Supporting Information

Synthesis of (-)-Nakamurol A and Assignment of Absolute Configuration of Diterpenoid (+)-Nakamurol A

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Contents

Table 1. ^{13}**C NMR Chemical shifts of compounds 1-21**[a,b]

	1	**3**	**4**	**5**	**7**[c]	**8**[d]	**9**	**10**	**12**
C1	31.9	33.3	41.8	31.8	32.1	30.4	28.9	33.3	31.8
C2	21.4	26.5	21.9	21.4	21.2	22.9	21.7	21.6	21.4
C3	31.1	30.5	30.4	30.3	30.4	30.3	30.4	30.7	31.2
C4	30.4	43.1	31.0	30.7	31.0	31.5	32.6	30.9	30.4
C5	39.5	39.0	37.9	39.1	39.5	37.6	38.3	39.4	39.5
C6	33.9	35.5	32.2	32.2	33.0	27.4	32.2	32.2	33.9
C7	33.1	34.0	37.6	38.0	38.3	31.7	35.3	38.6	33.1
C8	149.6	199.5	213.4	216.2	213.1	146.7/147.0	203.2	213.6	149.3
C9	43.2	124.0	49.0	53.5	48.4	114.5/115.4	152.4	50.6	41.9
C10	42.4	171.2	35.9	44.6	46.5	40.8/41.0	44.8	46.4	42.1
C11	18.2	---	---	58.3	22.7	23.8/24.0	120.5	21.7	23.6
C12	41.7	---	---	---	50.2	46.1/46.4	---	33.4	33.3
C13	73.6	---	---	---	---	165.2	---	139.0	139.5
C14	145.3	---	---	---	---	---	---	---	---
C15	111.5	---	---	---	---	---	---	---	---
C16	27.6	---	---	---	---	---	---	114.8	114.1
C17	106.5	---	---	---	---	---	---	---	106.2
C18	16.3	15.2	16.1	16.3	16.3	16.3	15.7	16.5	16.4
C19	16.4	16.0	15.3	15.2	16.0	15.5	15.7	16.0	16.5
C20	18.3	---	24.6	19.7	18.6	24.1/24.9	27.2	18.9	18.4

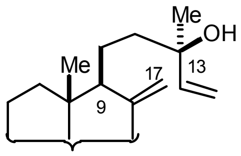
[a] Diterpene numbering is used in this table. [b] Values for compounds **1**, **3-5**, **10**, **12**, **13**, **15**, and **21** were assigned on the basis of HSQC spectra. [c] (COOMe): 170.3, 170.0, 52.4, 52.5. [d] **(**COOMe): -two epimers- 168.6, 169.1, 52.8, 52.9.

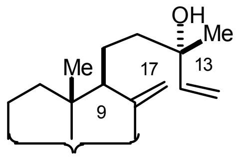
Table 1 (continued). ^{13}C NMR Chemical shifts of compounds 1-21[a,b]

	13	**14**[e]	**15**[f,g]	**16**[h]	**17**[i]	**18**[j]	**19**	**20**	**21**
C1	31.9	31.9	32.4	32.0	32.1	31.2	31.2	30.8	31.9
C2	21.3	21.4	21.3	21.2	20.4	21.4	21.4	22.6	21.4
C3	31.1	31.2	30.3	30.9	30.7	32.0	31.9	31.1	31.1
C4	30.5	30.4	30.7	30.4	30.5	30.4	30.4	30.5	30.4
C5	39.5	39.5	39.5	39.6	39.7	39.5	39.5	39.5	39.5
C6	34.0	33.9	33.0	33.5	33.2	33.9	33.9	33.0	33.9
C7	33.1	33.1	38.2	32.5	32.2	33.1	33.1	31.9	33.0
C8	149.2	149.6	211.6	148.8	146.1	149.2	149.5	149.5	149.4
C9	42.2	43.1	52.8	43.5	37.8	42.4	42.2	42.0	42.7
C10	42.4	42.4	46.7	42.6	42.6	42.3	42.4	42.2	42.3
C11	18.1	18.2	28.4	29.7	53.4	22.4	22.6	23.6	19.2
C12	43.0	41.6	---	---	---	40.1	38.7	33.9	37.6
C13	209.0	73.7	---	---	---	161.2	140.7	140.7	62.7
C14	---	145.0	---	---	---	114.7	122.9	124.4	62.5
C15	---	111.6	---	---	---	167.2	59.5	59.2	61.5
C16	30.1	28.1	---	---	---	19.1	16.5	21.2	16.9
C17	106.3	106.3	---	107.9	108.1	106.3	106.2	106.3	106.6
C18	16.4	16.4	16.3	16.3	16.2	16.3	16.3	16.4	16.3
C19	16.4	16.5	15.8	16.4	16.6	16.4	16.4	16.4	16.4
C20	18.2	18.4	18.8	18.3	18.8	18.3	18.3	18.4	18.3

[e] Values taken from an NMR spectrum of a mixture of **1** and **14**. [f] The COSY and HSQC spectra of the corresponding sulfone were recorded. [g] (SPh): 136.5, 130.0, 129.3, 128.7, 126.1. [h] (SPh): 128.2, 127.7, 124.8. [i] (SO_2Ph): 140.3, 133.4, 129.0, 128.1. [j] (OCH_3): 50.8.

Table 2. ^{1}H NMR Chemical Shifts of Vinylic Protons at C(17) for Labdane-type Diterpenoids and Compounds 1 and 14. Comparison Between C(13) Epimers





Compounds with configuration 9*S*,13*R*	=CH_2	Δδ	ref	Compounds with configuration 9*S*,13*S*	=CH_2	Δδ	ref
compound **14**	4.45 / 4.80	0.35	*	nakamurol-A (**1**)	4.50 /4.82	0.32	1, *
manool	4.46 / 4.80	0.34	22	13-epimanool	4.50 / 4.80	0.30	22
3α-hydroxymannol	4.49 / 4.82	0.33	23	3α-hydroxy-13-epimanool	4.53 / 4.83	0.30	20
3α-OTBS manool	4.46 / 4.79	0.33	20	3α-OTBS 13-epimanool	4.50 /4.80	0.30	20

* This work

Experimental Section[35]

General: All reactions were carried out under an argon atmosphere with dry, freshly distilled solvents under anhydrous conditions. Analytical thin-layer chromatography was performed on SiO_2 (silica gel 60 F_{254}, Merck), and the spots were located with iodoplatinate reagent or 1% aqueous $KMnO_4$. Chromatography refers to flash chromatography and was carried out on SiO_2 (silica gel 60, SDS, 230-240 mesh ASTM). Drying of organic extracts during workup of reactions was performed over anhydrous Na_2SO_4. Evaporation of solvent was accomplished with a rotatory evaporator. Chemical shifts of ^{1}H and ^{13}C NMR spectra are reported in ppm downfield (δ) from Me_4Si. The ^{13}C NMR spectra, when unambiguous assignation was not available, are reported as follows: chemical shift (multiplicity determined from DEPT spectra). Only noteworthy IR absorptions (cm^{-1}) are listed. Microanalyses and HRMS were performed by the Centro de Investigación y Desarrollo (CSIC), Barcelona.

(4a*S*,5*R*,8a*S*)-4a,5,8a-Trimethyl-3,4,4a,5,6,7,8,8a-octahydro-1*H*-naphthalen-2-one (4): ^{1}H NMR (500 MHz, COSY) 0.84 (s, 3H, Me-19), 0.88 (s, 3H, Me-20), 0.89 (d, *J* = 6.5 Hz, 3H, Me-18), 1.07 (dm, *J* = 10.5 Hz, H-1_{eq}), 1.3-1.4 (m, 1H, H-3), 1.50-1.60 (m, 4H, H-1_{ax}, H-2, H-3), 1.68 (td, *J* = 14.5, 4.5 Hz, 1H, H-6_{ax}), 1.69 (dd, *J* = 14.5, 2.1 Hz, 1H, H-9_{eq}), 1.89 (ddd, *J* = 14.5, 6.5, 2.1 Hz, 1H, H-6_{eq}), 2.14 (dm, *J* = 12 Hz, 1H, H-4_{ax}), 2.18 (dm, *J* = 14 Hz,1H, H-7_{eq}), 2.39 (td, *J* = 14.5, 5 Hz, 1H, H-7_{ax}), 3.04 (d, *J* = 14.5 Hz, 1H, H-9_{ax}); ^{13}C NMR (75 MHz, HSQC), see Table 1.

(1*S*,4a*S*,5*R*,8a*S*)-4a,5,8a-Trimethyl-1-(2,2-dimethoxycarbonylethyl)-3,4,4a,5,6,7,8,8a-octahydro-1*H*-naphthalen-2-one (7). To a solution of dimethyl malonate (0.09 mL, 0.78 mmol) in benzene (2 mL) and MeOH (0.5 mL) was added sodium methoxide (86 mg, 1.59 mmol), and the mixture was heated at reflux. Then, a solution of mesylate **6** (94 mg, 0.31 mmol) in benzene (3 mL) was slowly added and the stirring was maintained for 1 h. The reaction mixture was cooled to room temperature and, after addition of 2 N HCl (25 mL), extracted with Et_2O. The dried organic extracts were concentrated and purified by chromatography (5% EtOAc in hexane) to give, in order of elution, enol lactone **8** (32 mg, 33%), as a mixture of epimers, and malonate **7** (15 mg, 14%).

Compound **7**: IR (NaCl) 1708, 1736 cm^{-1}; ^{1}H NMR (300 MHz) 0.68 (s, 3H), 0.82 (s, 3H), 0.88 (d, *J* = 6.6 Hz, 3H), 1.38–1.55 (m, 3H), 1.65 (td, *J* = 14.4, 4.5 Hz, 1H), 1.78–1.92 (m, 2H), 2.13–2.23 (m, 2H), 2.26–2.35 (m, 1H), 2.43 (td, *J* = 14, 6 Hz, 1H), 3.06 (d, *J* = 11 Hz, 1H), 3.50 (dd, *J* = 11.4, 3.9 Hz, 1H), 3.71 and 3,72 (2 s, 3H each); ^{13}C NMR (75 MHz, DEPT), see Table 1.

Methyl (2*RS*,6a*S*,7*R*,10a*R*)-6a,7,10a-Trimethyl-3-oxo-2,3,5,6,6a,7,8,9,10,10a-decahydro-1*H*-benzo[*f*]chromene-2-carboxylate **(8)**: IR (NaCl) 1743, 1771 cm^{-1}; ^{1}H NMR (300 MHz): 0.81 and 0.82 (2 s, 3H), 0.82 and 0.83 (2 d, *J* = 6.5 Hz, 3H), 0.88 and 0.94 (2 s, 3H), 2.39-2.75 (m, 2H), 3.46 (dd, *J* = 12.9, 6.9 Hz, 0.5H), 3.63 (dd, *J* = 6.3, 4.8 Hz, 0.5H), 3.75 and 3.82 (2 s, 3H); ^{13}C NMR (75 MHz, DEPT), see Table 1.

(1*R*,4a*S*,5*R*,8a*S*)-1-(But-3-enyl)-4a,5,8a-trimethyl-3,4,4a,5,6,7,8,8a-octahydro-1*H*-naphthalen-2-one (11): ^{13}C NMR (75 MHz, DEPT) 17.7 (q), 19.3 (q), 21.6 (t), 23.9 (q), 28.4 (t), 29.7 (d), 31.1 (t), 33.5 (t), 35.9 (t), 37.5 (s), 39.0 (t), 45.1 (s), 56.8 (d), 114.6 (t), 138.8 (d), 213.6 (s). Values taken from an NMR spectrum of a mixture of **10** and **11**.

(1*S*,4a*S*,5*R*,8a*S*)-1-Phenylsulfanylmethyl-4a,5,8a-trimethyl-3,4,4a,5,6,7,8,8a-octahydro-1*H*-naphthalen-2-one (15). To a solution of enone **9** (125 mg, 0.6 mmol) in THF (3 mL) were added thiophenol (0.09 mL, 0.9 mmol) and triethylamine (4 µl, 0.03 mmol). The reaction mixture was stirred at room temperature for 24 h, poured into saturated aqueous $NaHCO_3$ and extracted with Et_2O. The dried organic extracts were concentrated and purified by chromatography (2% EtOAc in hexane) to give **15** (128 mg, 67%): ^{1}H NMR (300 MHz) 0.69 (s, 3H), 0.81 (s, 3H), 0.87 (d, *J* = 6.6 Hz, 3H), 1.0-1.5 (m, 7H), 1.69 (dd, *J* = 14, 4.6 Hz, 1H), 1.90 (ddd, *J* = 14.4, 6, 2.6 Hz, 1H), 2.27 (m, 1H), 2.49 (td, *J* = 13.6, 6.2 Hz, 1H), 2.73 (d, *J* = 11 Hz, 1H), 3.29 (d, *J* = 9 Hz, 1H), 3.35 (dd, *J* = 11, 9 Hz, 1H), 7.28 (m, 5H); ^{13}C NMR (75 MHz, DEPT), see Table 1.

(1*R*,4a*S*,5*R*,8a*S*)-2-Methylene-1-phenylsulfanylmethyl-4a,5,8a-trimethylperhydronaphthalene (16). *n*-BuLi (1.6 M in hexane, 1.98 mL, 3.16 mol) was added to a cooled (0 ºC) dispersion of methyltriphenylphosphonium bromide (1.13g, 3.16 mol) in THF (10 mL). After stirring for 1 h, a solution of **15** (100 mg, 0.316 mmol) in THF (12 mL) was added dropwise, and the reaction mixture was heated at reflux for 24 h. The reaction mixture was cooled at room temperature and quenched with water, and the aqueous layer was extracted with EtOAc. The organic extracts were washed with brine, concentrated, and purified by chromatography (hexane) to give **16** (75 mg, 75%): ^{1}H NMR (200 MHz) 0.70 (s, 3H), 0.75 (s, 3H), 0.79 (d, *J* = 6.6 Hz, 3H), 1.05-1.50 (m, 8H), 1.61 (dq, *J* = 13.8, 4.6, 2.5 Hz, 1H), 2.11 (ddd, *J* = 13.2, 5.0, 2.8 Hz, 1H), 2.25 (m, 1H), 3.03 and 3.05 (2d, *J* = 12 Hz, 1H each), 3.04 (s, 1H), 4,63 (s, 1H), 4.98 (s, 1H), 7.25 (m, 5H); ^{13}C NMR (50 MHz, DEPT), see Table 1.

(1*R*,4a*S*,5*R*,8a*S*)-1-Benzenesulfonylmethyl-2-methylene-4a,5,8a-trimethylperhydronaphthalene (17). **Method A.** To a solution of sulfide **16** (250 mg, 0.8 mmol) in MeOH (5 mL) was added dropwise a solution of oxone® (1.47 g, 2.34 mmol) in water (5 mL). The reaction mixture was stirred at room temperature for 16 h, diluted with CH_2Cl_2 and extracted. The organic layer was dried and concentrated, and the resulting oil was purified by chromatography (10% EtOAc in hexane) to give **17** (275 mg, 98%): ^{1}H NMR (300 MHz, COSY) 0.56 (s, 3H, Me-20), 0.74 (s, 3H, Me-19), 0.80 (d, *J* = 6.6 Hz, 3H, Me-18), 1.10-1.55 (m, 7H), 1.6 (ddd, *J* = 13.8, 4.4, 2.8 Hz, 1H, H-6_{eq}), 2.03 (ddd, *J* = 13.6, 4.8, 2.6 Hz, H-7_{eq}); 2.20 (m, 1H, H-4), 2.22 (td, *J* = 14, 4.2 Hz, H-7_{ax}), 3.19 and 3.37 (2m, 1H each, H-11), 3.40 (d, *J* = 9.2 Hz, 1H, H-9), 4.47 and 4.78 (2s, 1H each, H-17), 7.58 (m, 3H), 7.89 (m, 2H); ^{13}C NMR (75 MHz, HSQC, DEPT), see Table 1.

Method B. To a solution of sulfide **15** (110 mg, 0.35 mmol) in MeOH (2 mL) was added dropwise a solution of oxone® (0.6g, 1.05 mmol) in water (2 mL). The reaction mixture was stirred at room temperature for 4 h and extracted with CH_2Cl_2. The dried organic extracts were dried, concentrated, and purified by chromatography (10% EtOAc in hexane) to give (1*S*,4a*S*,5*R*,8a*S*) 1-benzenesulfonylmethyl-4a,5,8a-trimethyl-3,4,4a,5,6,7,8,8a-octahydro-1*H*-naphthalen-2-one, not shown, (120 mg, 99%): ^{1}H NMR (600 MHz, COSY): 0.54 (s, 3H, Me-20), 0.82 (s, 3H, Me-19), 0.91 (d, *J* = 6.6 Hz, 3H, Me-18), 1.35 (m, 1H, H-1), 1-40 (m, 1H, H-3), 1.50 (m, 1H, H-1), 1.55 (m, 1H, H-2), 1.60 (m, 1H, H-3), 1.65 (m, 1H, H-6_{ax}), 1.76 (m, 1H, H-2), 1.91 (ddd, *J* = 14.5, 6.2, 2.5 Hz, 1H, H-6_{eq}), 2.16 (ddd, *J* = 13.2, 4.5, 2.4 Hz, H-7_{eq}), 2.41 (dqd, *J* = 12.3, 6.6, 4 Hz, 1H, H-4), 2.47 (td, *J* =13.4, 6.4 Hz, H-7_{ax}), 2.85 (d, *J* = 13.9 Hz, 1H, H-11), 3.75 (d, *J* = 8.5 Hz, 1H, H-9_{ax}), 3.99 (dd, *J* = 14.2, 8.5 Hz, 1H, H-11), 7.54 (td, *J*= 7.8, 1.2 Hz, 2H, *m*-ArH), 7.62 (tt, *J* =7.8, 1.2 Hz, 1H, *p*-ArH), 7.90 (dd, *J* = 7.8, 1.2 Hz, 2H, *o*-ArH); ^{13}C NMR (75 MHz, HSQC) 16.1 (C-19), 16.4 (C-18), 19.1 (C-20), 20.8 (C-2), 30.3 (C-3), 31.7 (C-4), 32.7 (C-1), 33.0 (C-6); 37.5 (C-7), 39.7 (C-5), 46.0 (C-9), 46.8 (C-10), 50.6 (C-11), 128.0 (*o*-Ar), 129.1 (*m*-Ar), 133.6 (*p*-Ar), 139.9 (*ipso*-Ar), 208.4 (C-8). A solution of $TiCl_4$ (0.1 mL, 0.95 mmol) in CH_2Cl_2 (2 mL) was added slowly to a cooled (-40 °C) mixture of zinc dust (0.3 g, 4.5 mmol) and CH_2Cl_2 (0.2 mL) in THF (3 mL). The mixture was stirred for 30 min and a solution of the above ketone sulfone (55 mg, 0.16 mmol) in THF (2 mL) was added dropwise. The reaction was allowed to reach room temperature and stirred for 20 h. The crude was poured into 2 N HCl and extracted with Et_2O. The dried organic extracts were concentrated and purified by chromatography (10% EtOAc in hexane) to yield **17** (25 mg, 46%).

