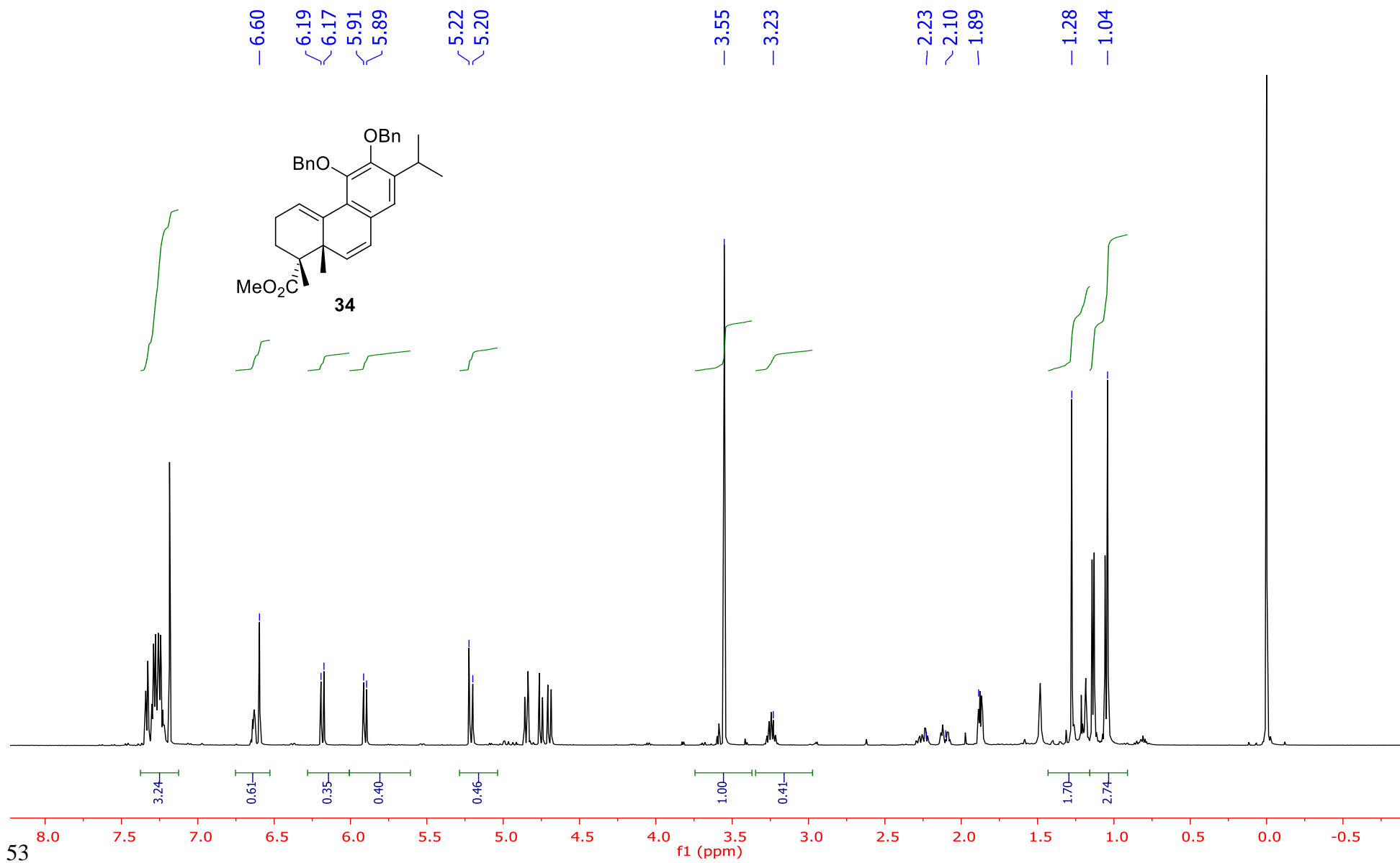
{ 29.91
 { 26.72
 { 24.27
 { 23.69
 { 23.23
 { 22.55
 { 20.83

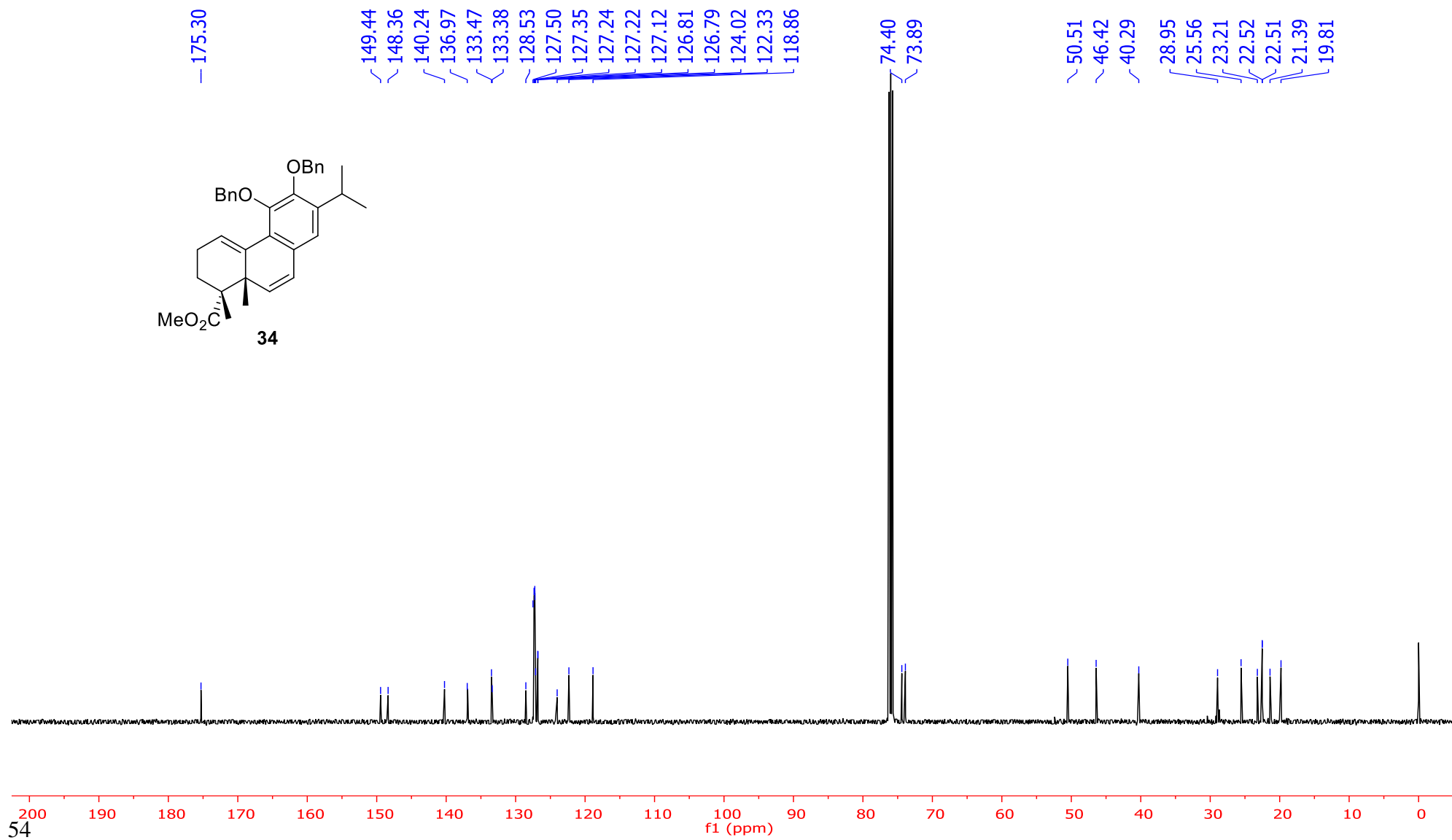
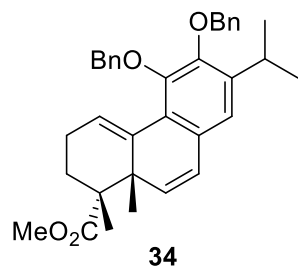