(*E*)-(1*R*,4a*S*,5*R*,8a*S*)-3-Methyl-5-(4a,5,8a-trimethyl-2-methylene-decahydronaphthalen-1-yl)-pent-2-en-1-ol (20): $[\alpha]_D$ -6.4 (*c* 0.05, CH_2Cl_2); ^{1}H NMR (300MHz) 0.62 (s, 3H), 0.73 (s, 3H), 0.79 (d, *J* = 6.6 Hz, 3H) 1.10-1.60 (m, 10H), 1.75 (s, 3H), 1.80-1.95 (m, 1H), 2.05 (m, 1H), 2.10-2.25 (m, 3H), 2.35 (m, 1H), 2.58 (d, *J* = 9 Hz, 1H), 4.09 (br d, *J* = 6 Hz, 2H), 4.54 (s, 1H), 4.86 (s, 1H), 5.43 (br t, *J* = 6 Hz, 1H); ^{13}C NMR (75 MHz, DEPT), see Table 1.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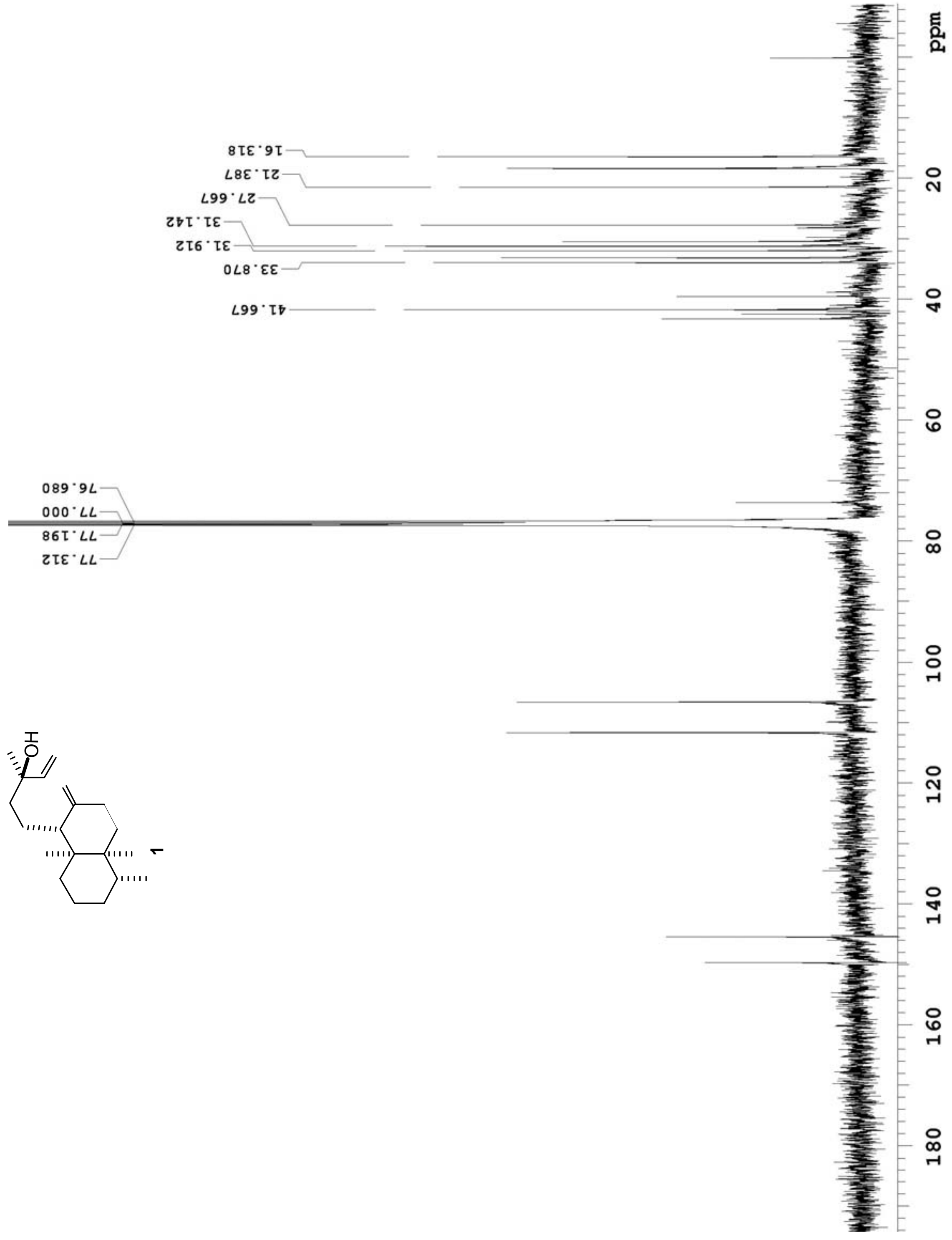
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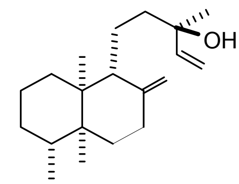

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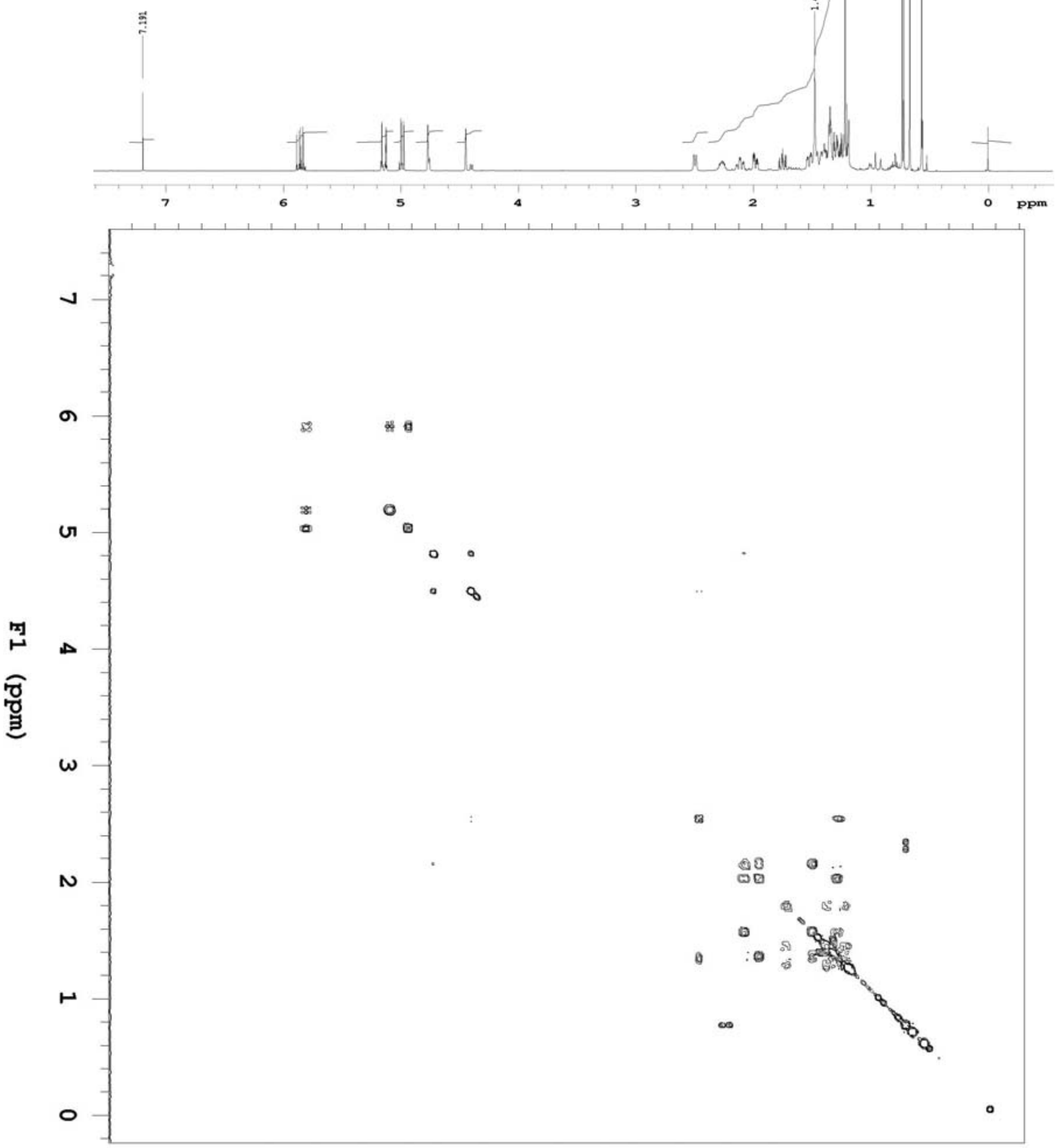

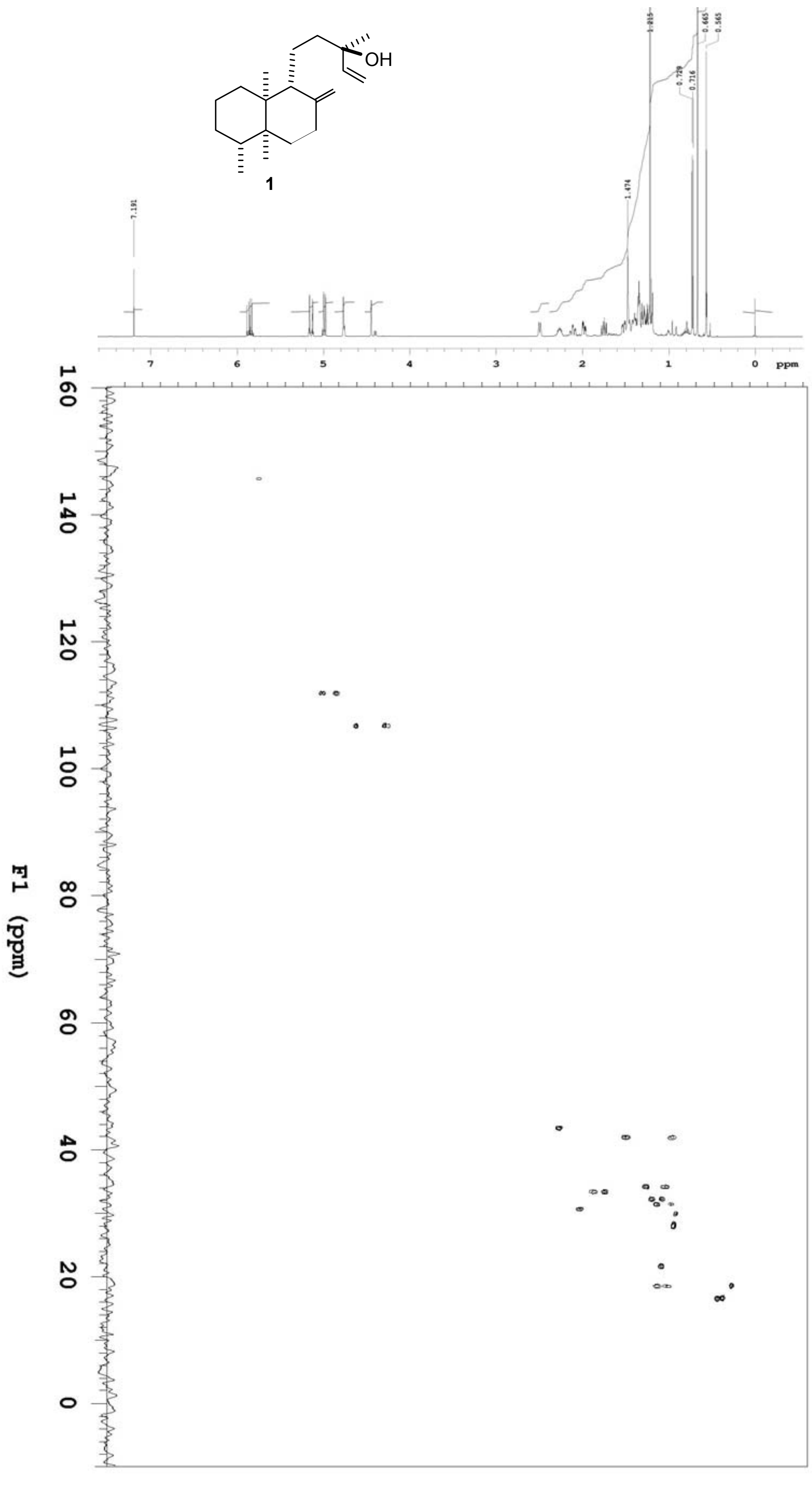
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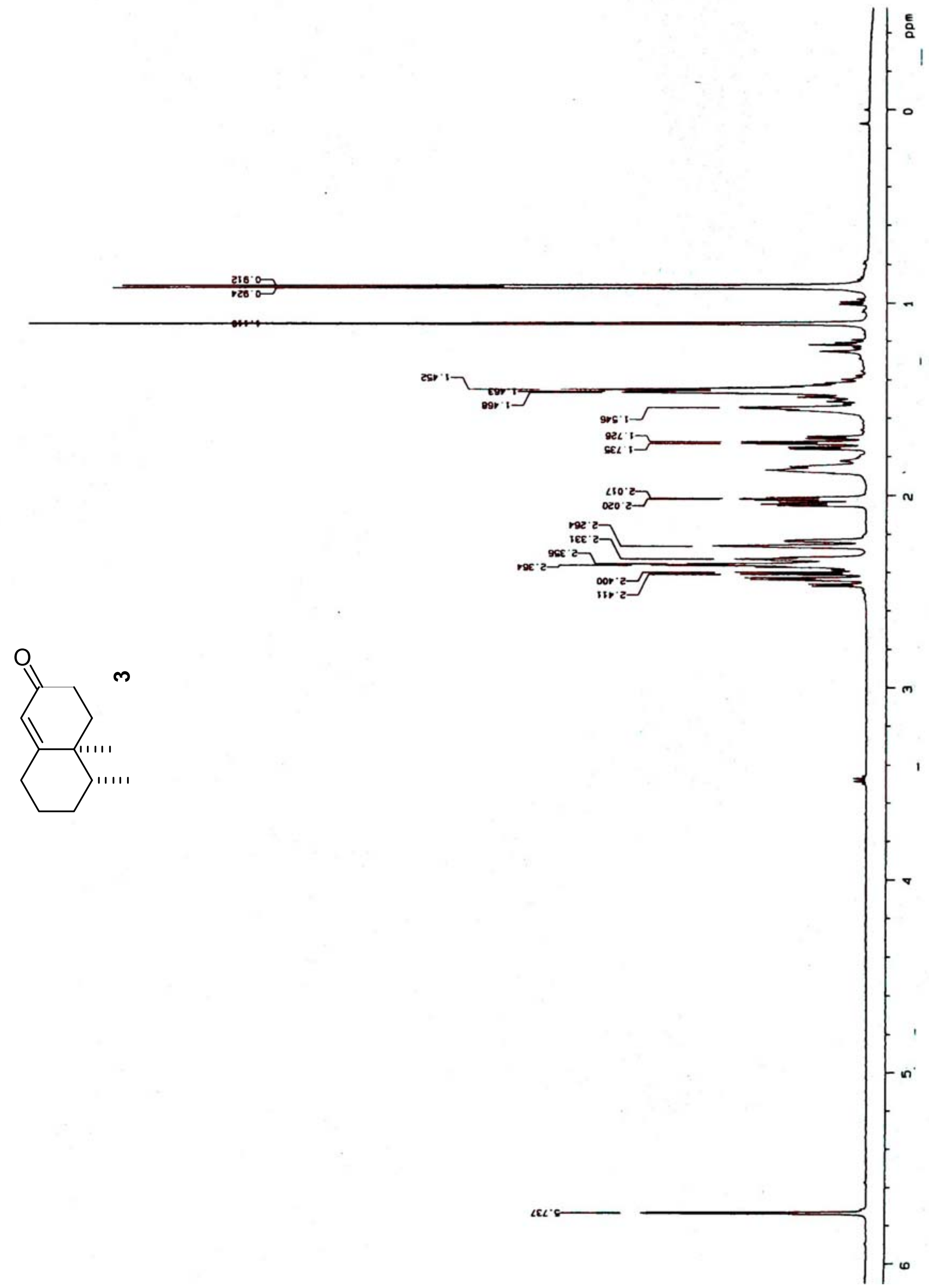

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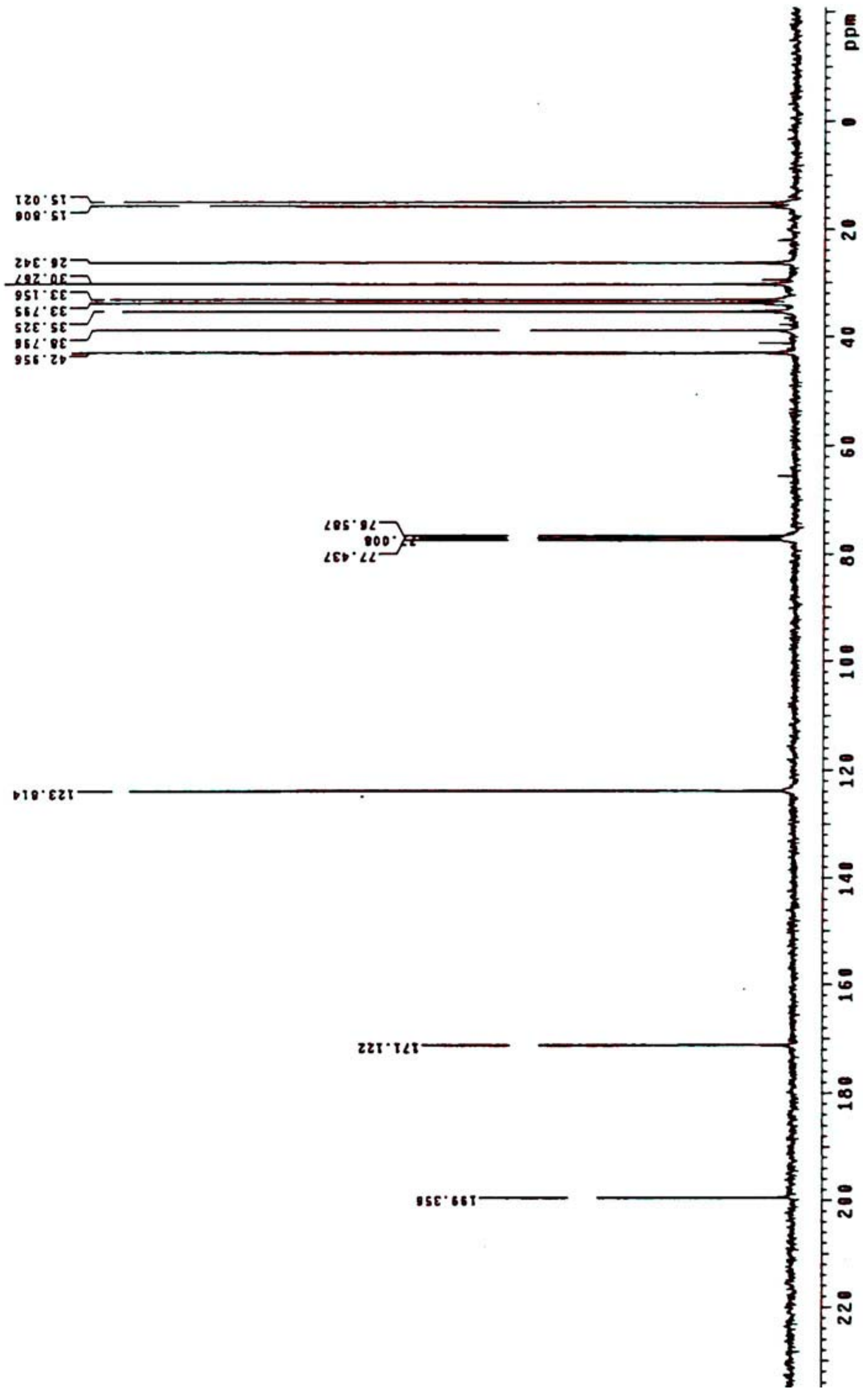
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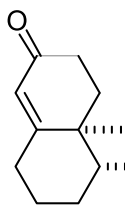

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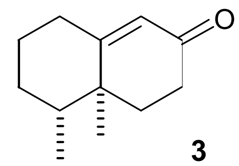

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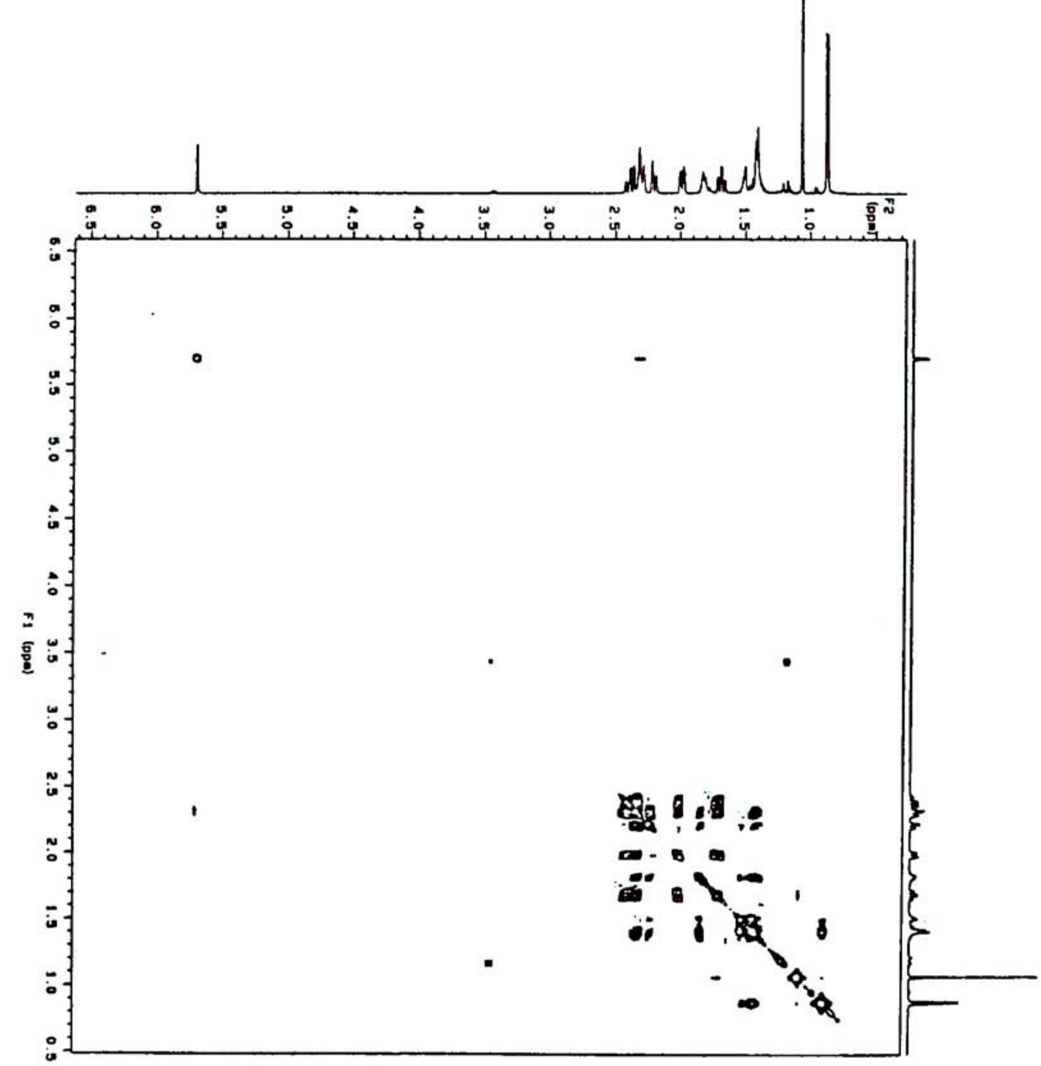

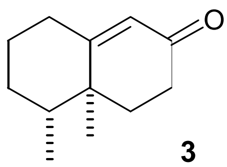

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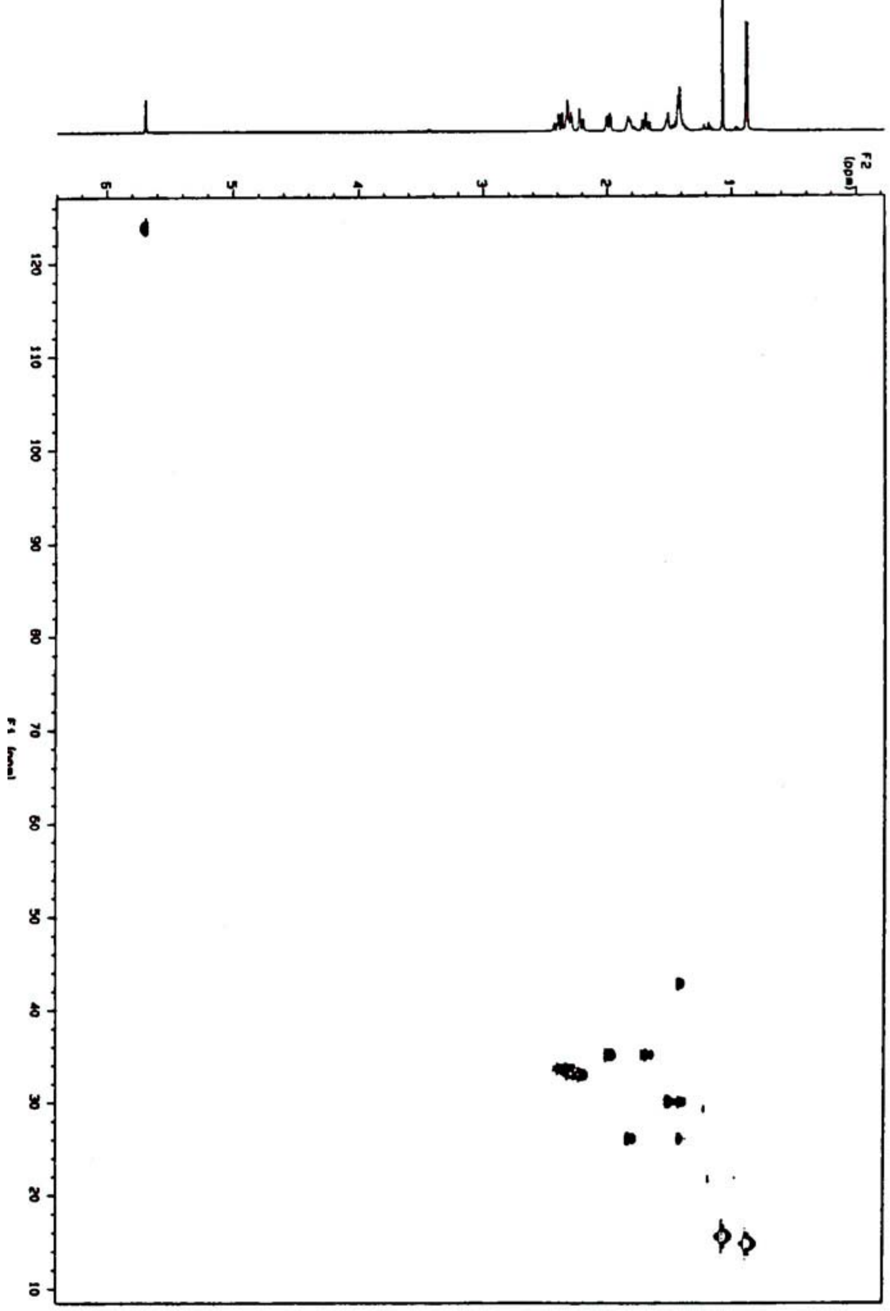

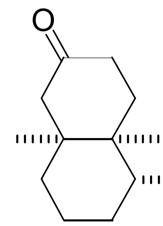

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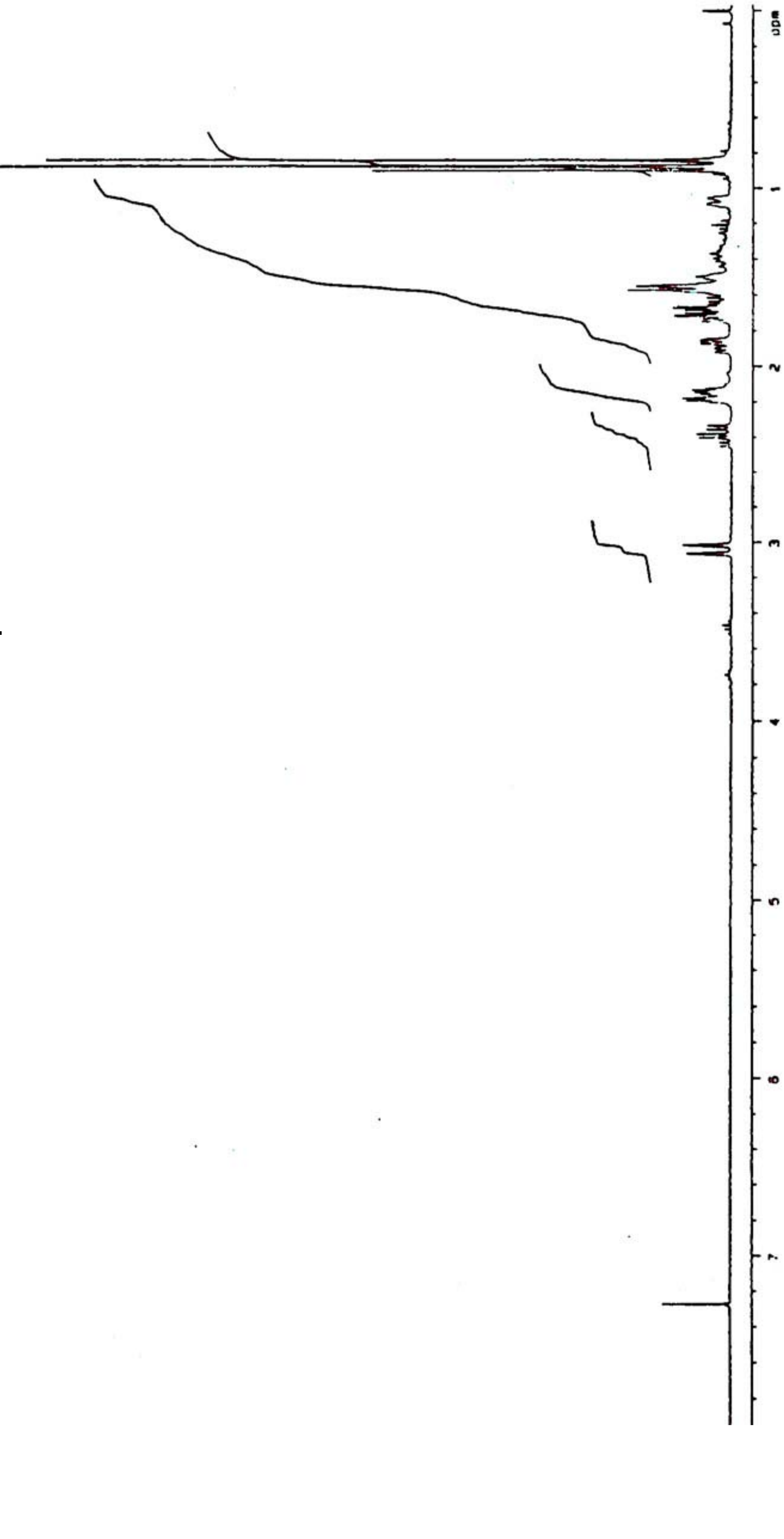

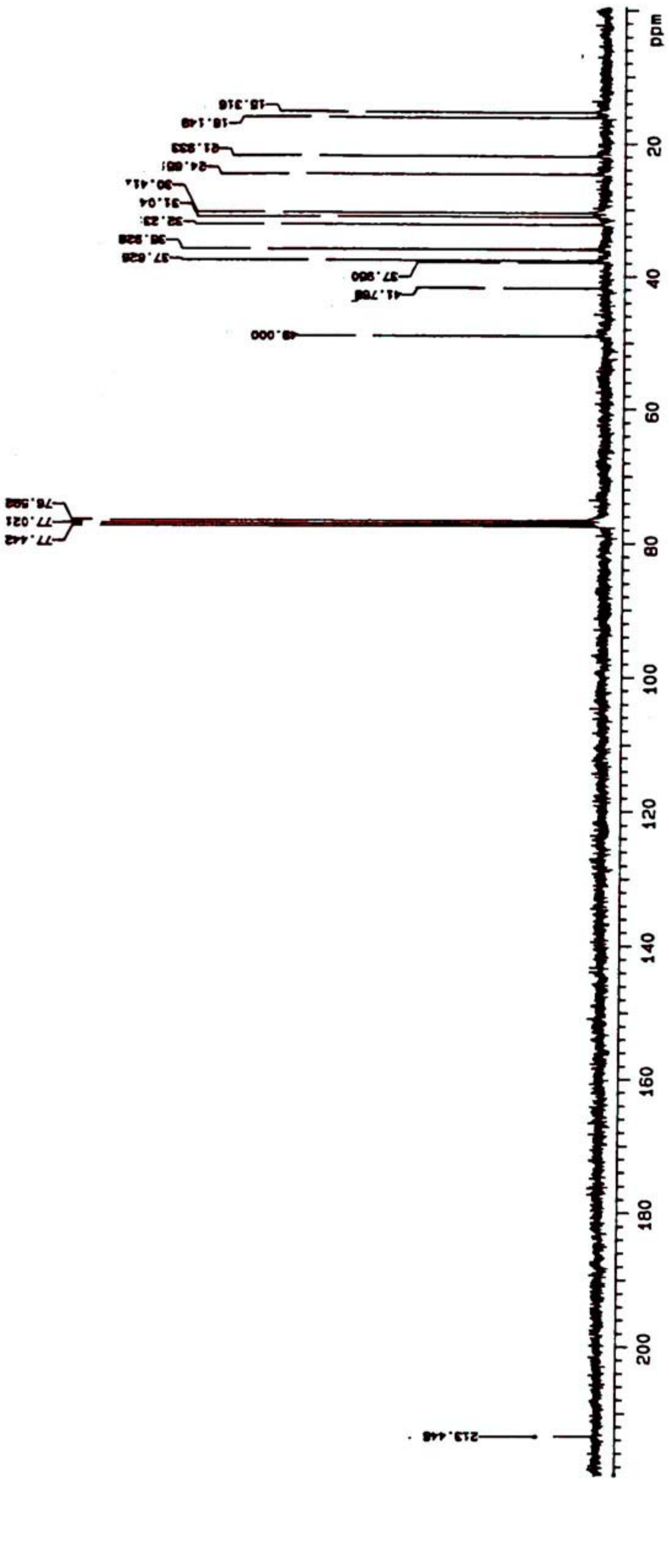
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36.528
37.628
37.950
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48.000
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77.021
77.442
213.446
ppm
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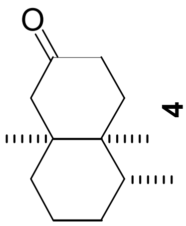
60
80
100
120
140
160
180
200



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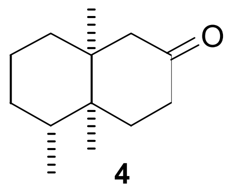

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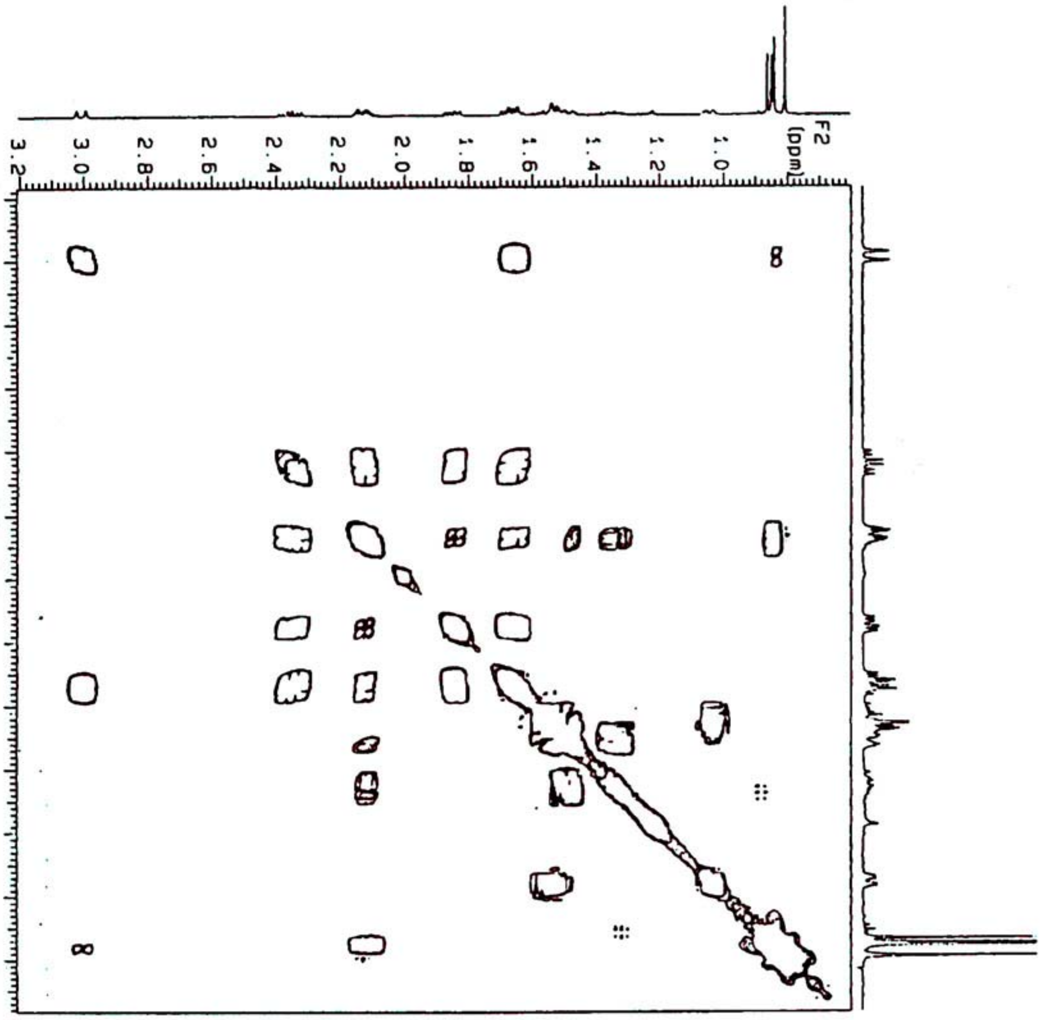

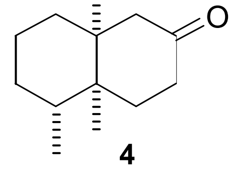

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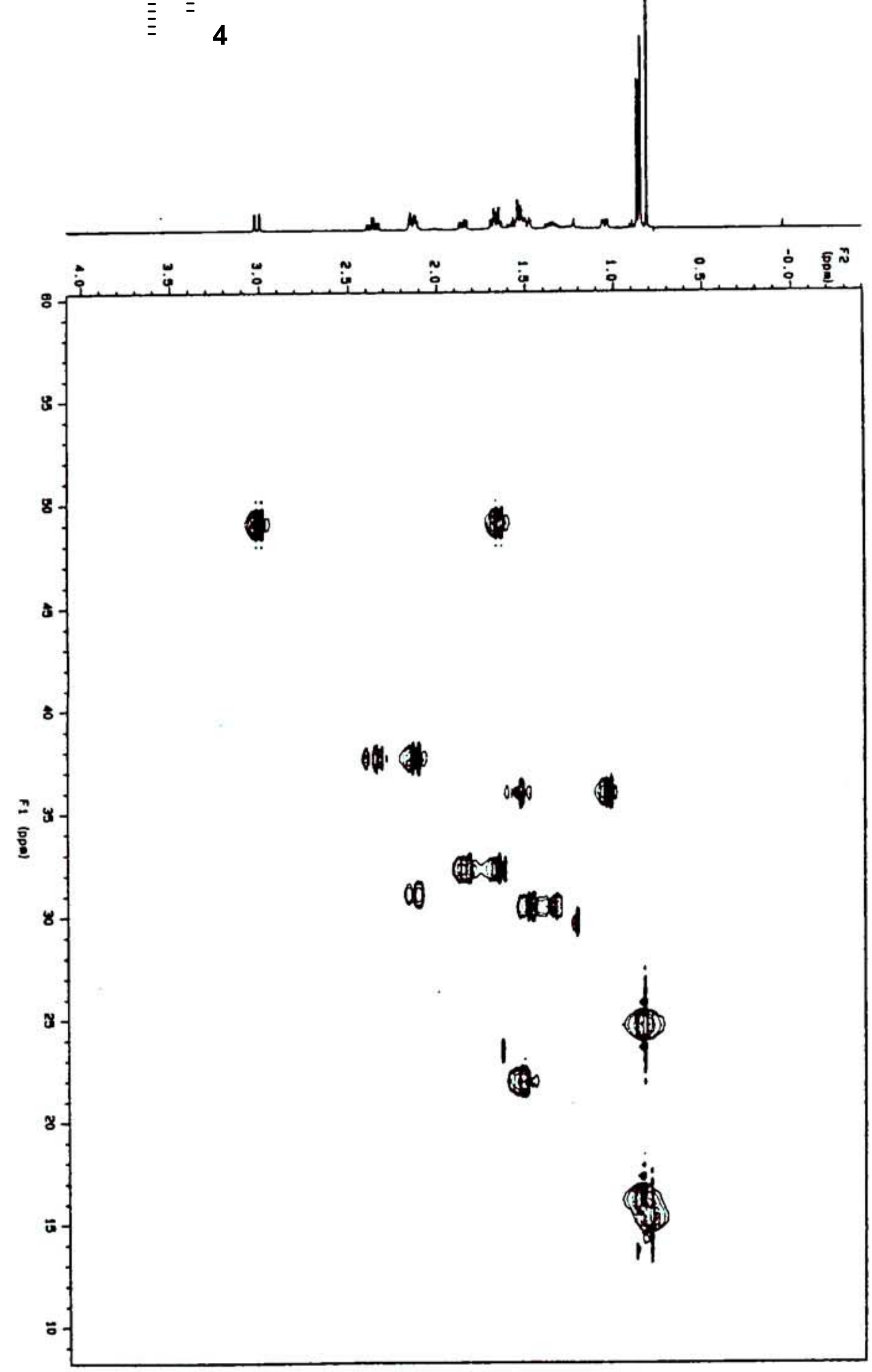

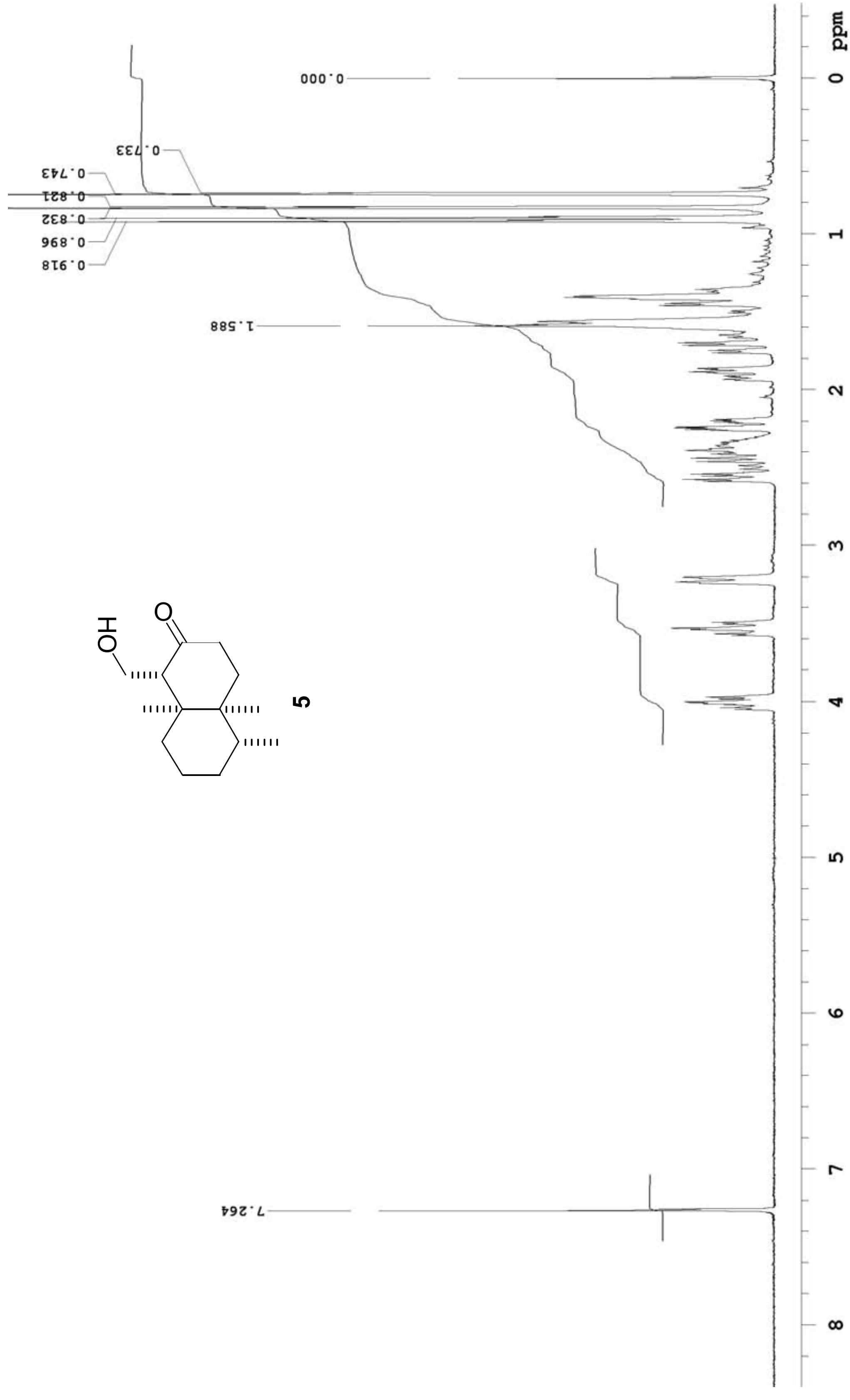
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0.821
0.832
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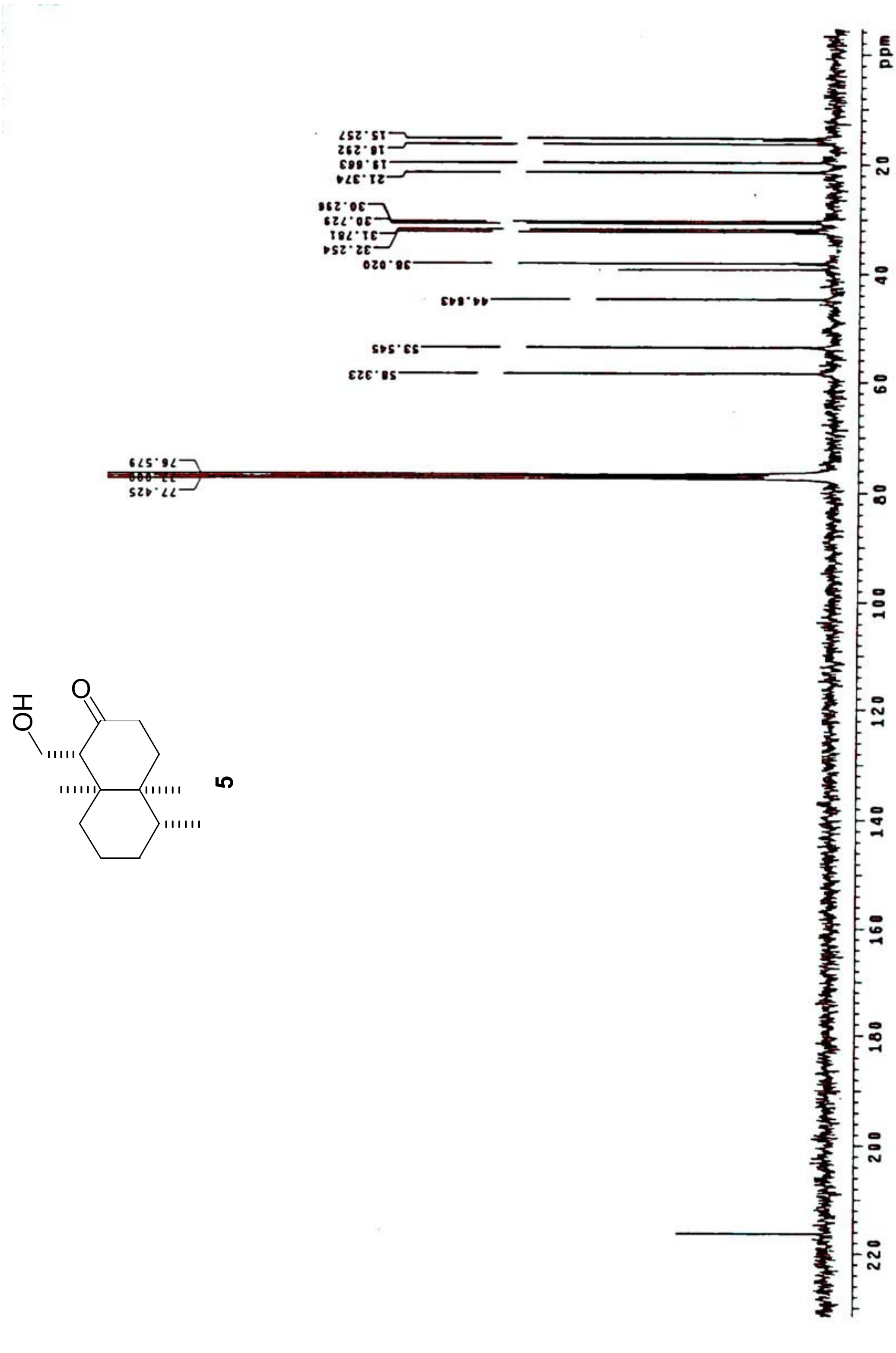
0.918
1.588
7.264
ppm
0
1
2
3
4
5
6
7
8
OH
O
5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19.683
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30.729
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32.254
38.020
44.843
53.545
58.323
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77.000
77.425
ppm
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60
80
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140
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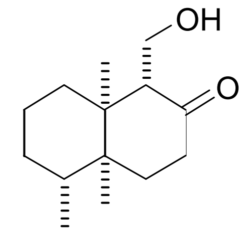
180
200
220
OH
O
5