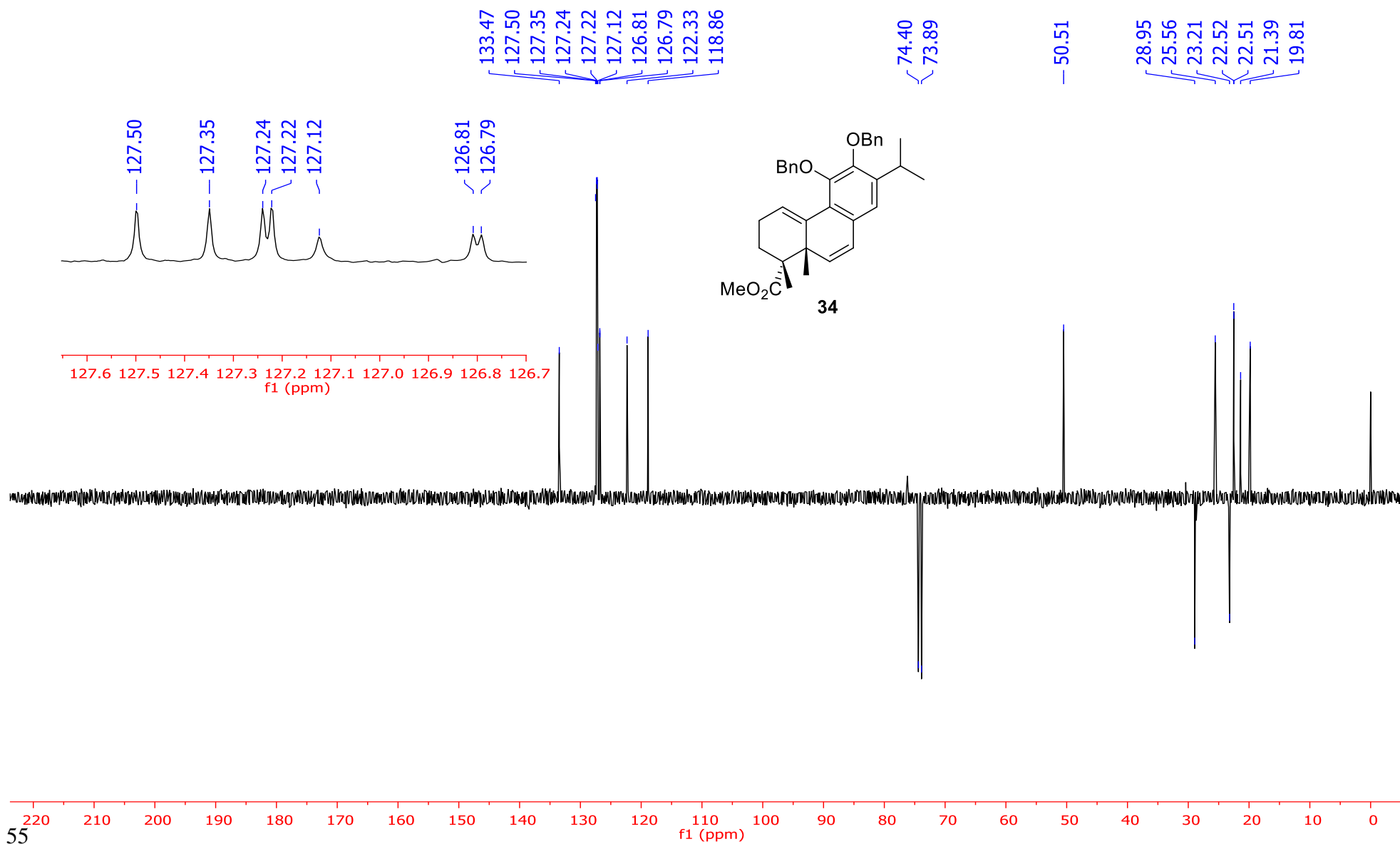
23_10_16 AMG 6 795 (6.074) Cm (789:807)

1: TOF MS ES+
1.47e7



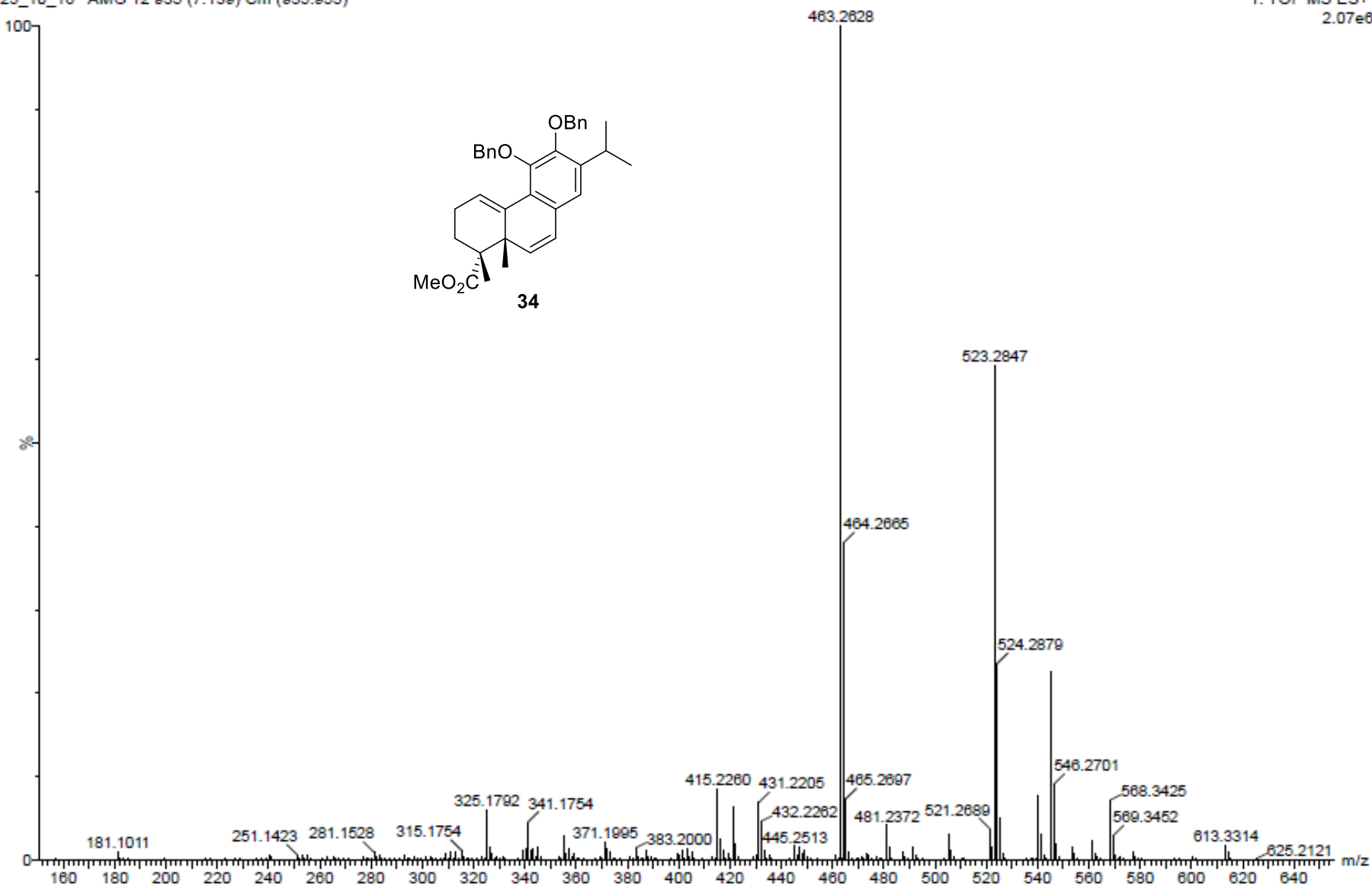
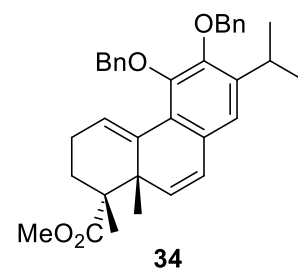


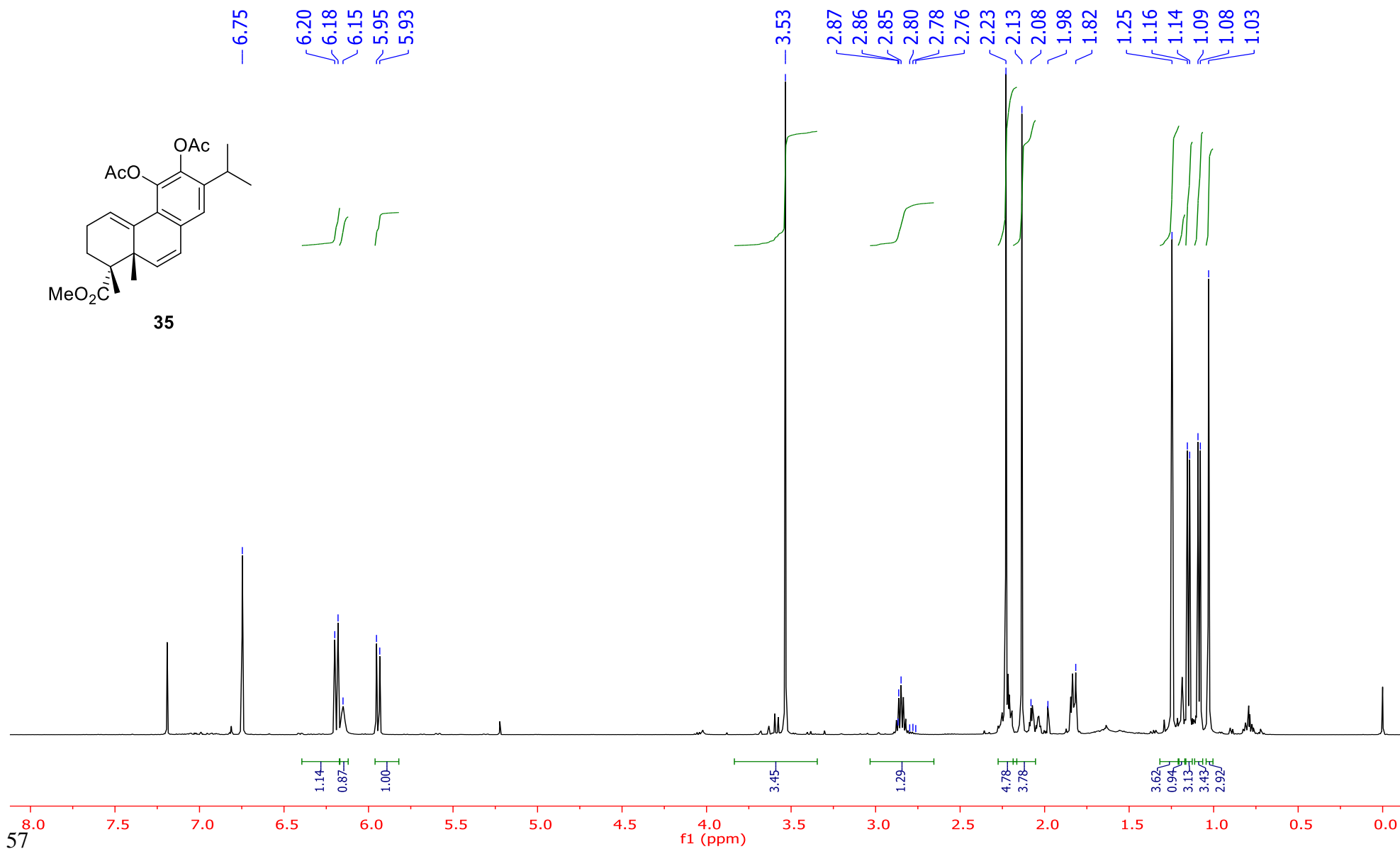


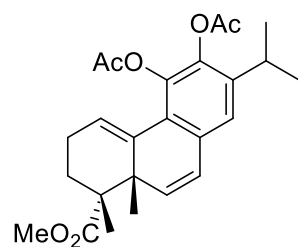


23_10_16 AMG 12 935 (7.139) Cm (935:955)