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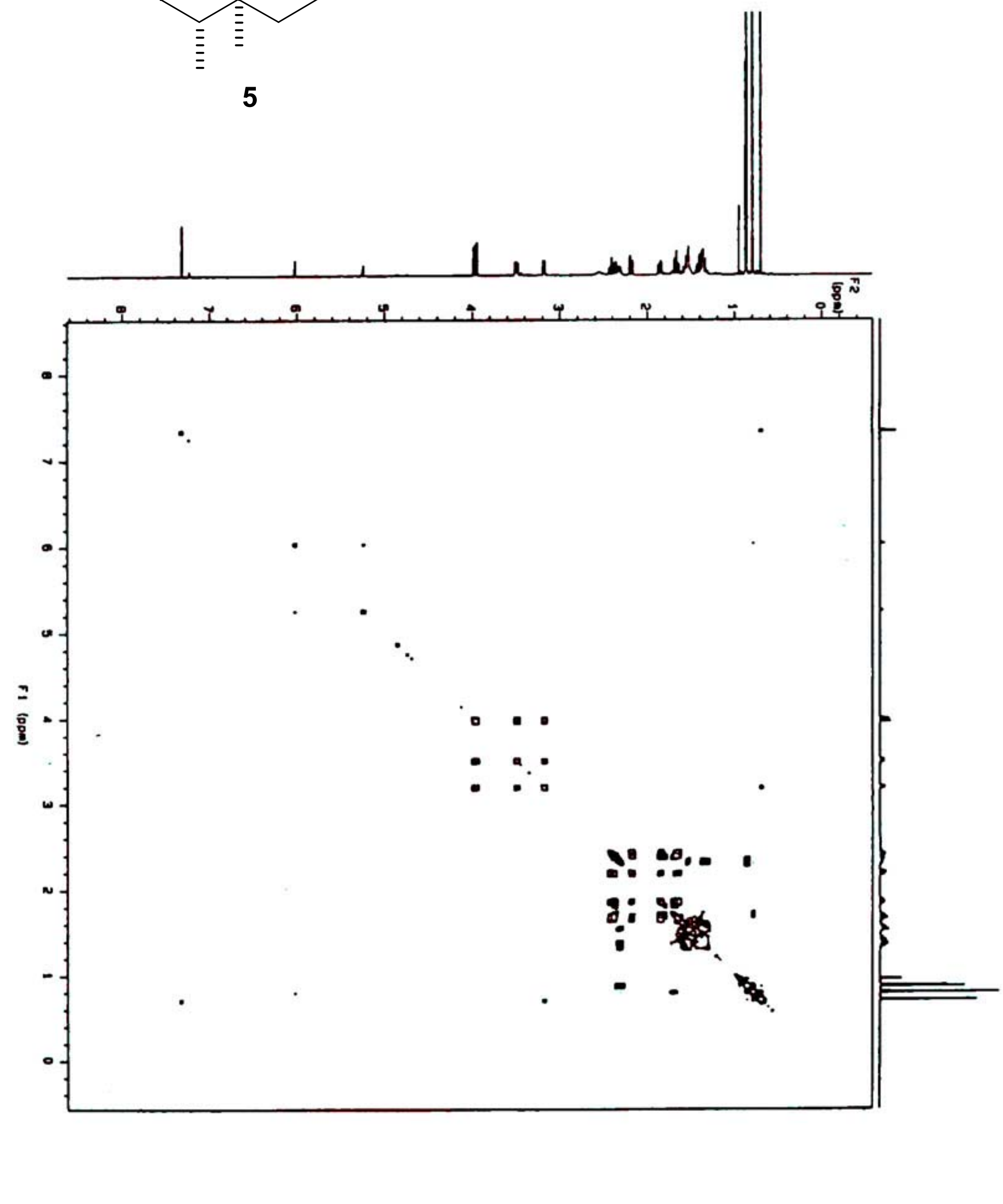

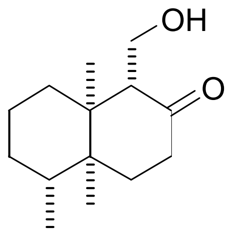

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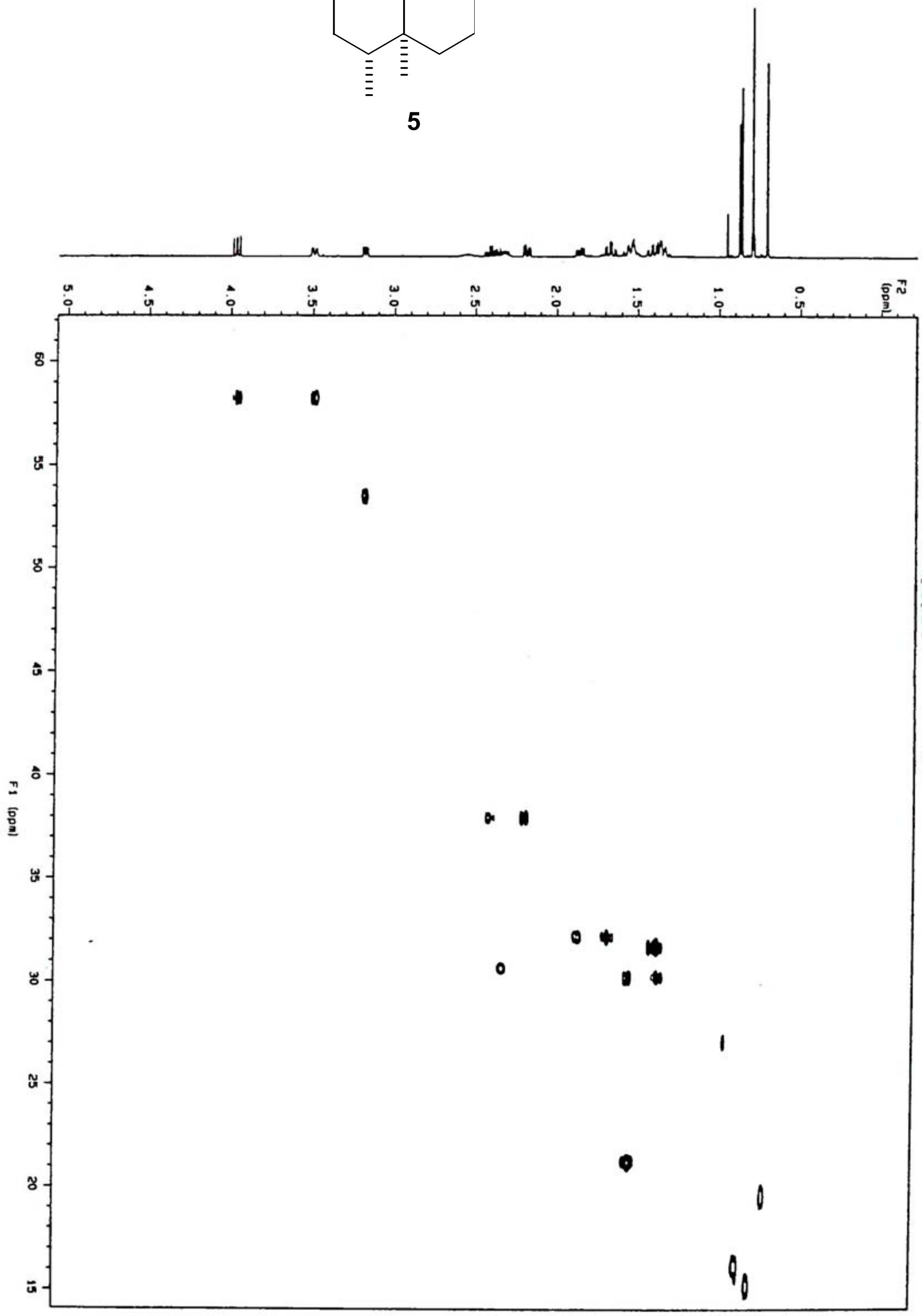

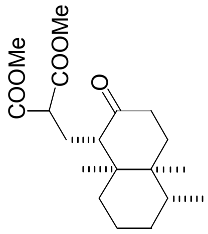

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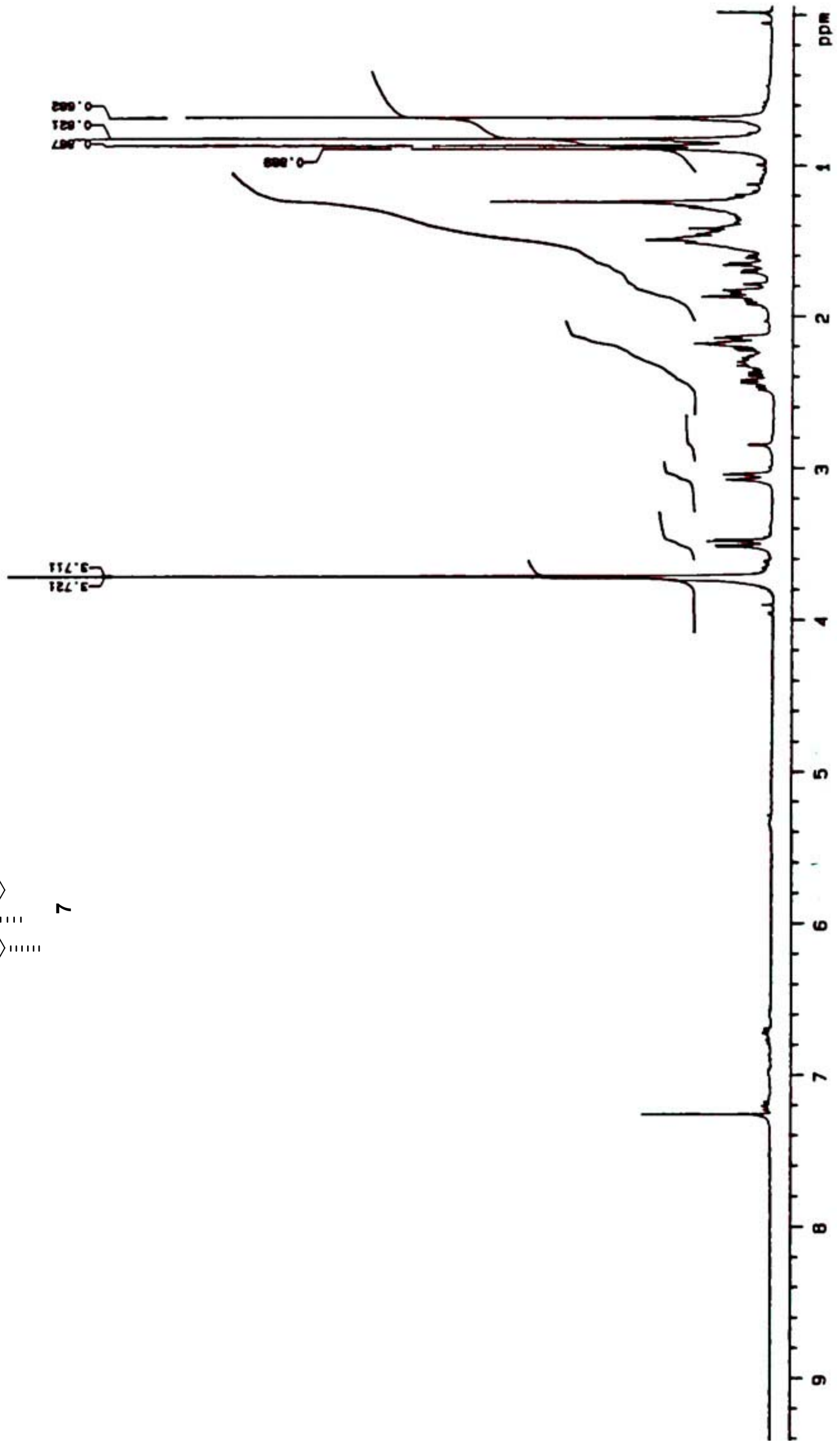
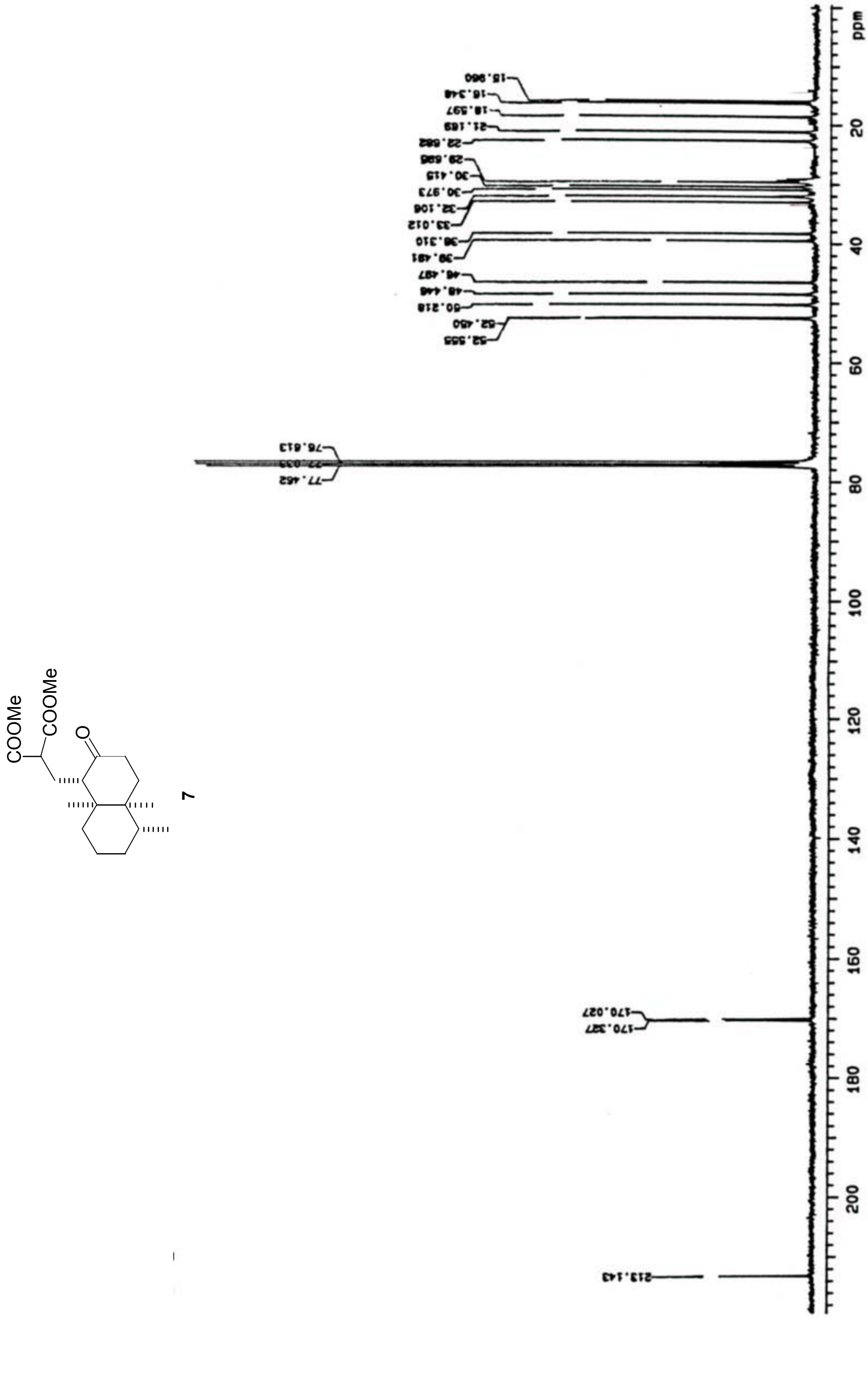
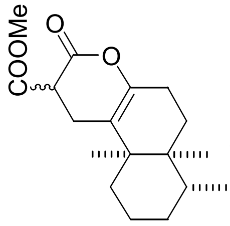



COOMe
COOMe
O
7
ppm



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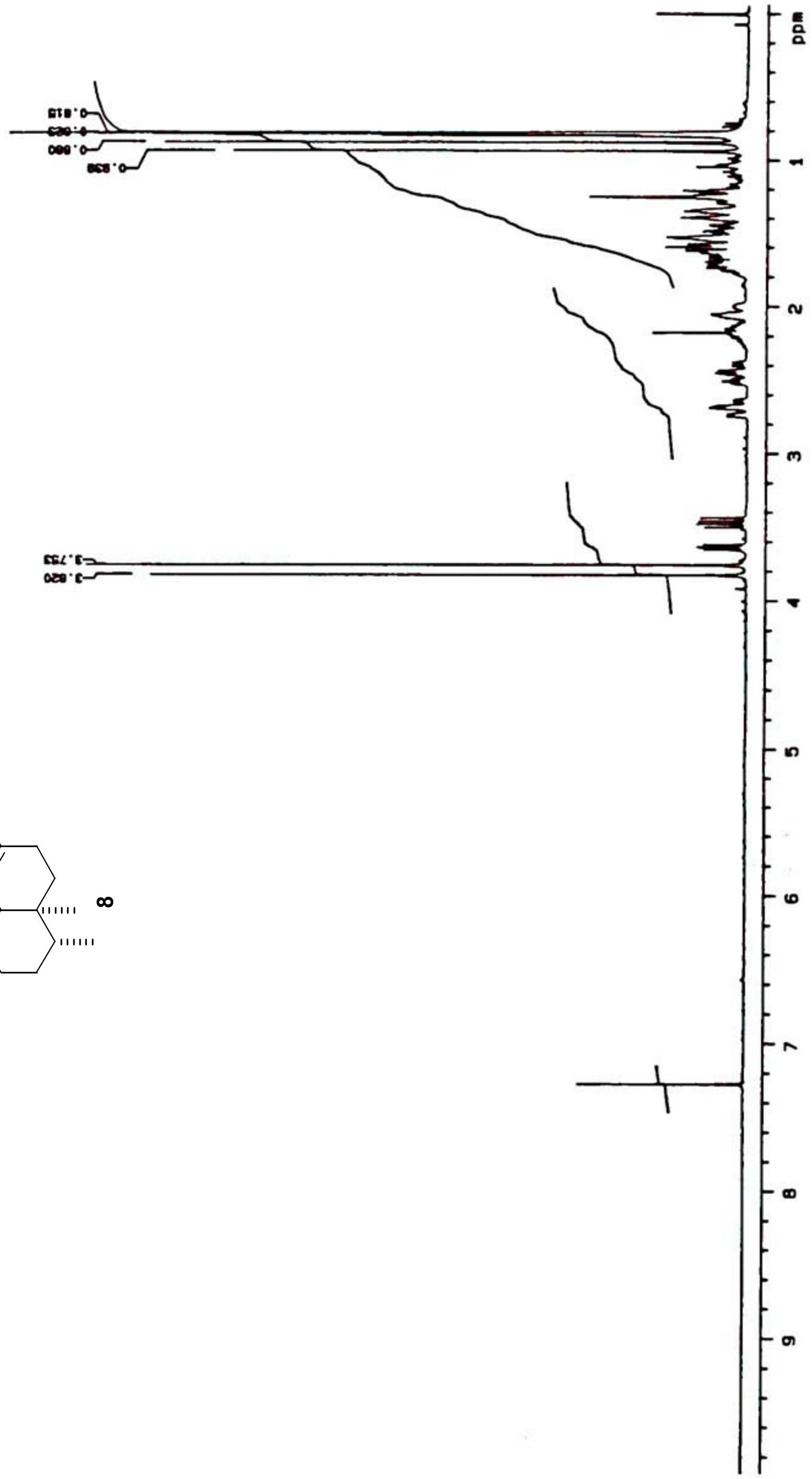

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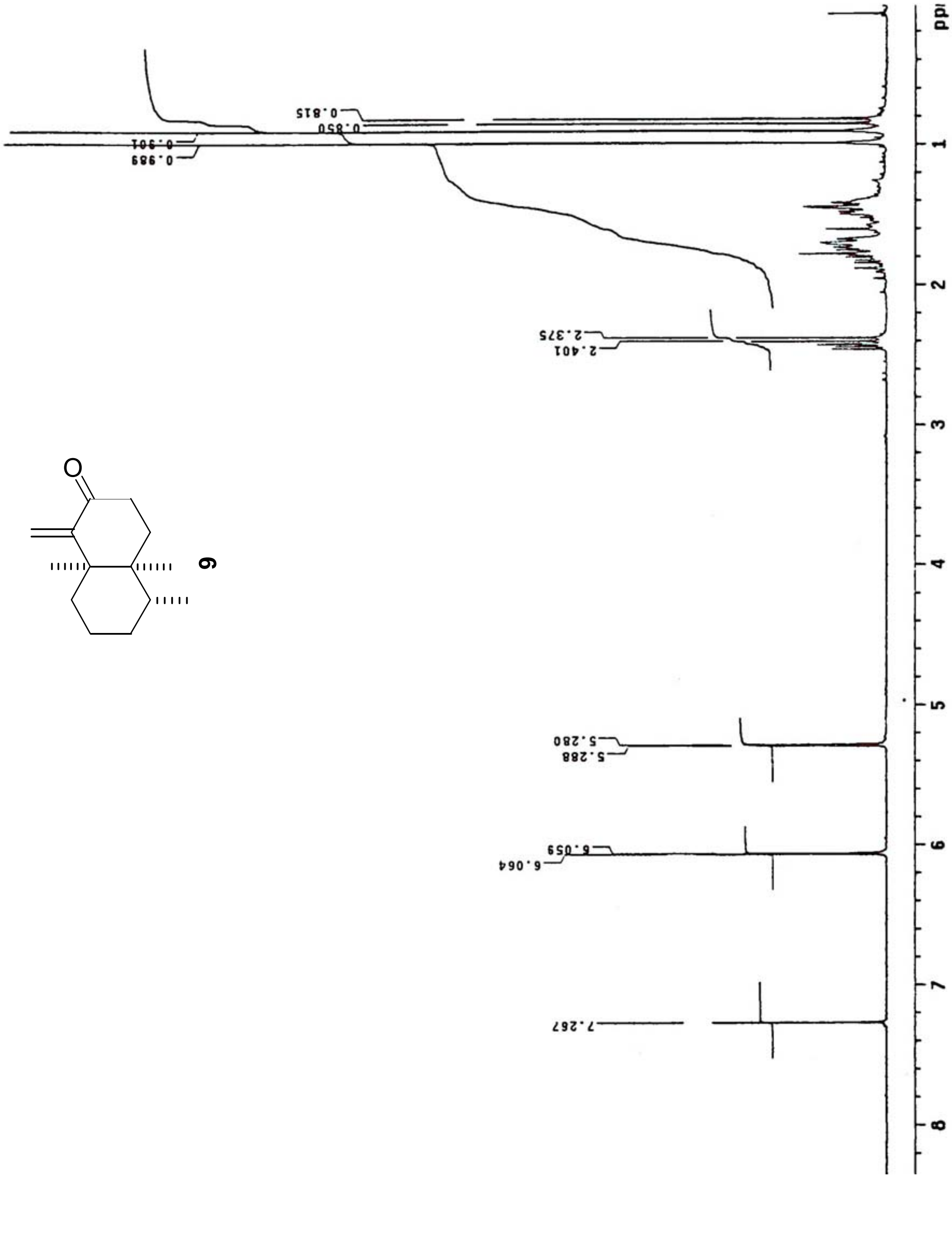

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0.850
0.901
0.989
2.375
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5.288
6.059
6.064
7.267
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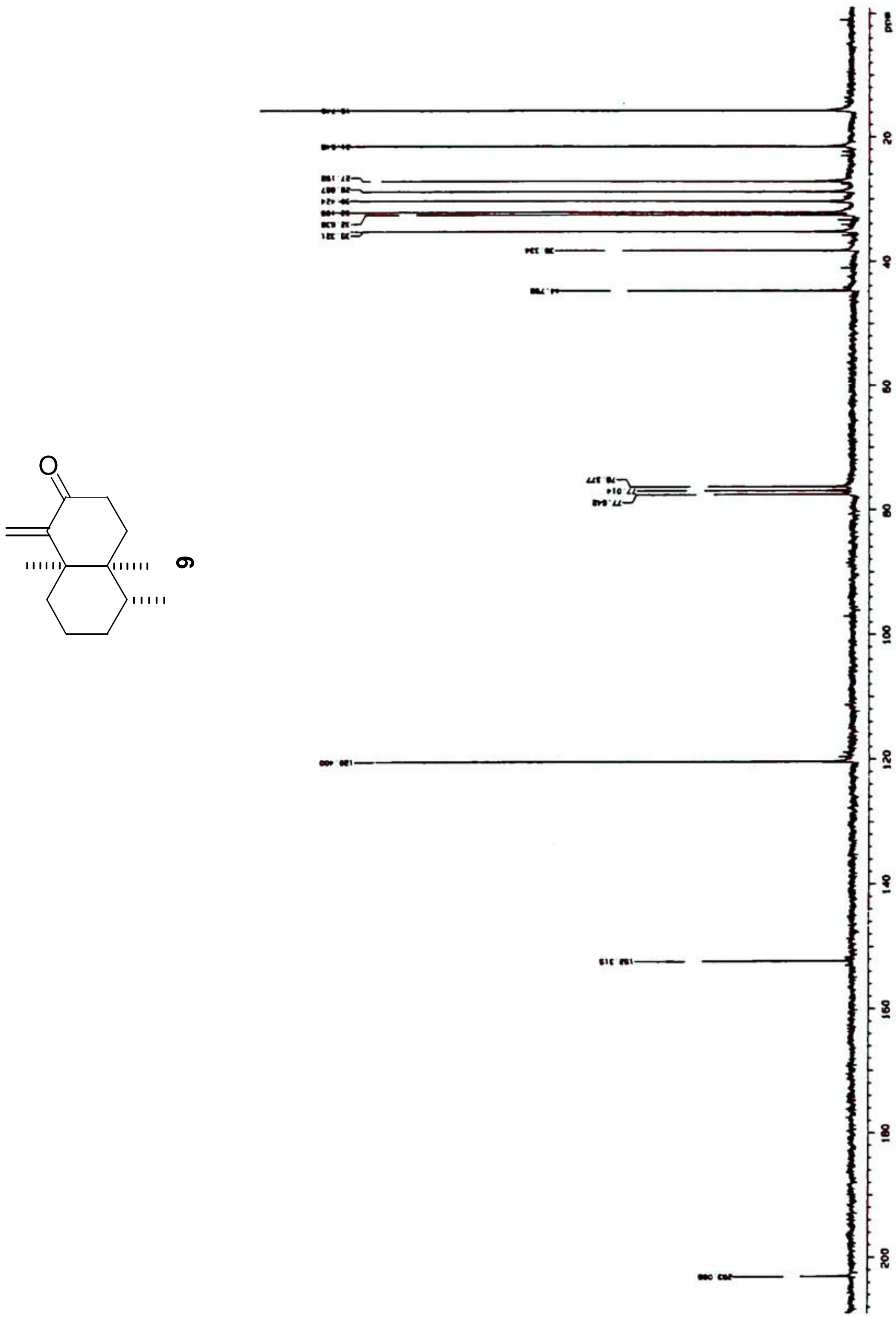
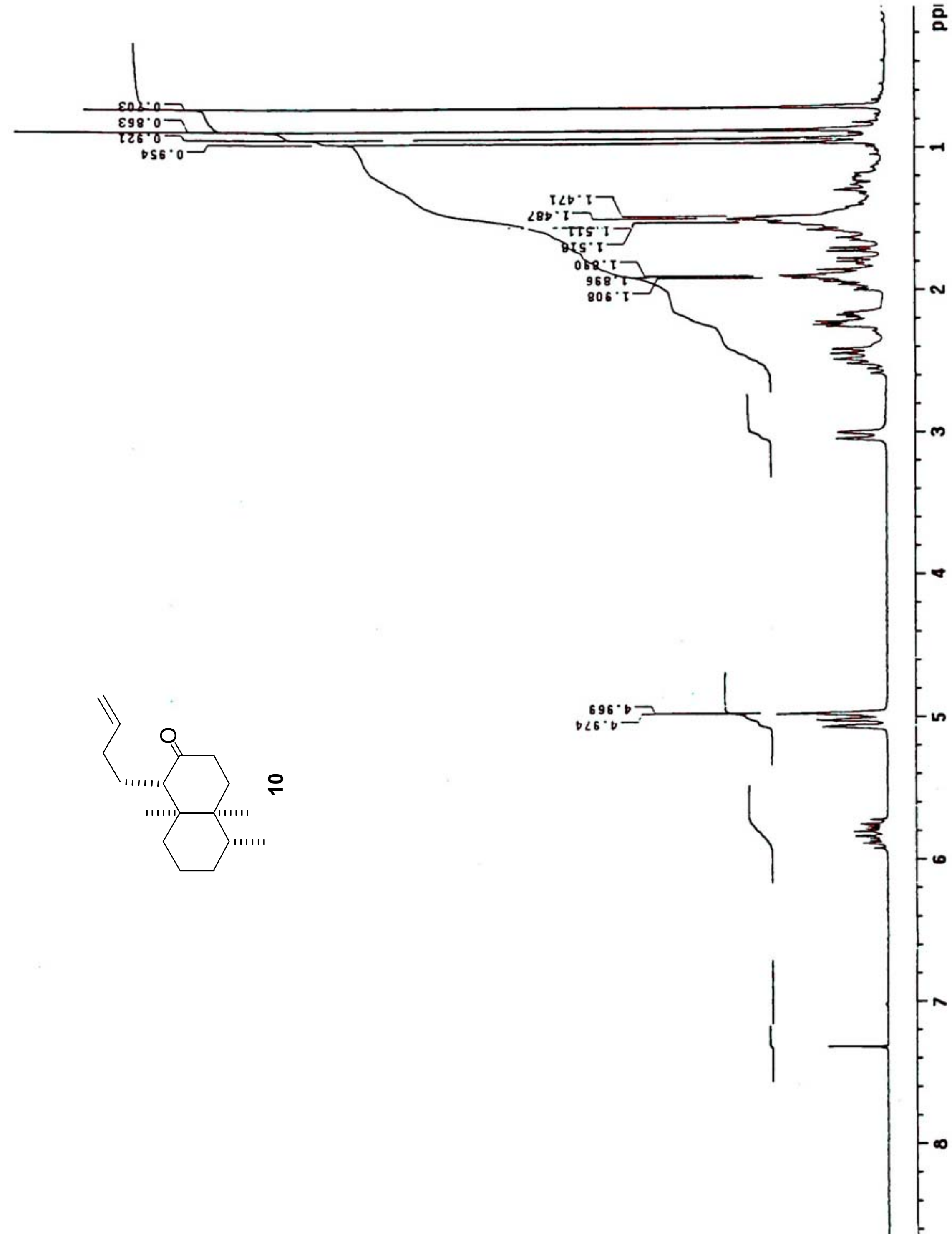
4
5
6
7
8

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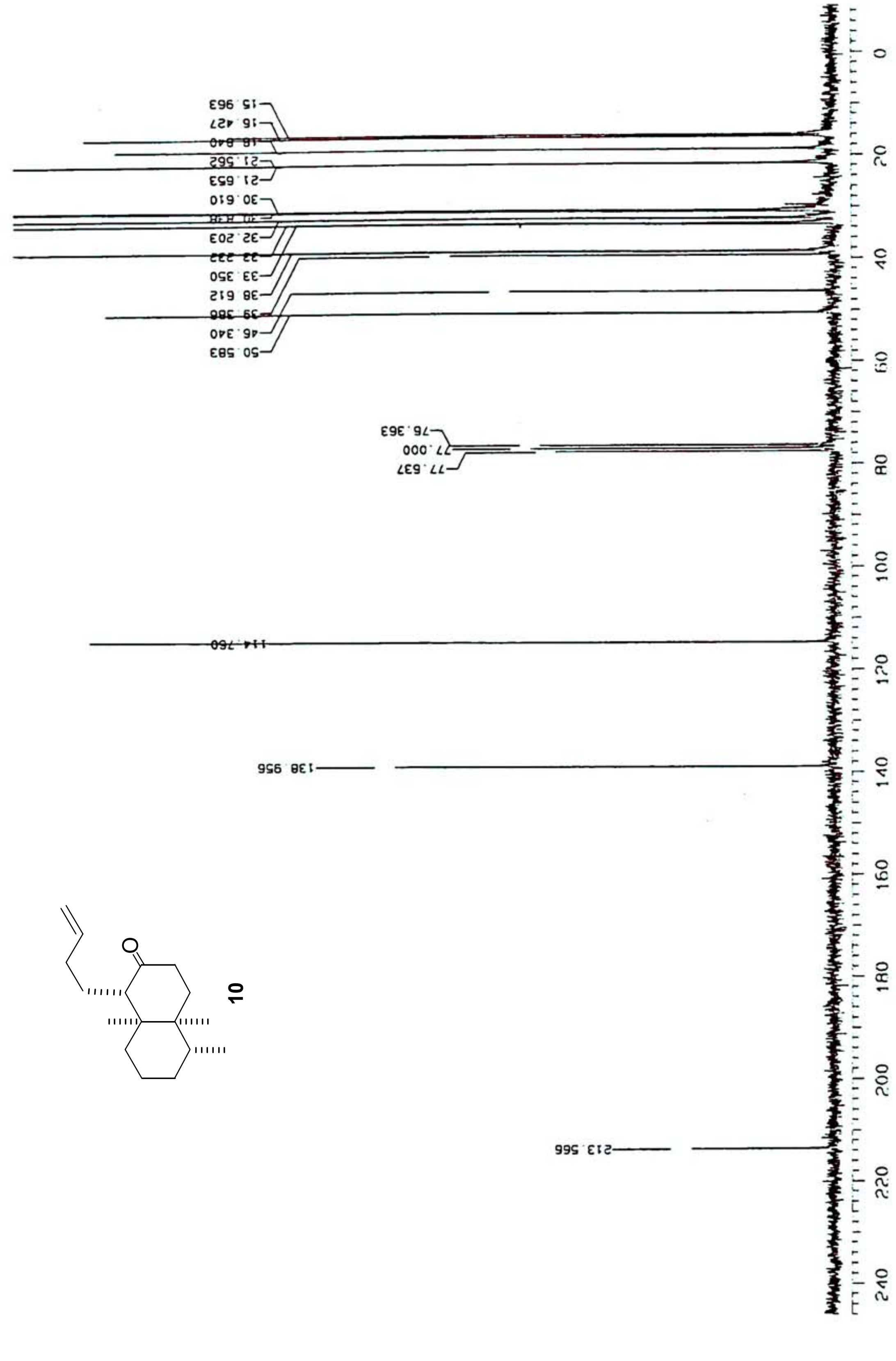
0.863
0.921
0.954
1.471
1.487
1.511
1.516
1.890
1.896
1.908
4.969
4.974
ppm
10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16.427
18.840
21.562
21.653
30.610
32.203
33.222
33.350
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39.386
46.340
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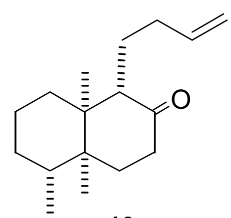
138.956
213.566
10



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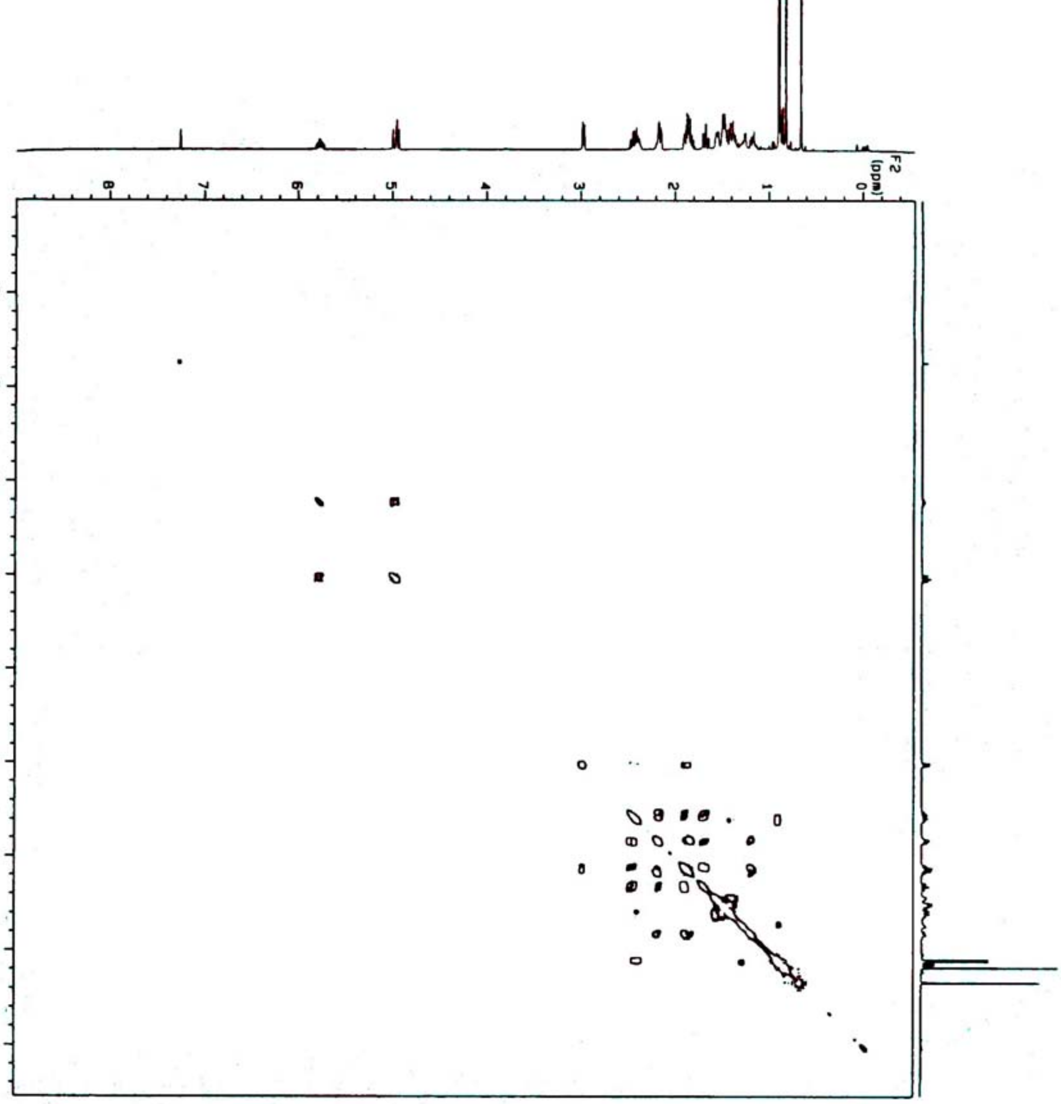