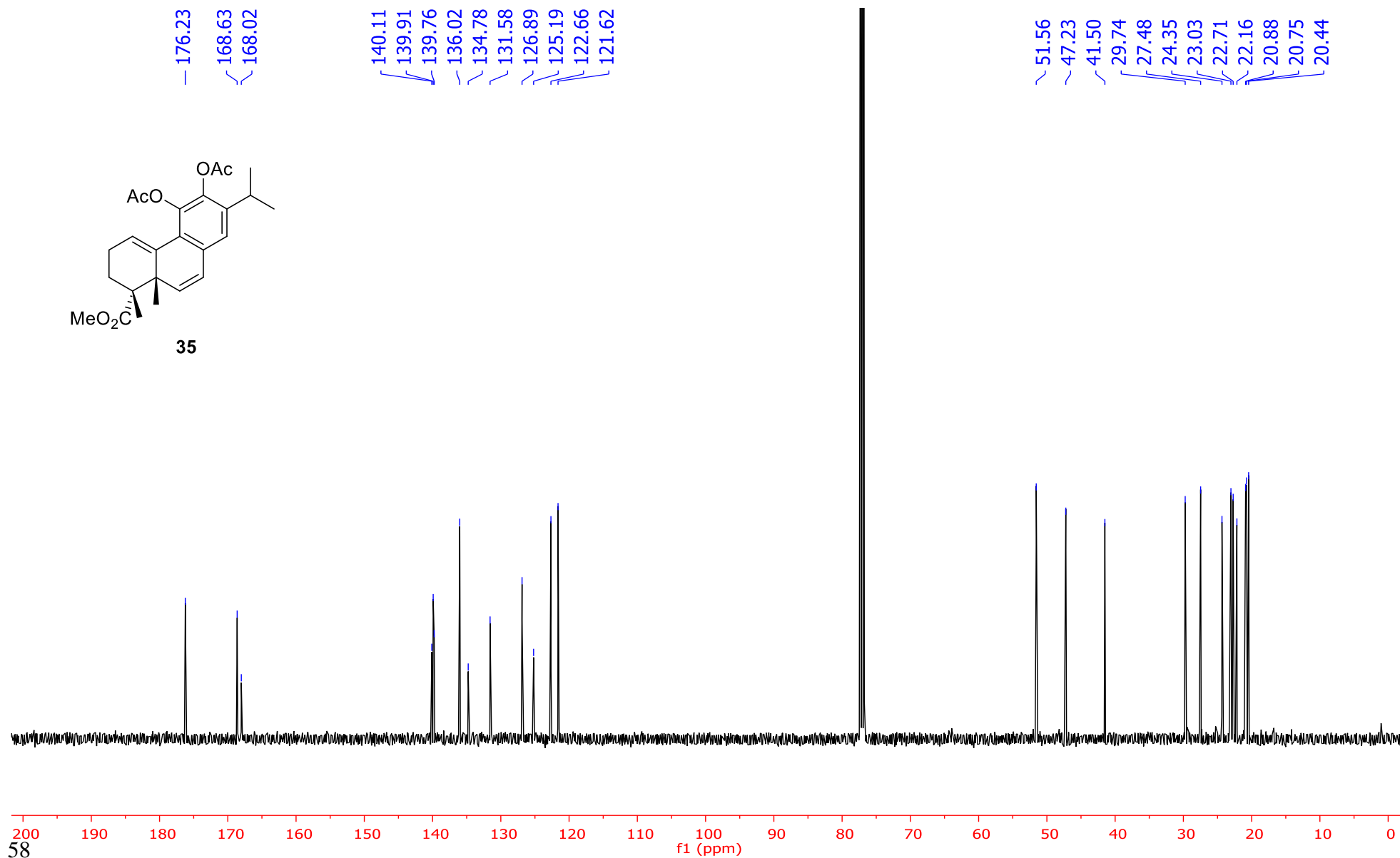
1: TOF MS ES+
2.07e6

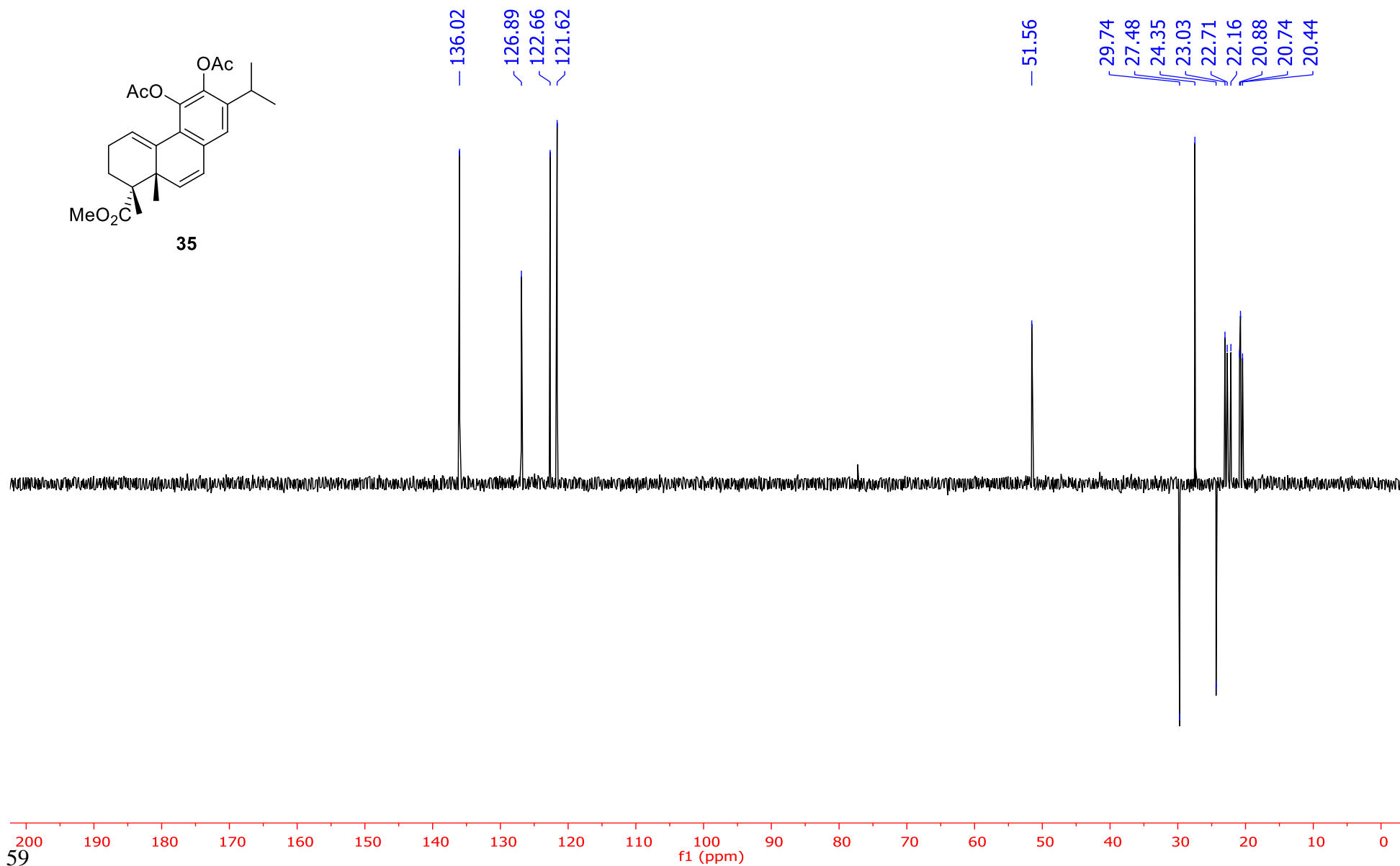