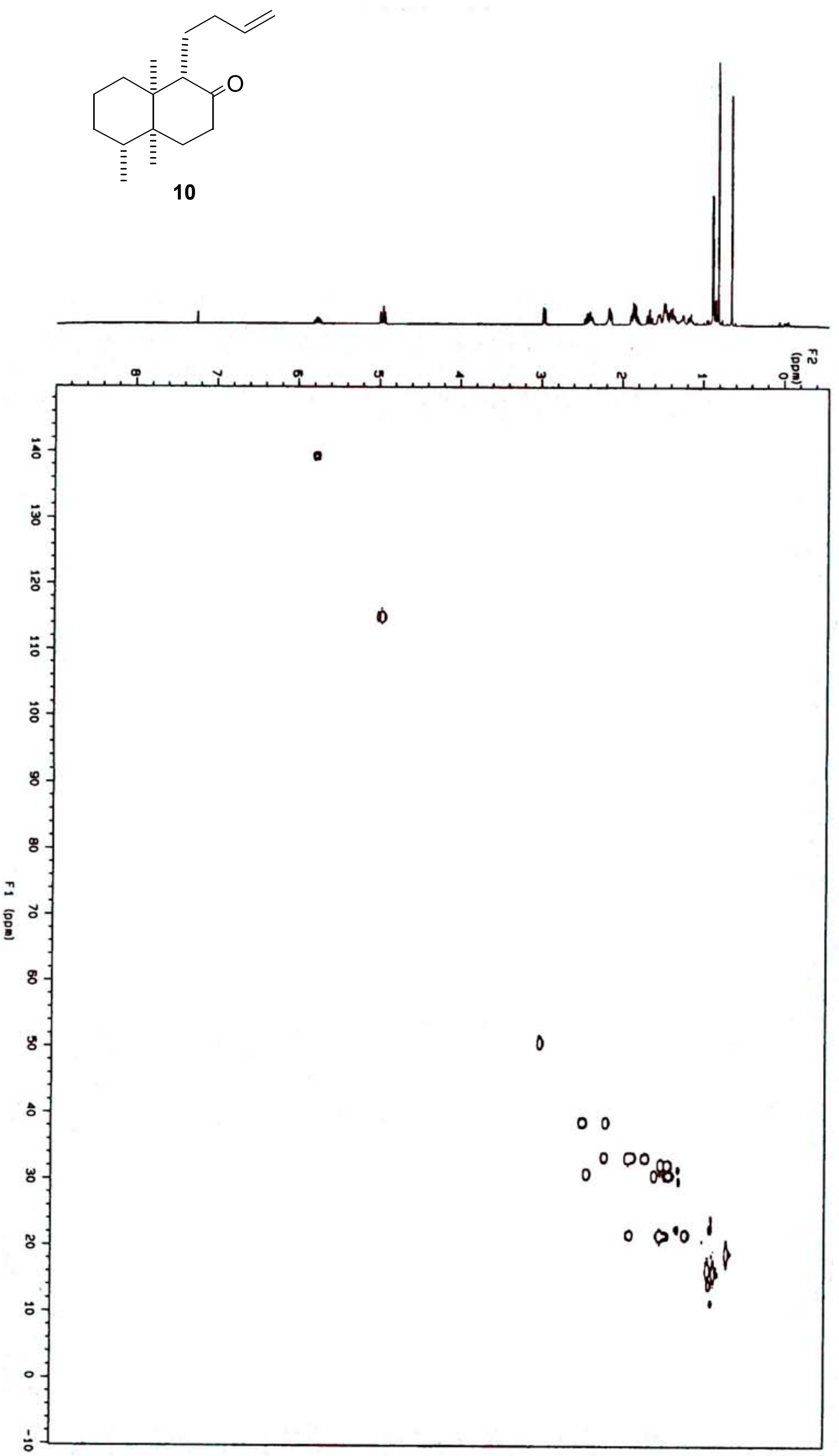

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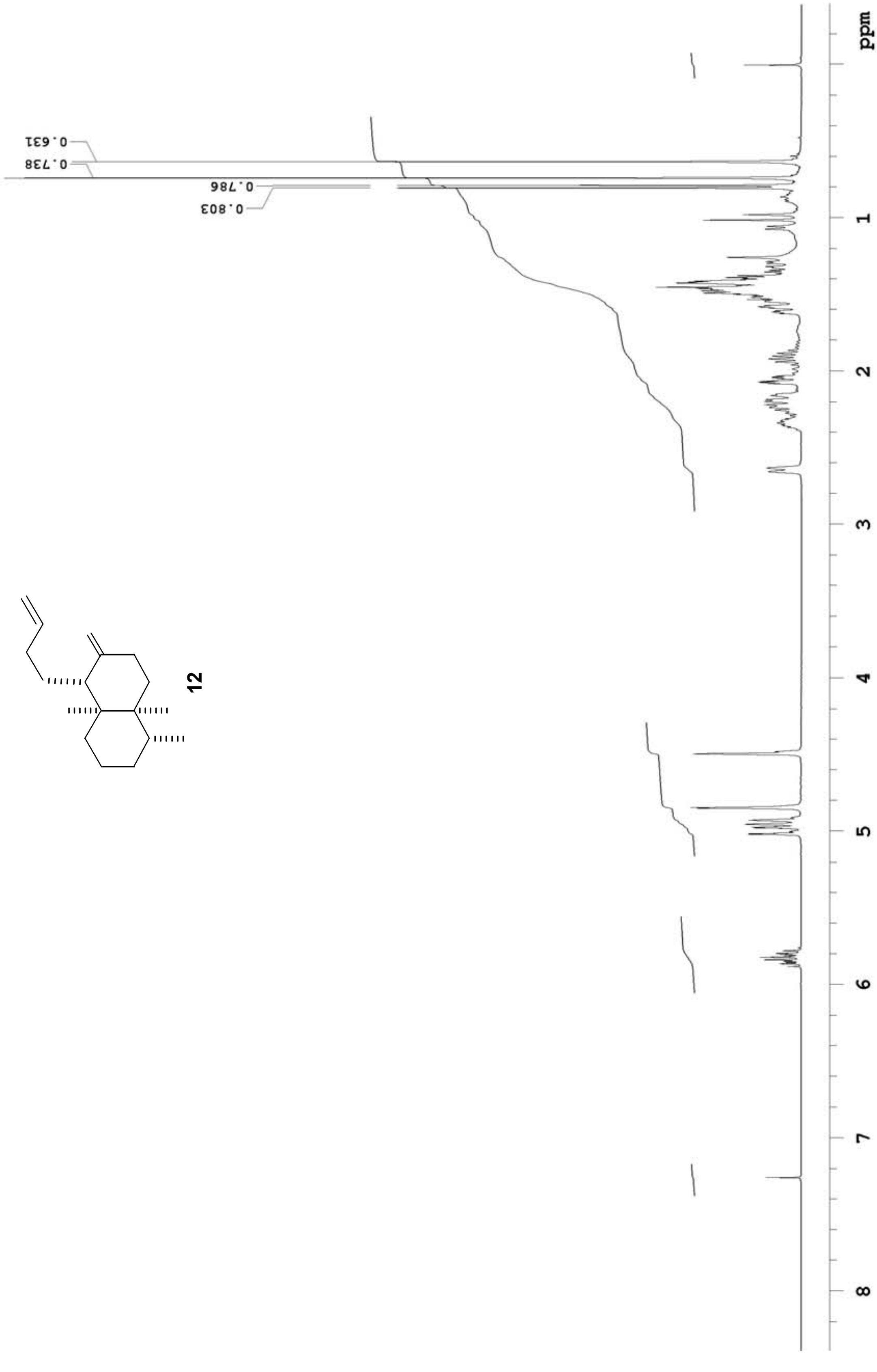
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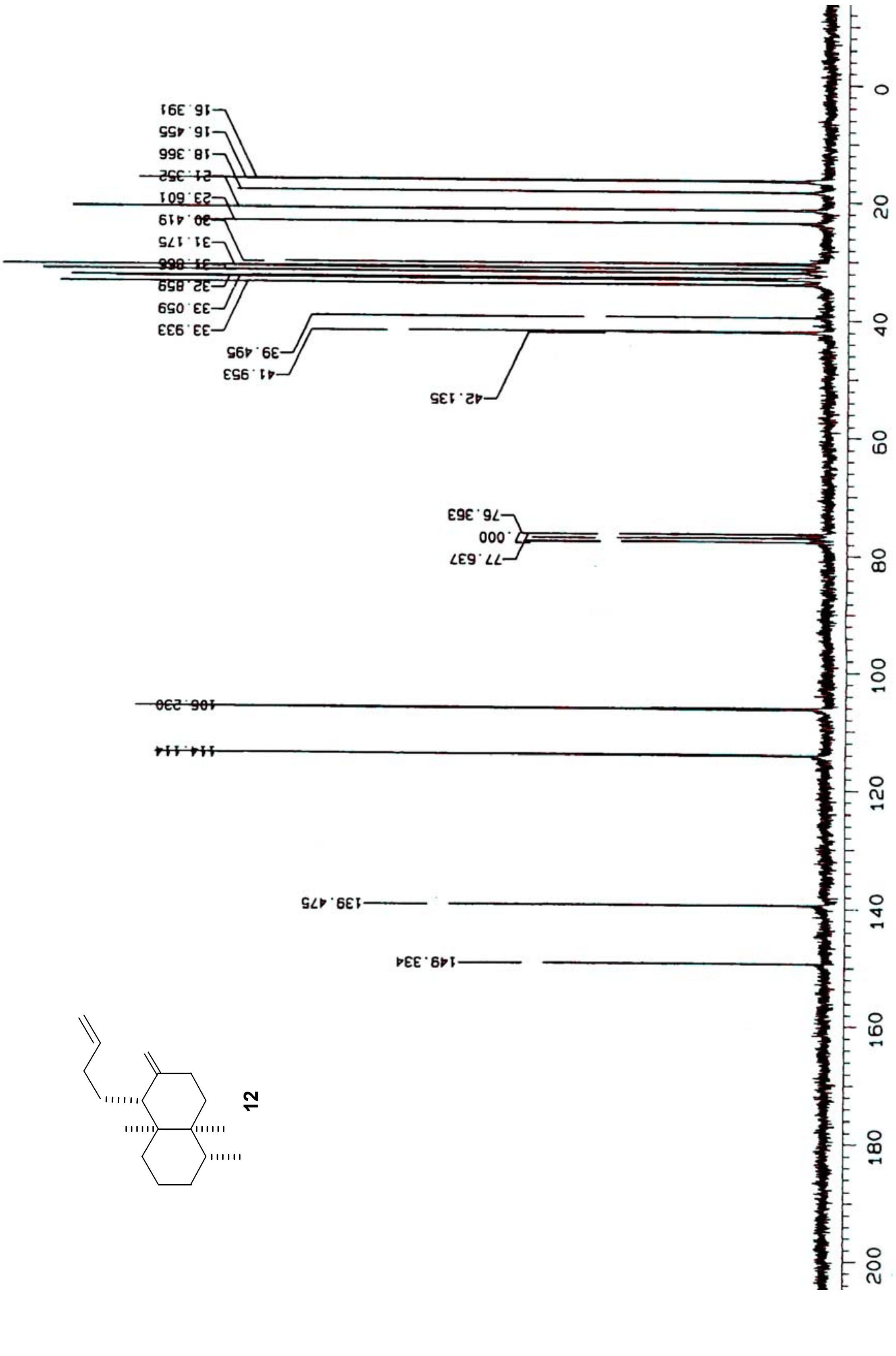
0.738
0.786
0.803
12
ppm
1
2
3
4
5
6
7
8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18.366
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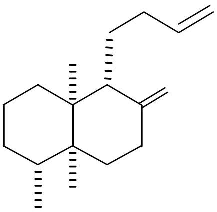
23.601
30.419
31.175
31.866
32.859
33.059
33.933
39.495
41.953
42.135
76.363
77.000
77.637
106.230
114.114
139.475
149.334
0
20
40
60
80
100
120
140
160
180
200
12



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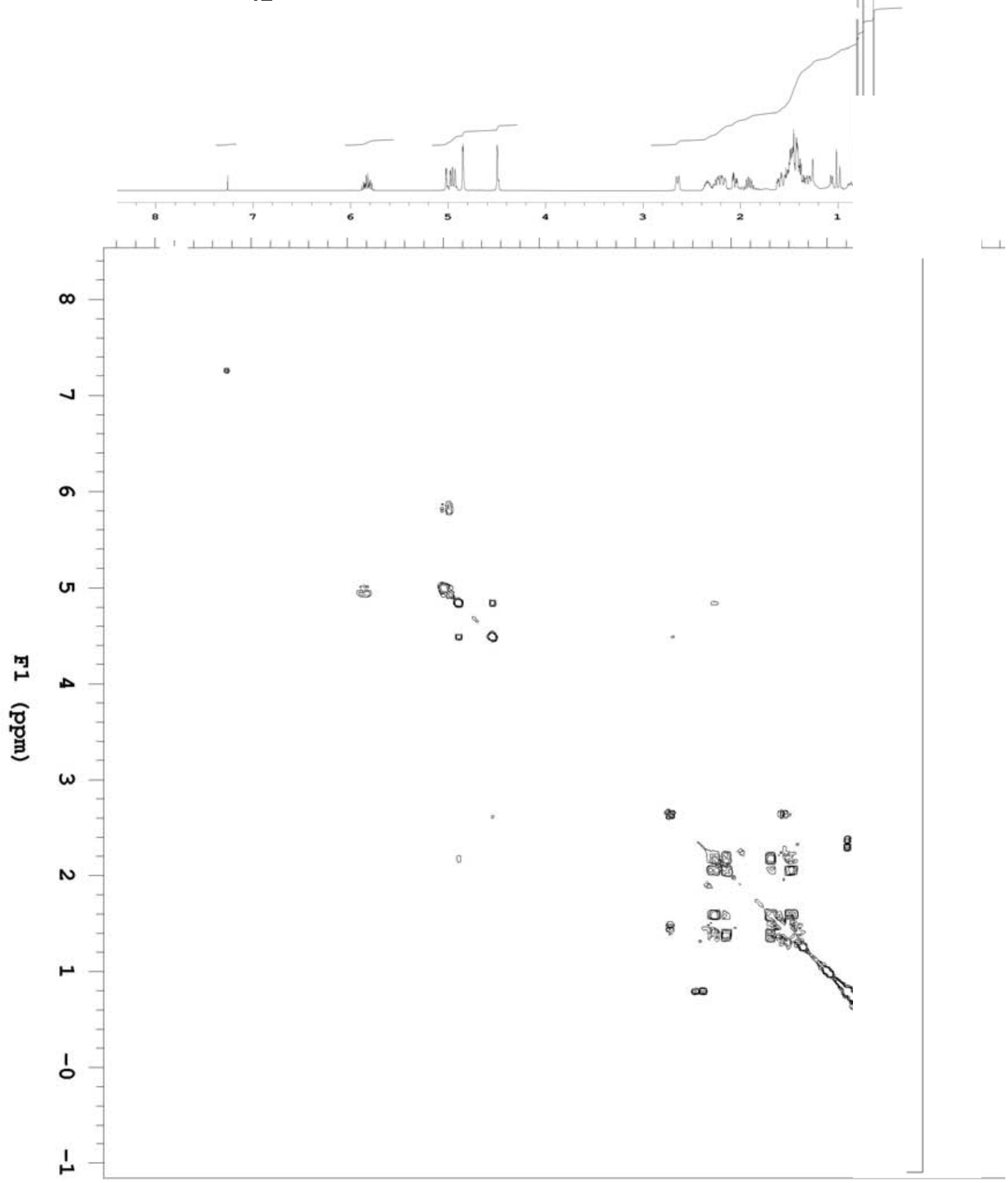

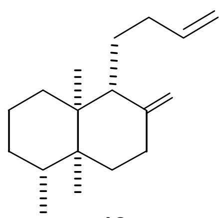

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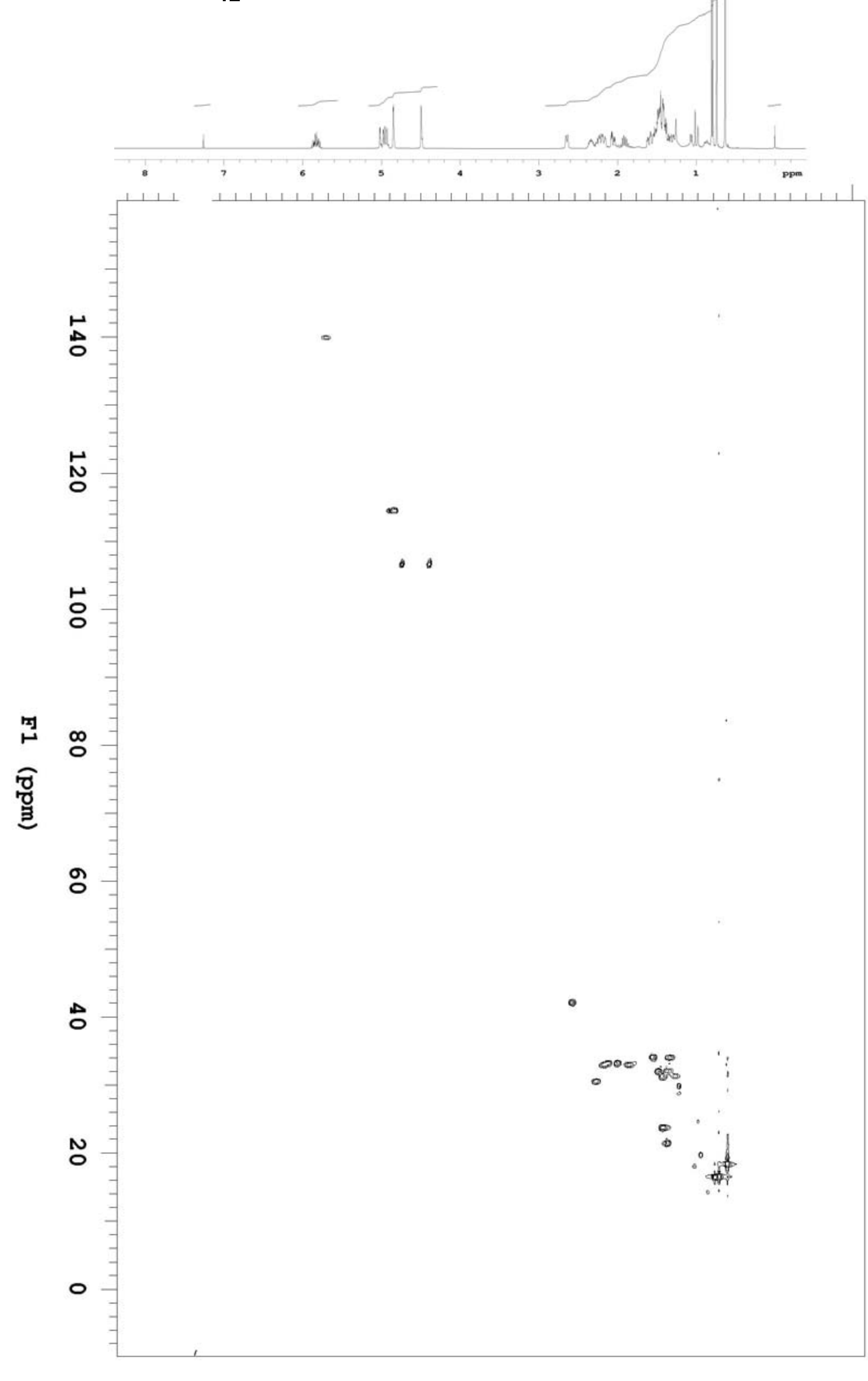

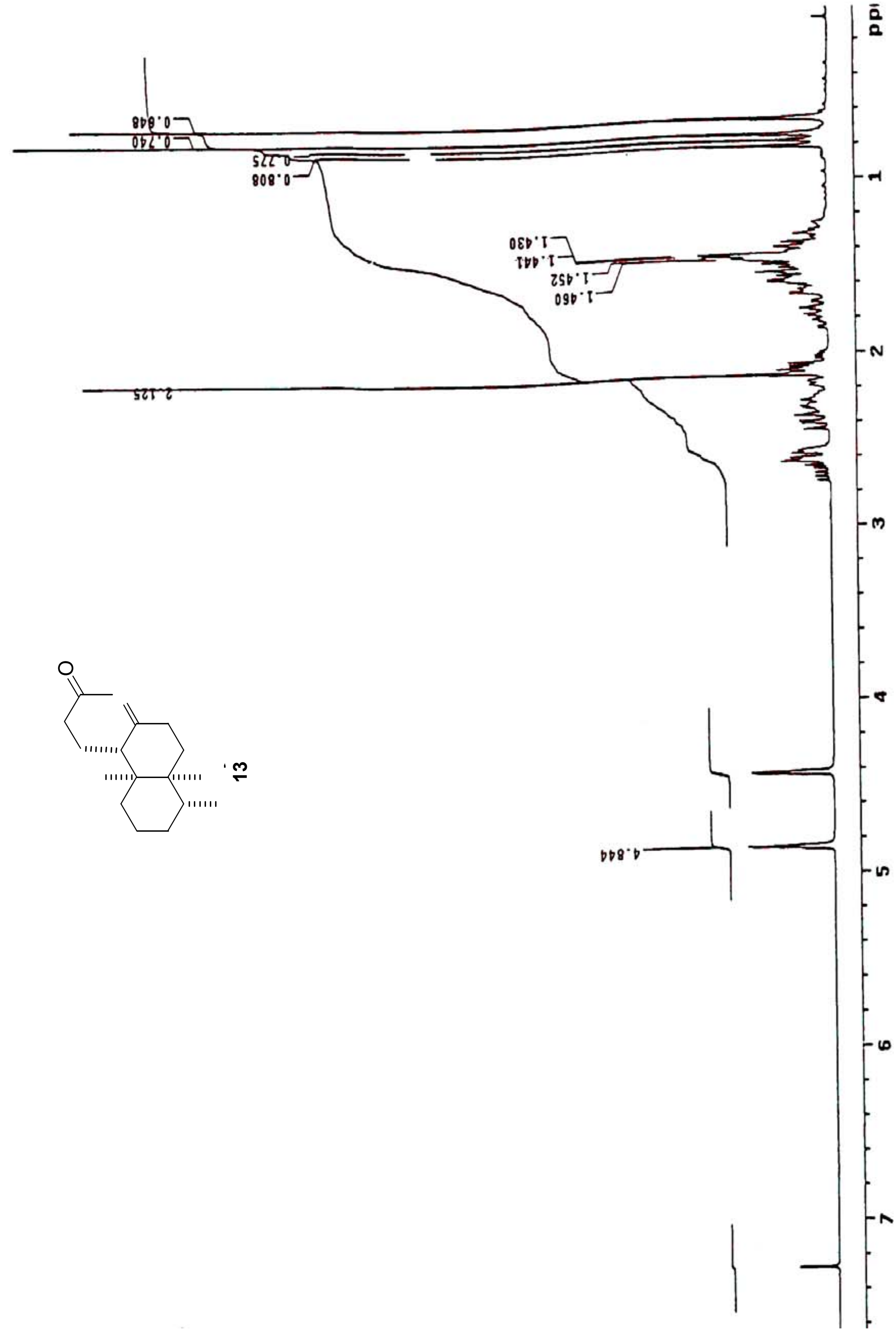

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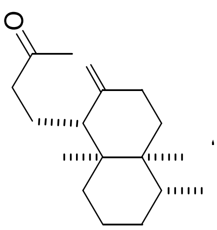