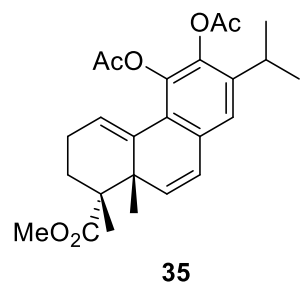






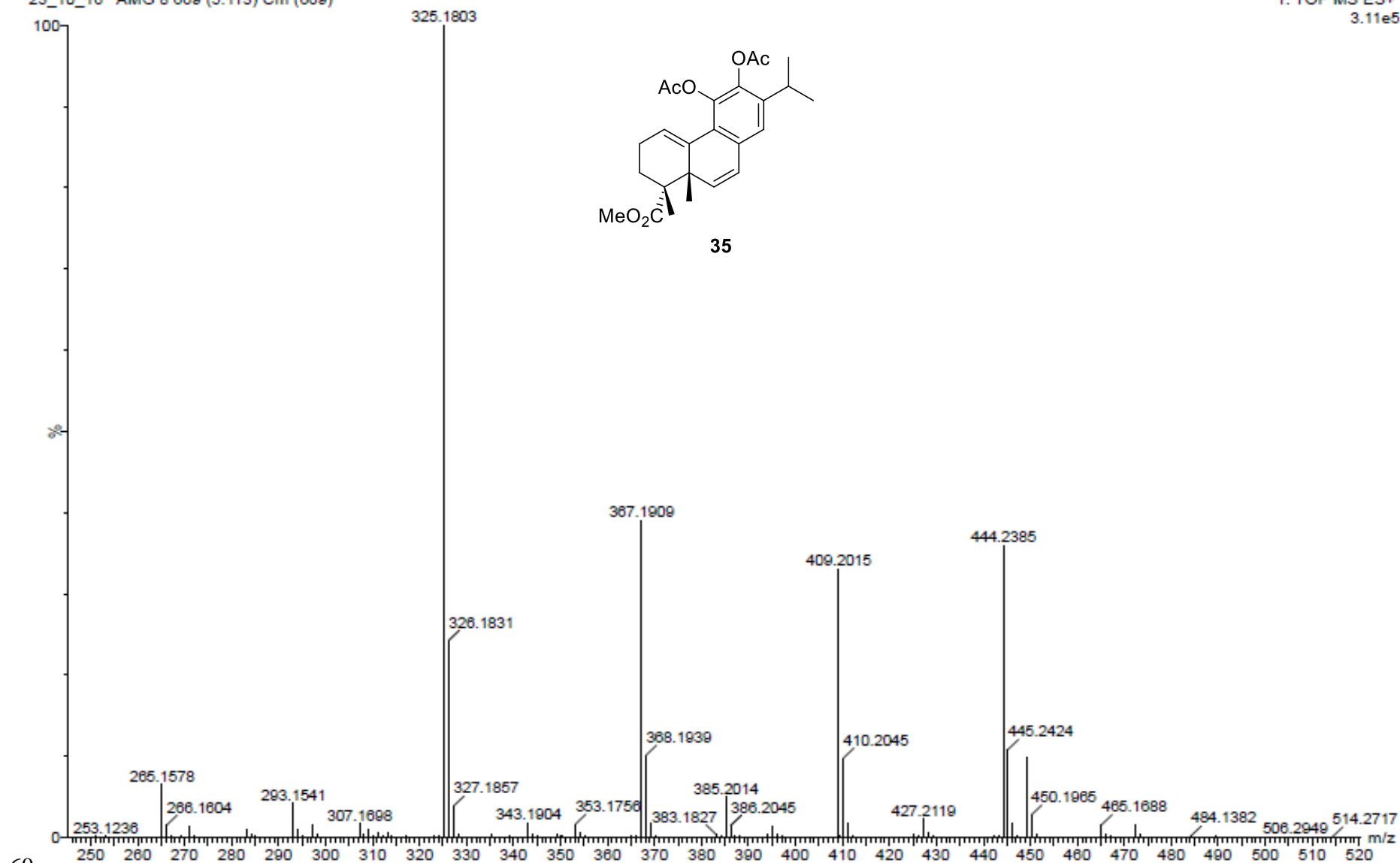
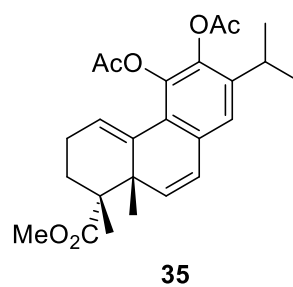
35