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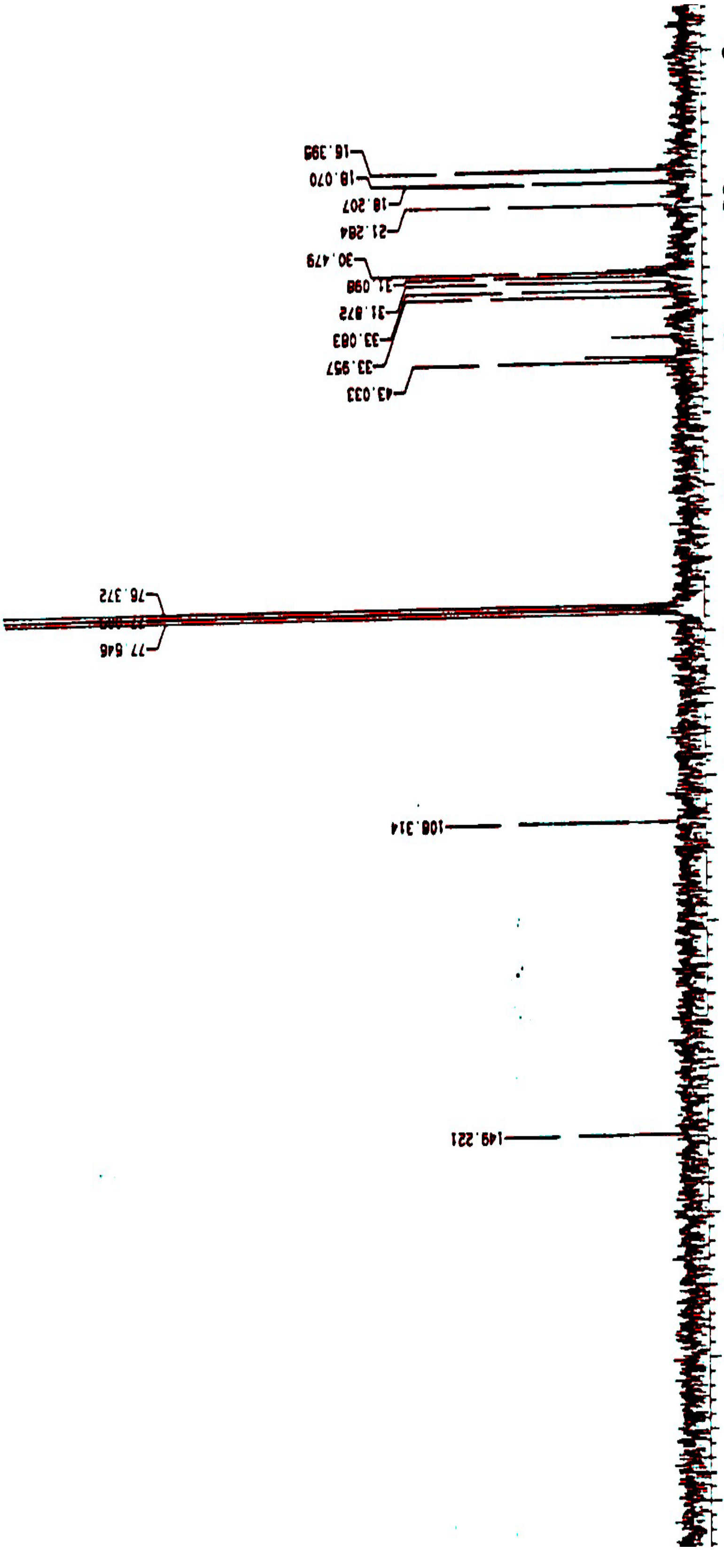
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33.083
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77.646
108.314
149.221
0
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60
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140
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180
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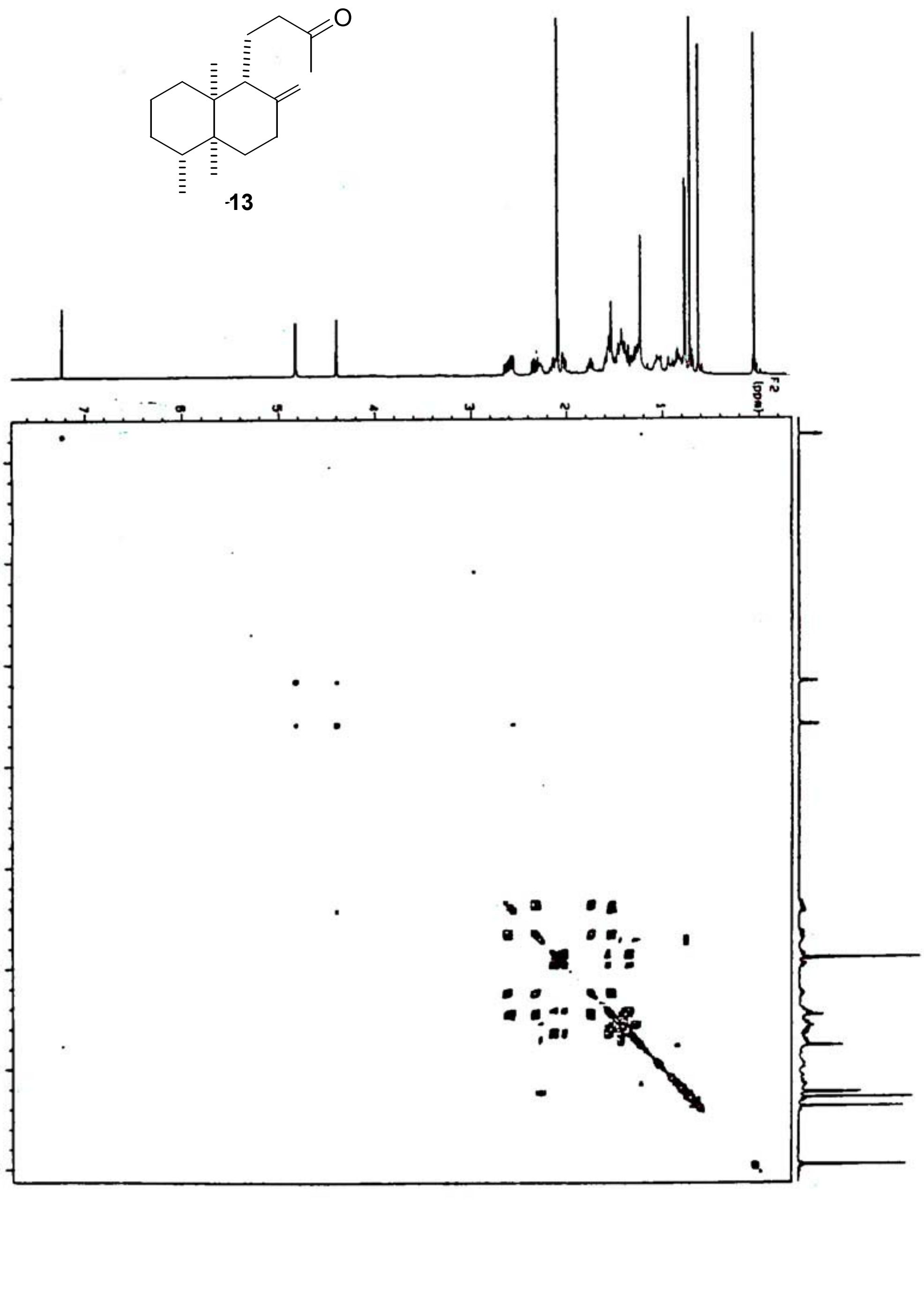

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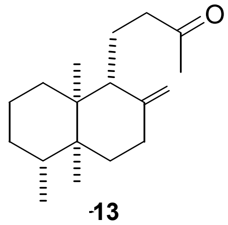

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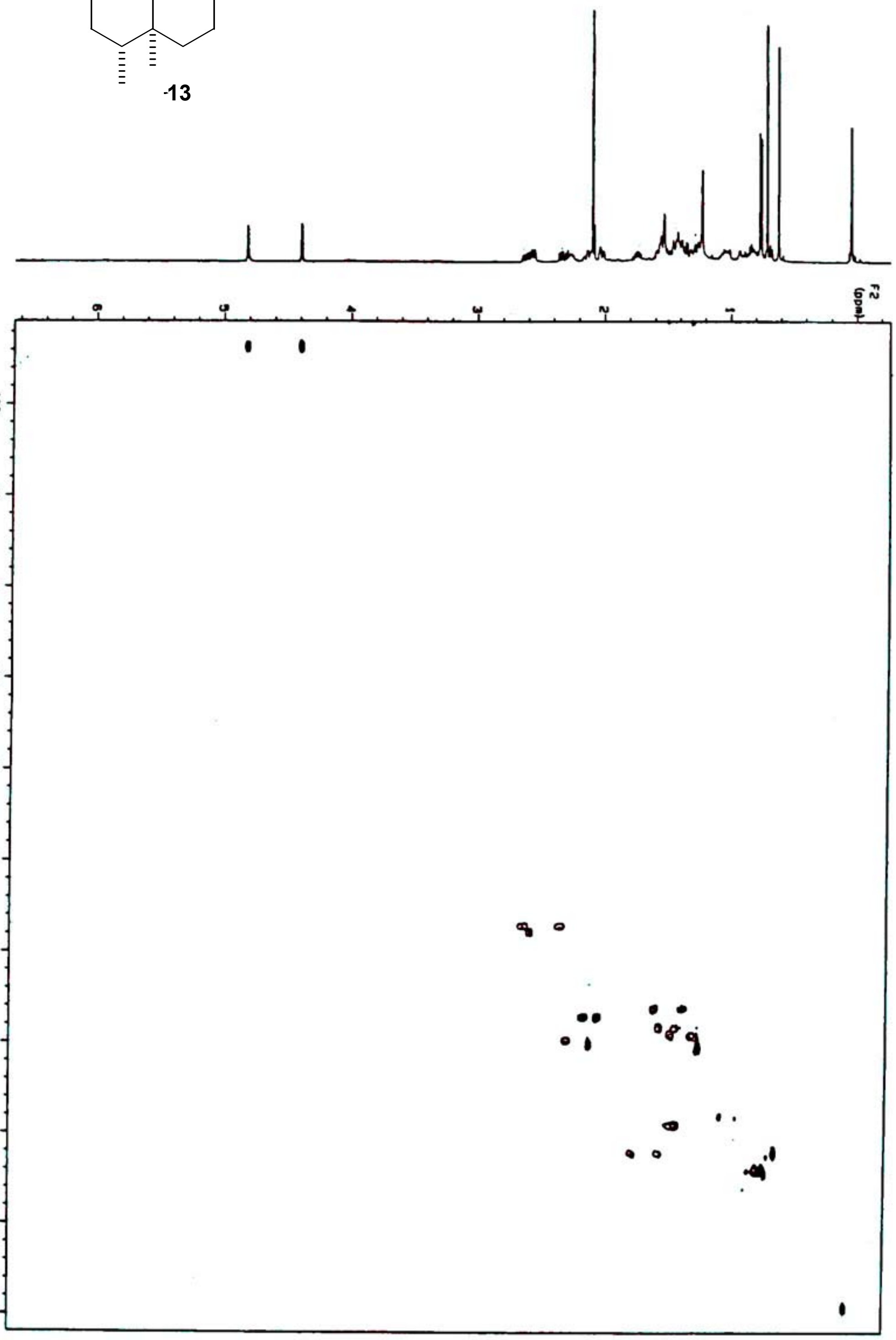

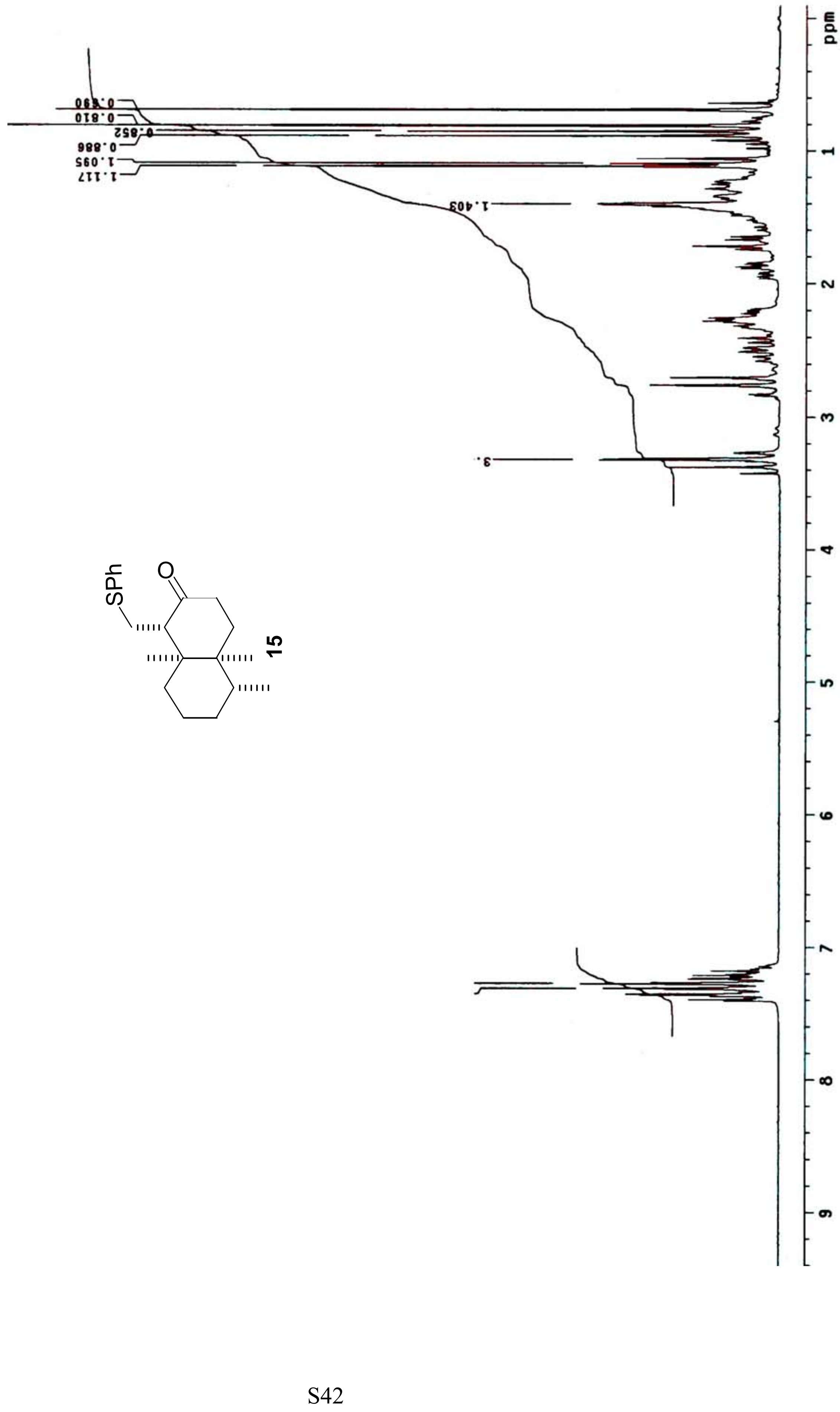
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O
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1.095
1.117
1.403
3.
ppm
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2
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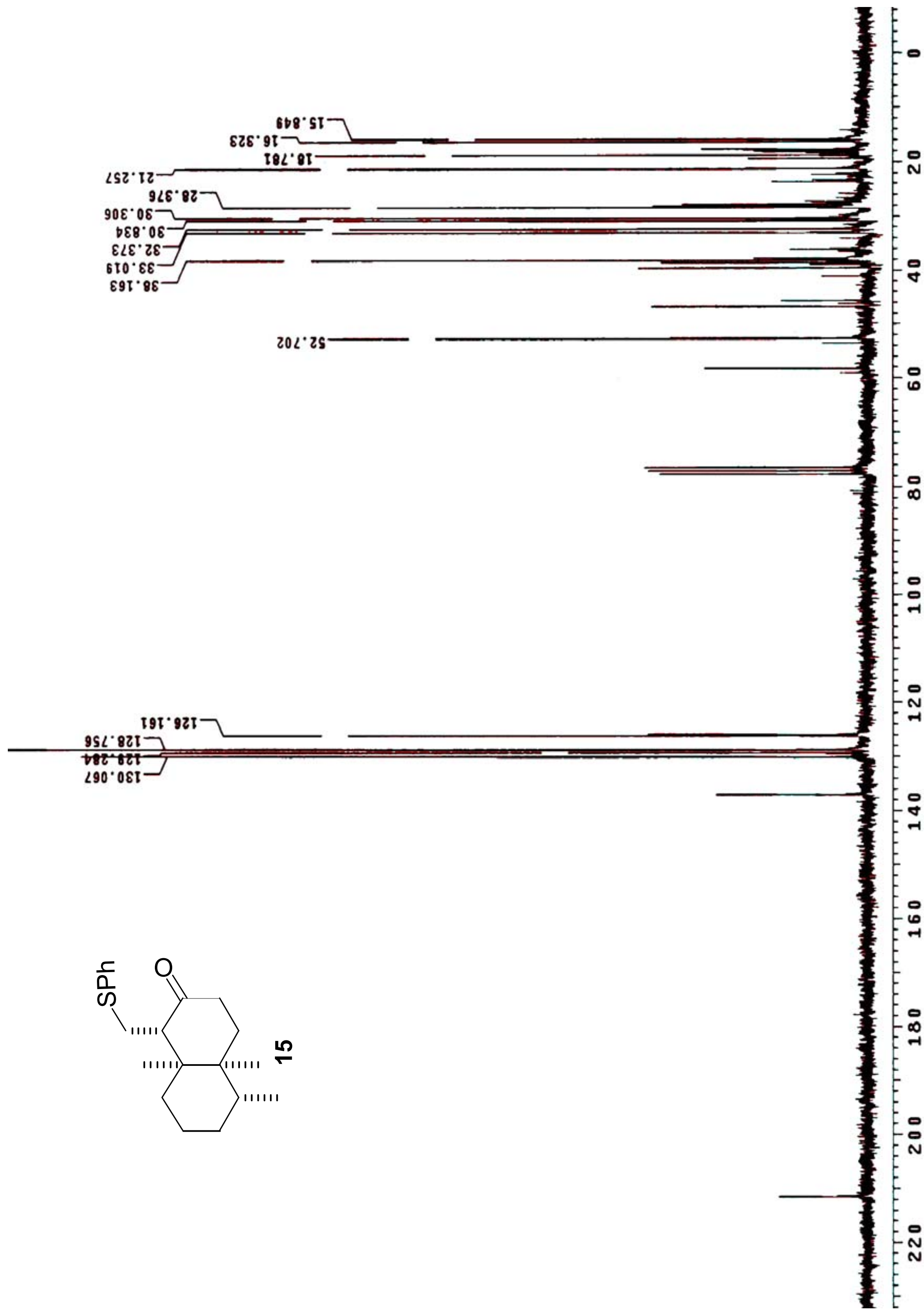
5
6
7
8
9