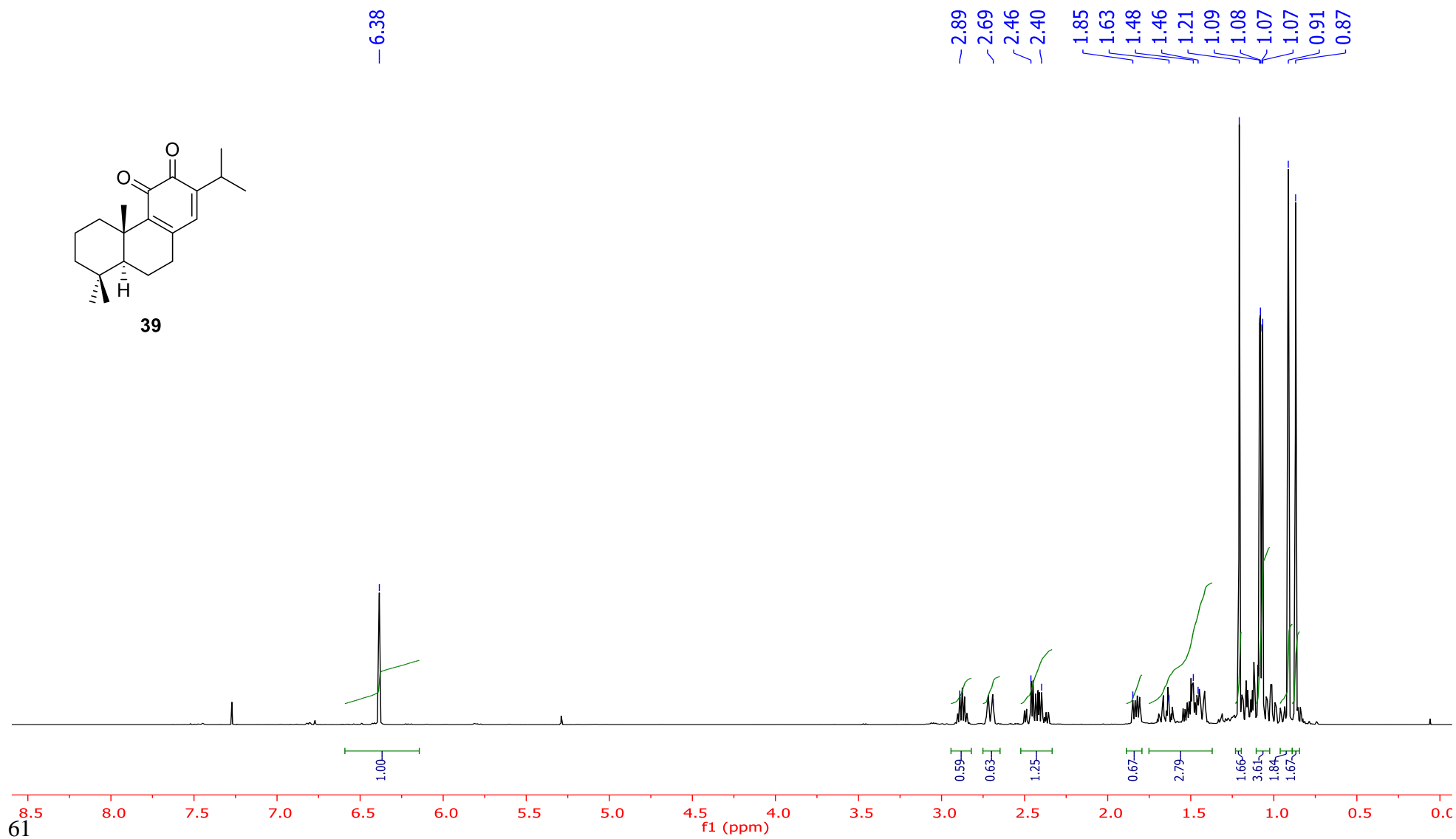


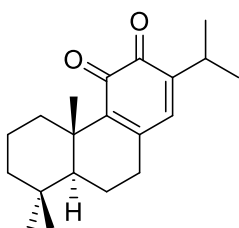


23_10_16 AMG 8 669 (5.113) Cm (669)

1: TOF MS ES+
3.11e5





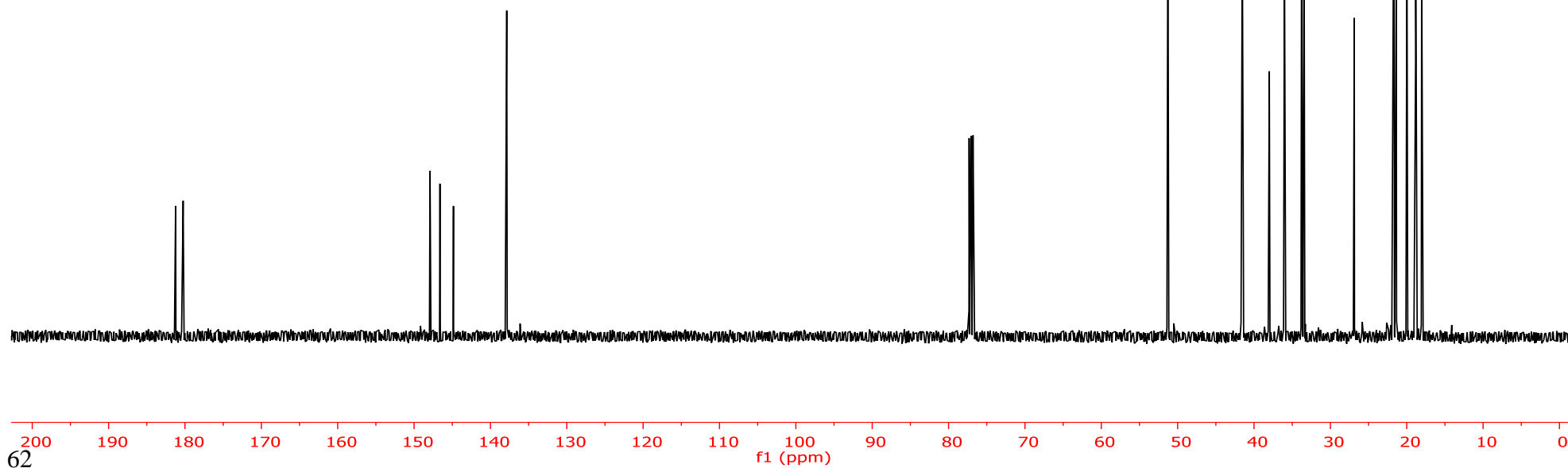


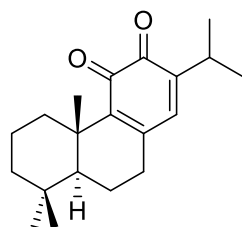
39

181.23
180.24

147.91
146.61
144.84
137.86

51.28
41.53
38.00
36.01
33.78
33.45
33.38
26.87
21.69
21.41
21.37
19.97
18.84
18.05





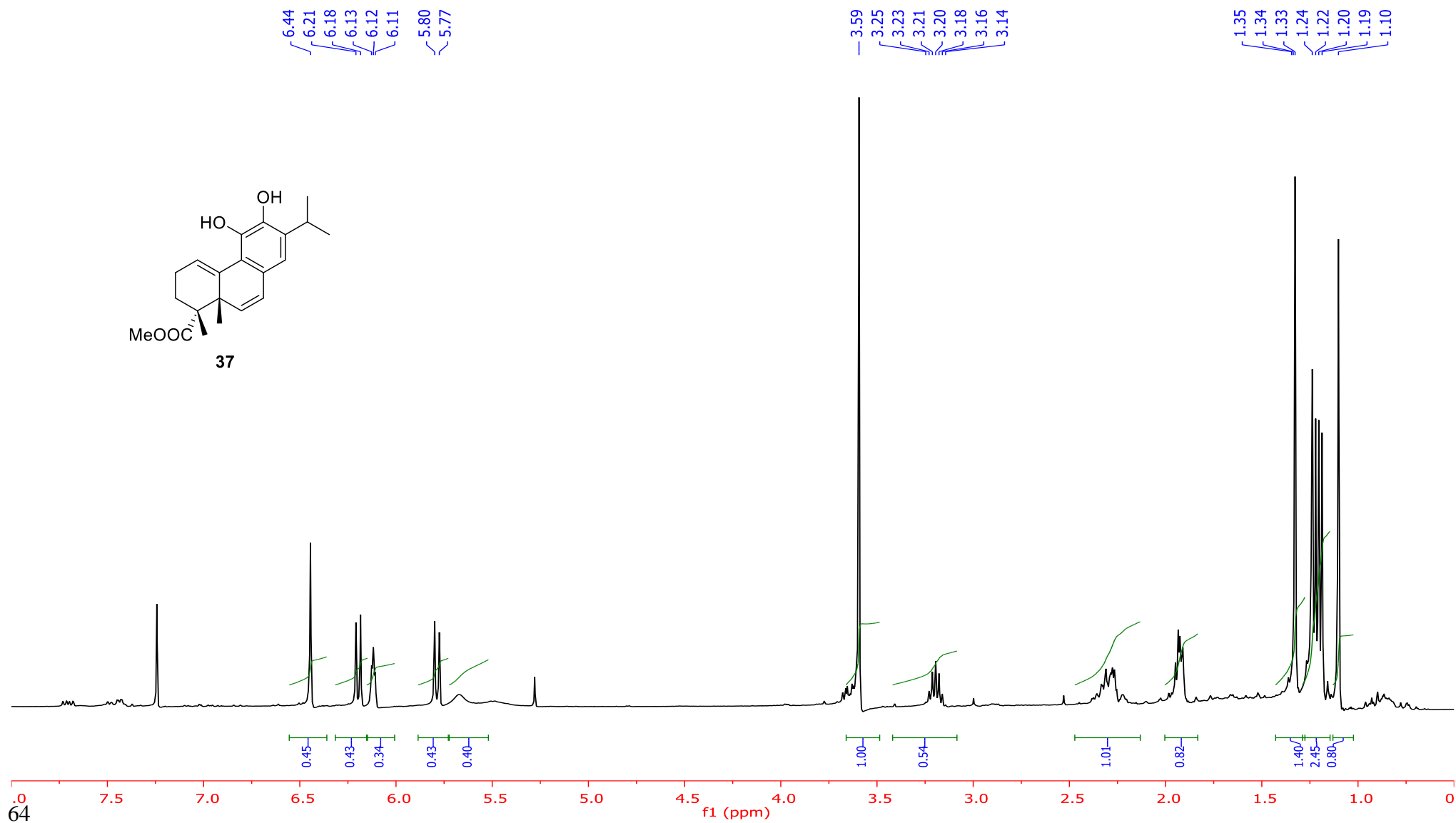
39

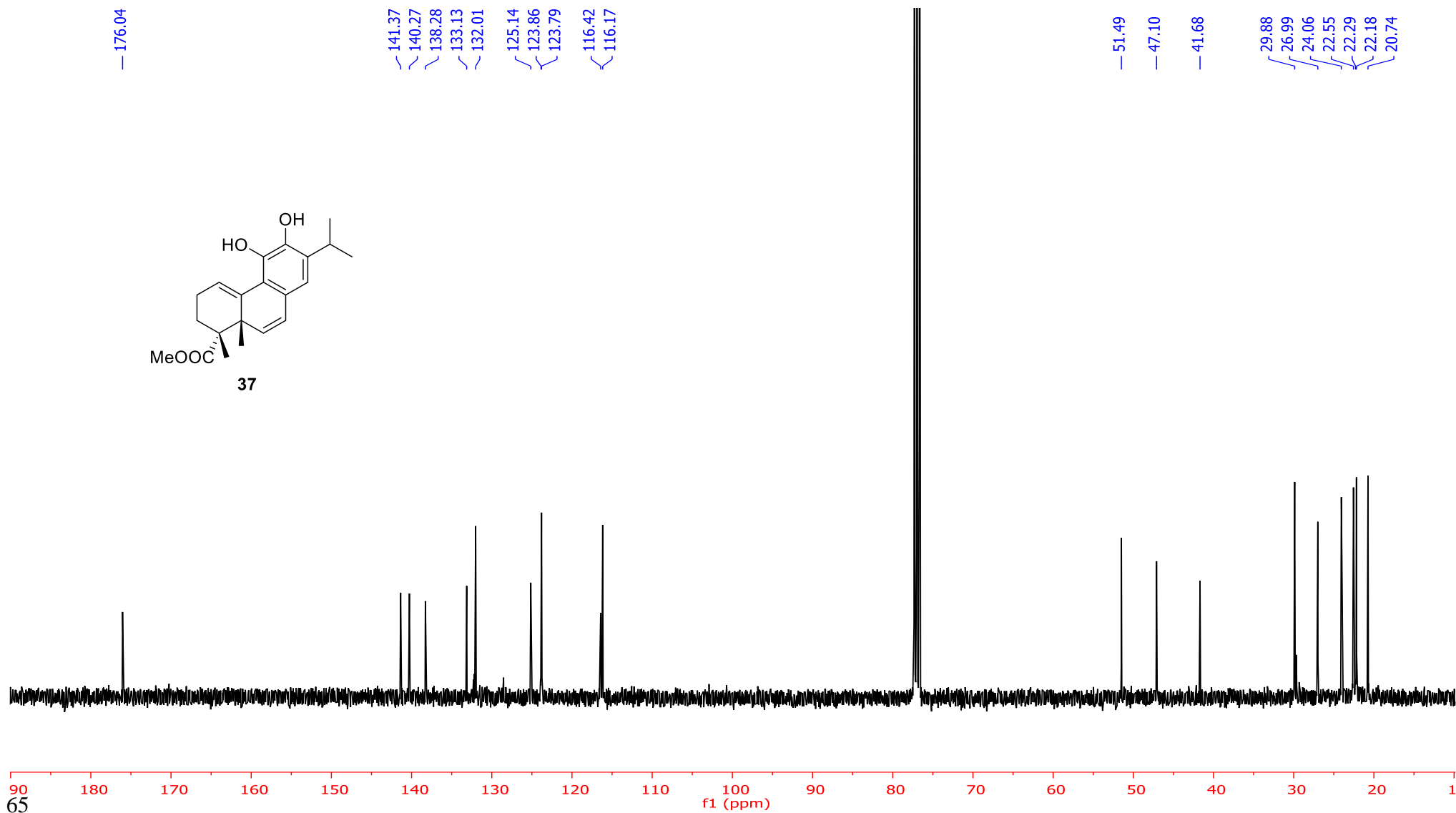
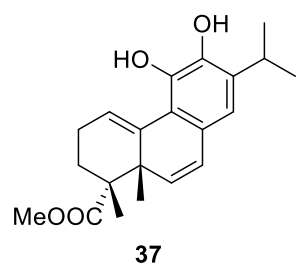
— 137.86

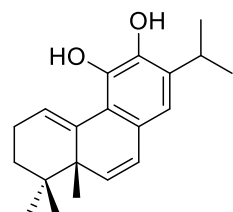
— 51.28
 — 41.53
 — 36.01
 — 33.78
 — 33.45
 — 26.87
 — 21.69
 — 21.41
 — 21.37
 — 19.97
 — 18.84
 — 18.05



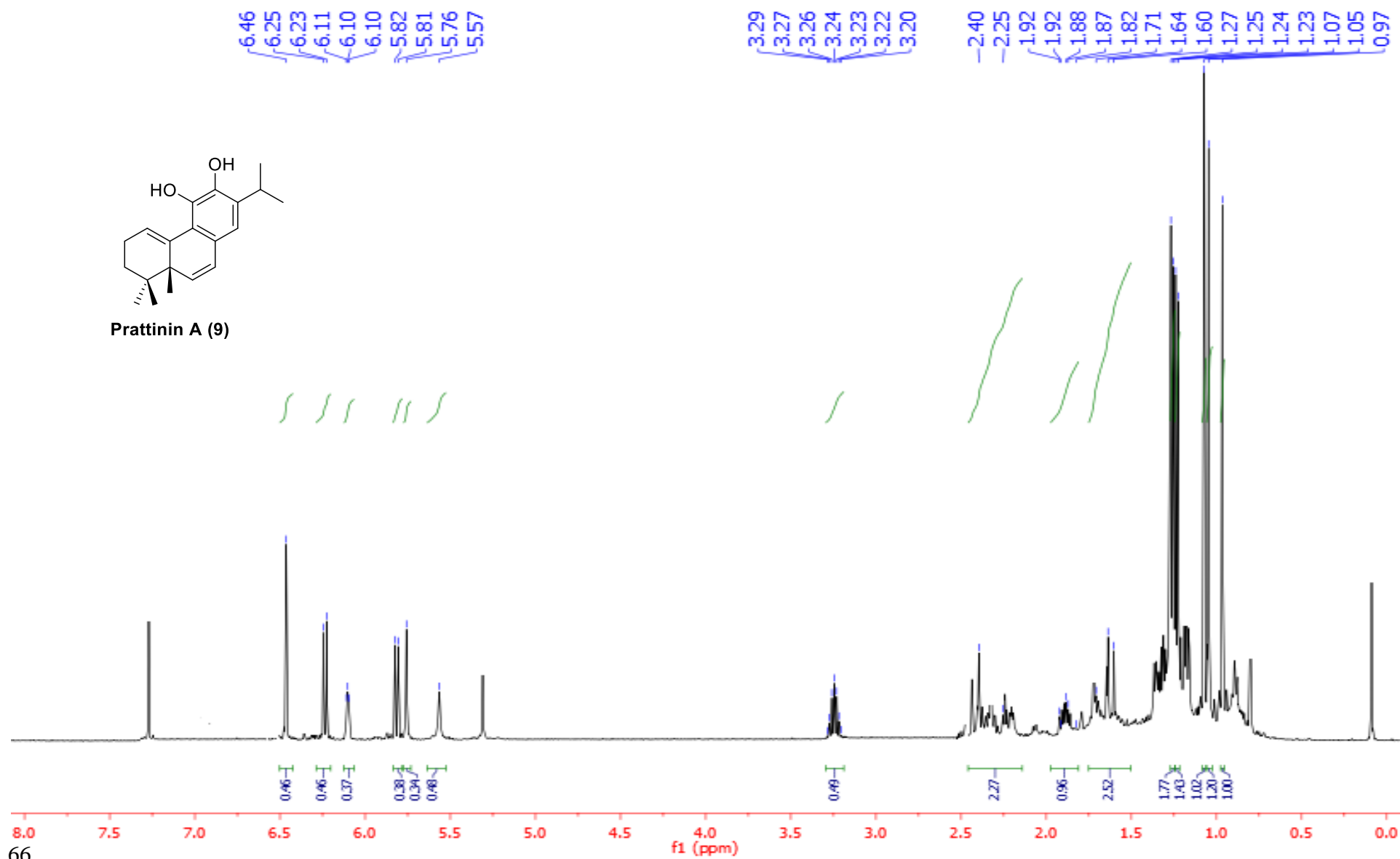
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
 63 f1 (ppm)



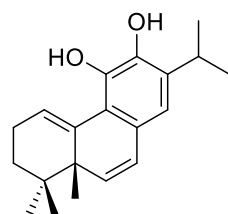




Prattinin A (9)







Prattinin A (9)