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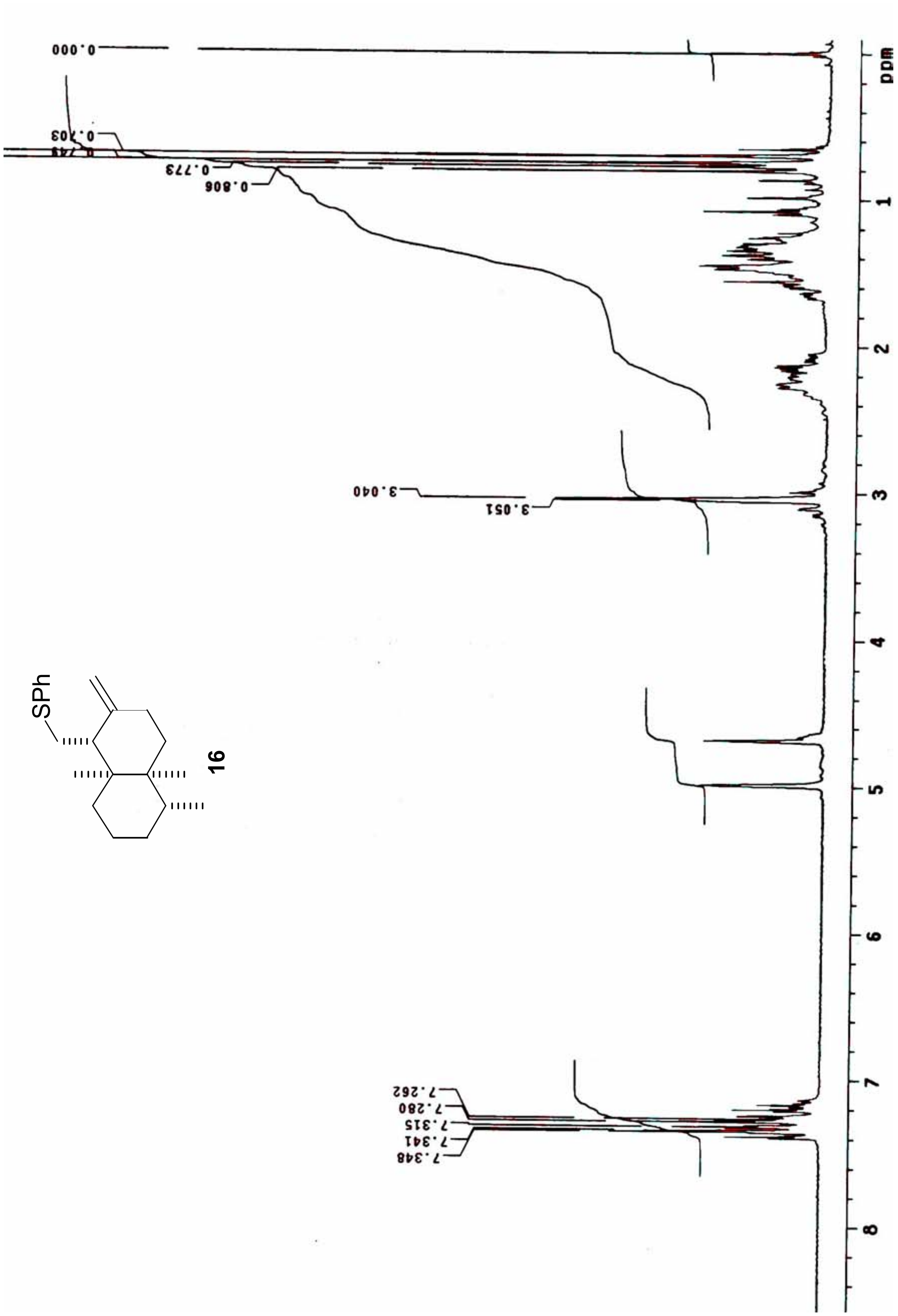
SPh
16
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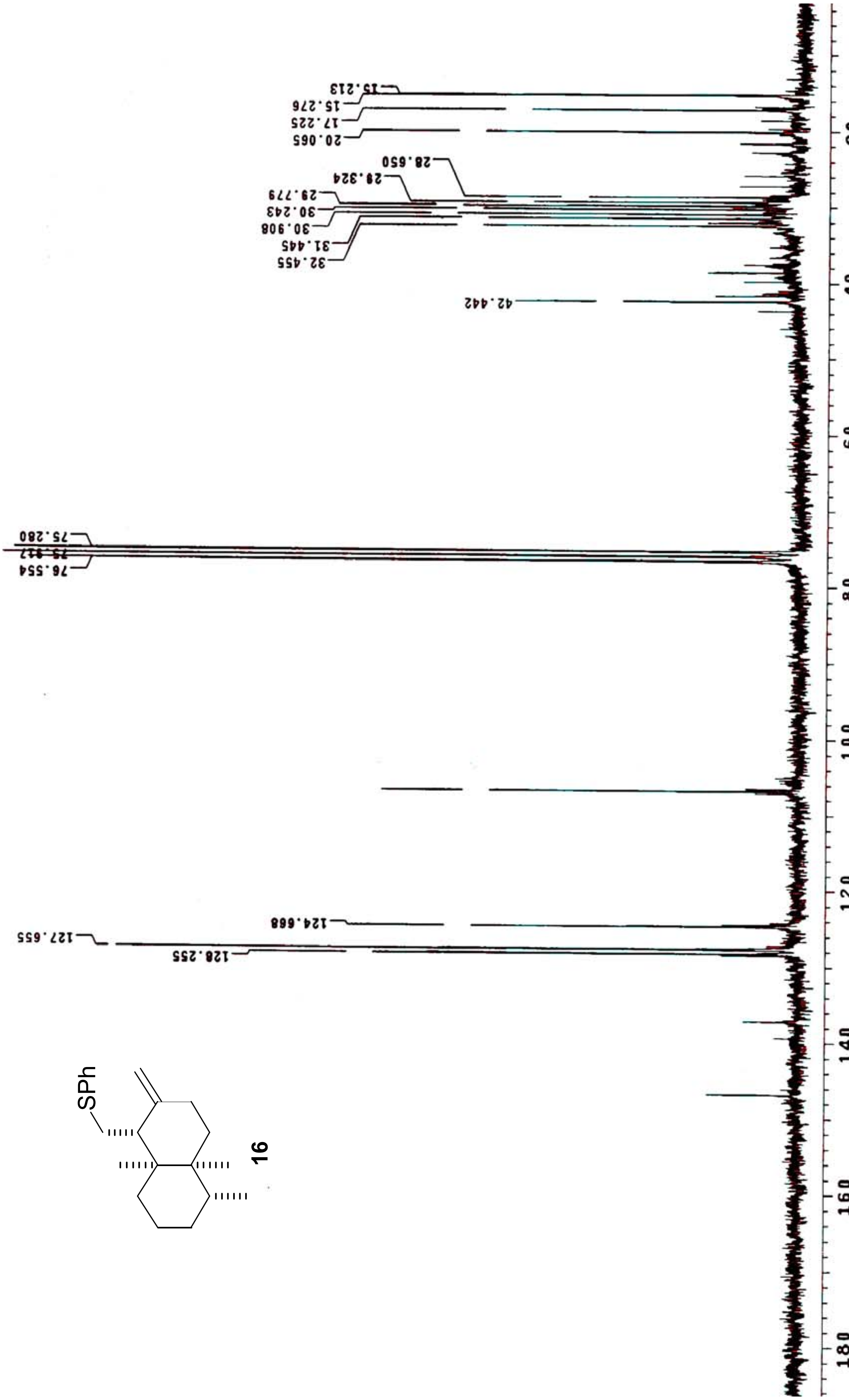
0.773
0.806
3.040
3.051
7.262
7.280
7.315
7.341
7.348
ppm
1
2
3
4
5
6
7
8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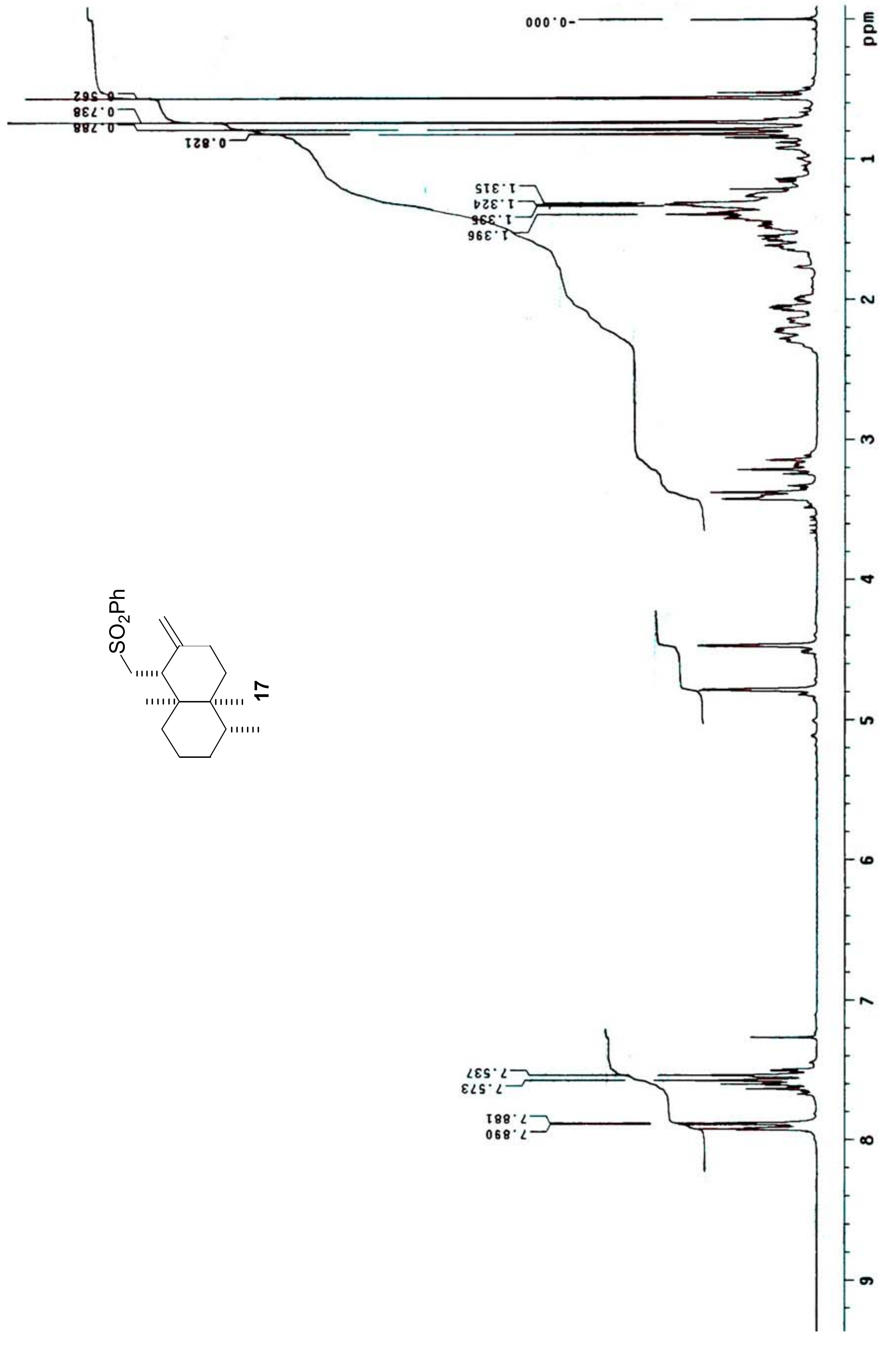
20.065
28.650
28.324
29.779
30.243
30.908
31.445
32.455
42.442
75.280
76.554
124.668
127.655
128.255
20
40
60
80
100
120
140
160
180
SPh
16


SO2Ph
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1.324
1.336
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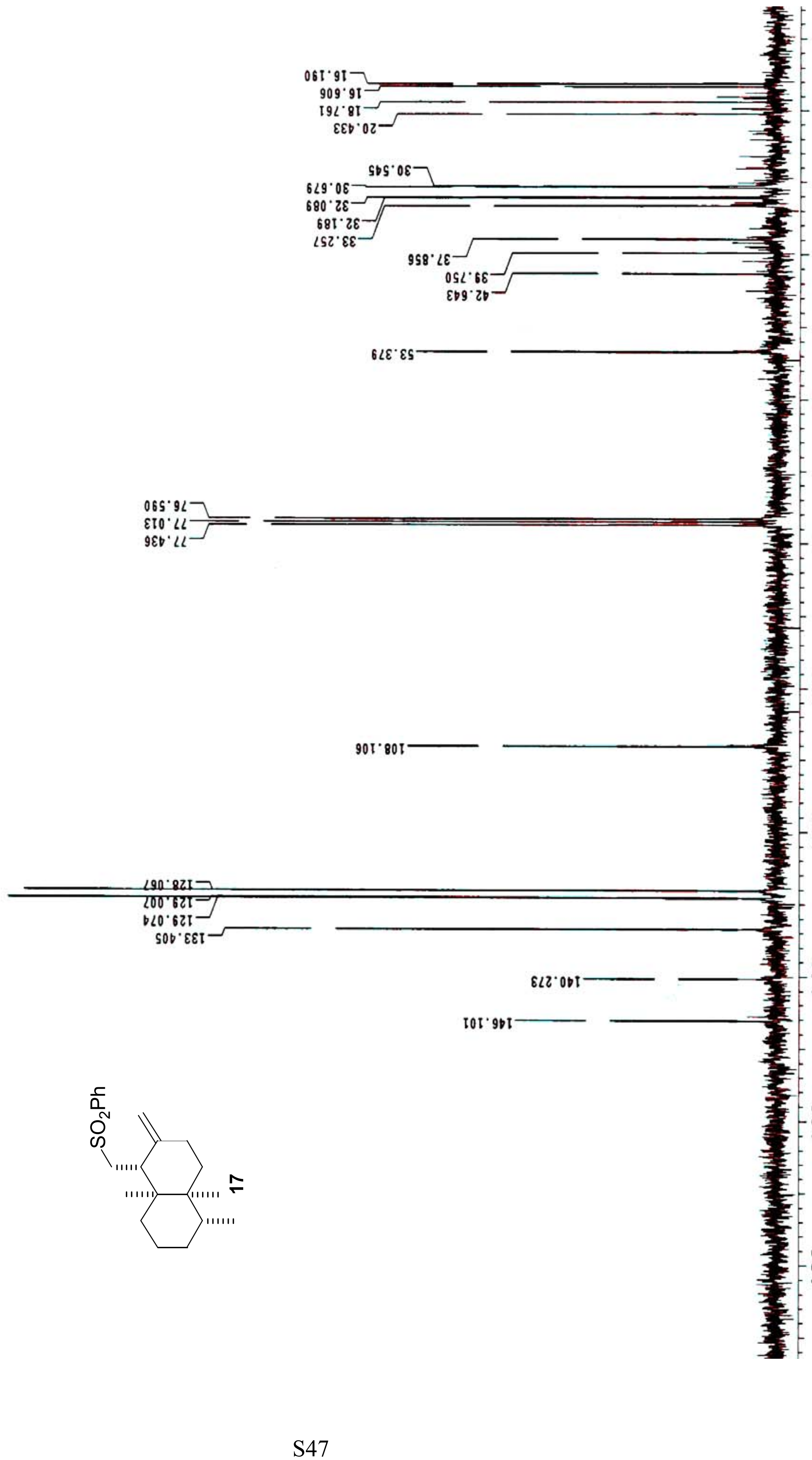
7.881
7.890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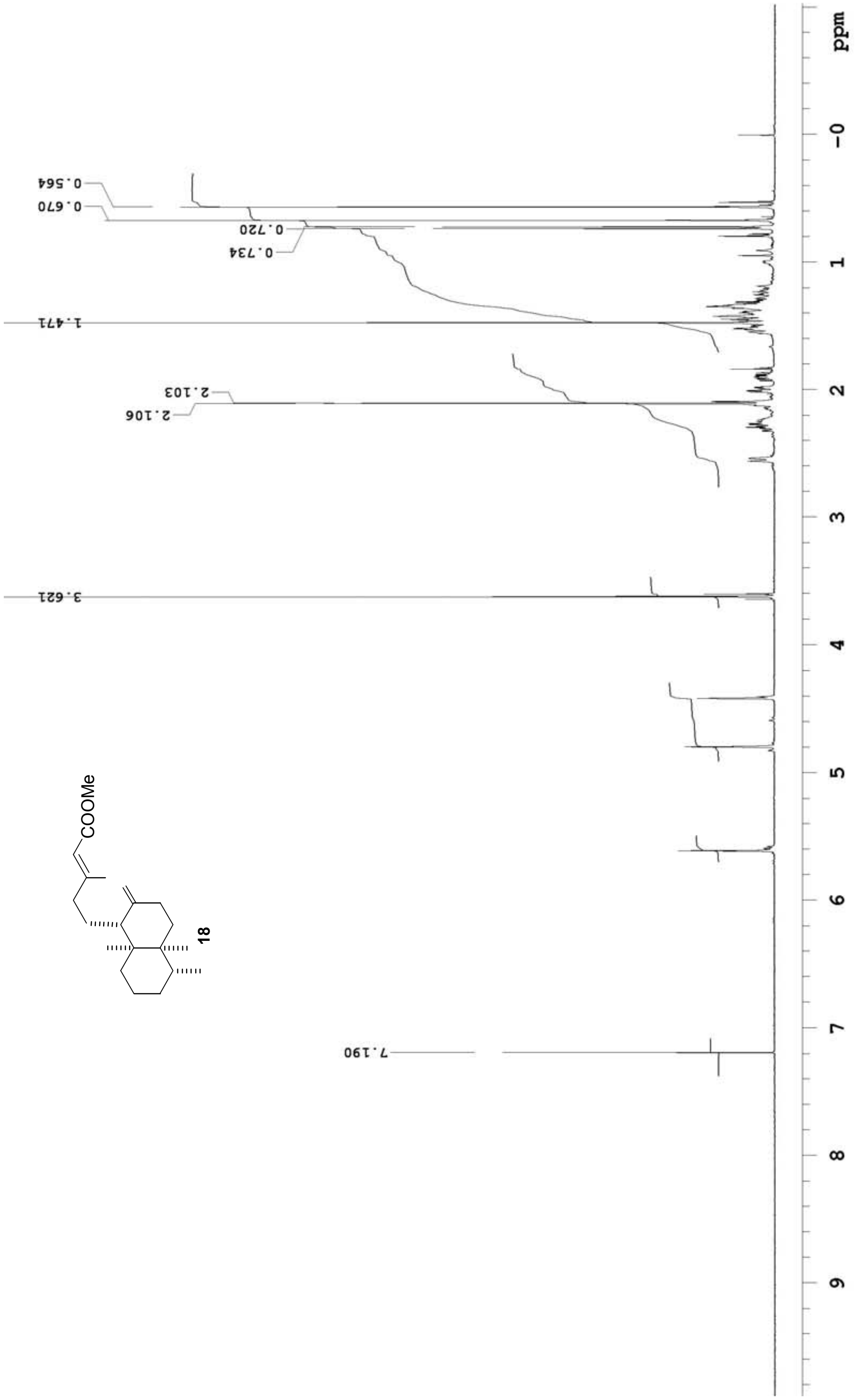
30.679
32.089
32.189
33.257
37.856
39.750
42.643
53.379
76.590
77.013
77.436
108.106
128.067
129.007
129.074
133.405
140.273
146.101
SO2Ph
17
20
40
60
80
100
120
140
160
180


COOMe
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0.734
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2.103
2.106
3.621
7.190
ppm
-0
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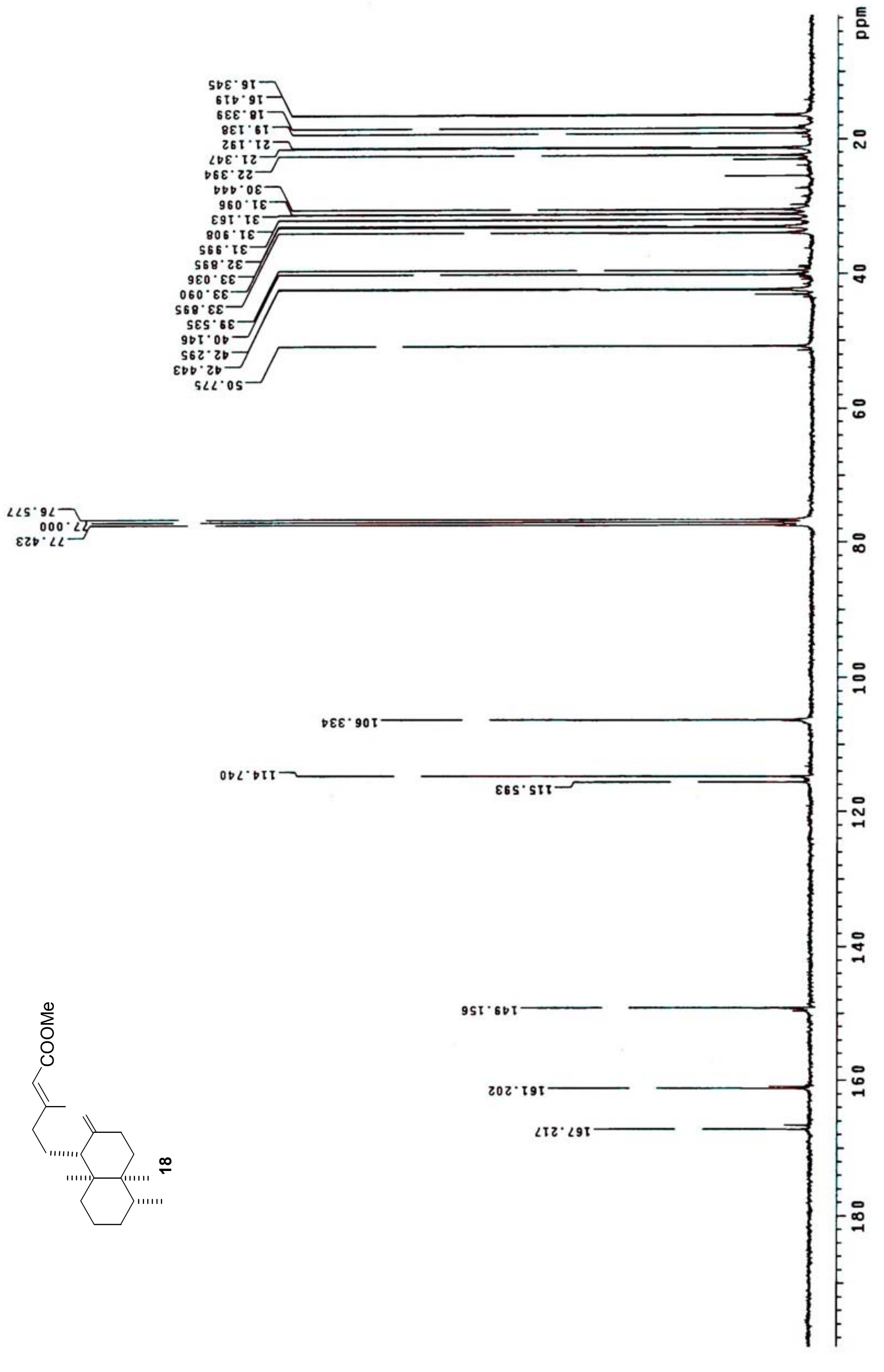
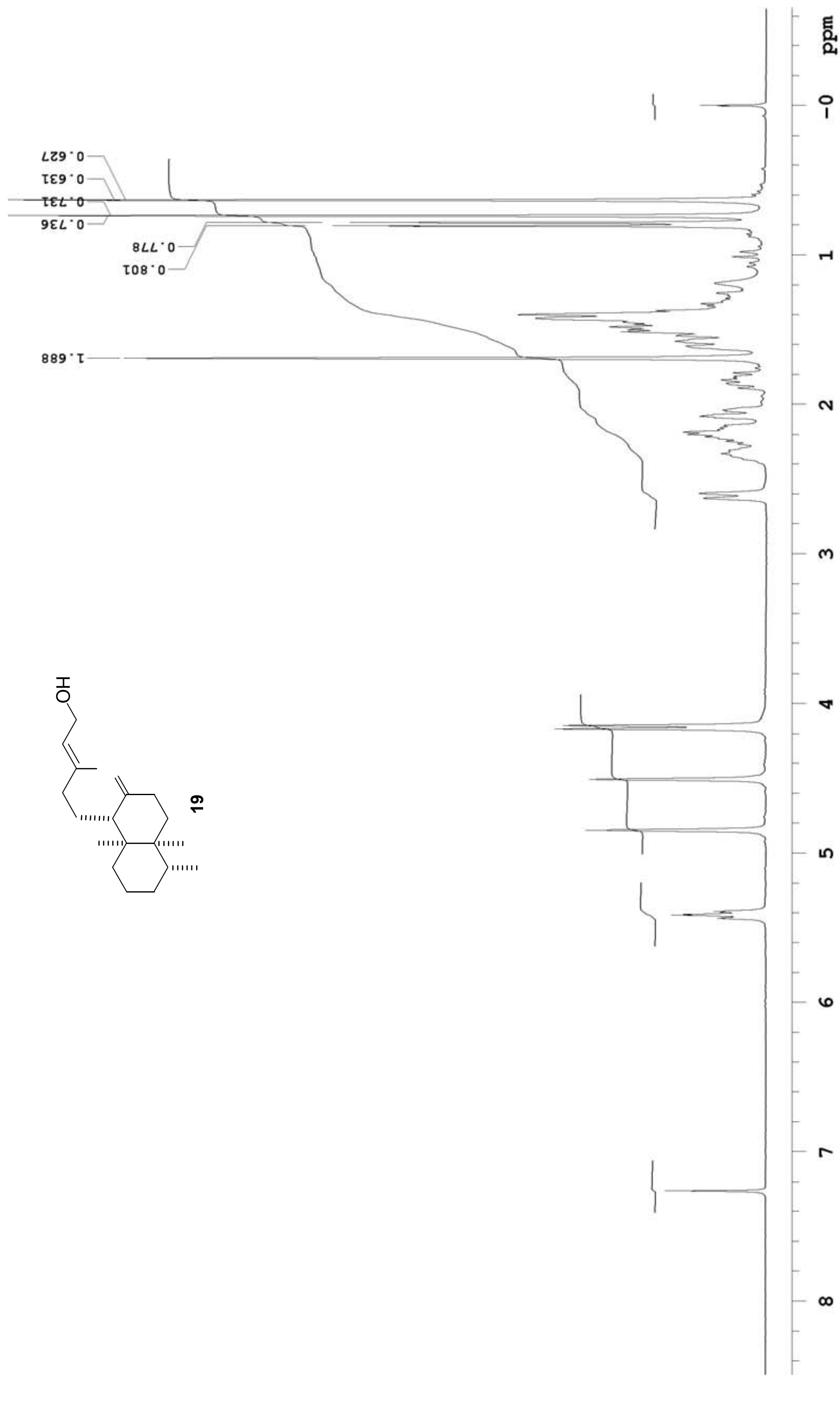
2
3
4
5
6
7
8
9



18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OH
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ppm
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3
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5
6
7
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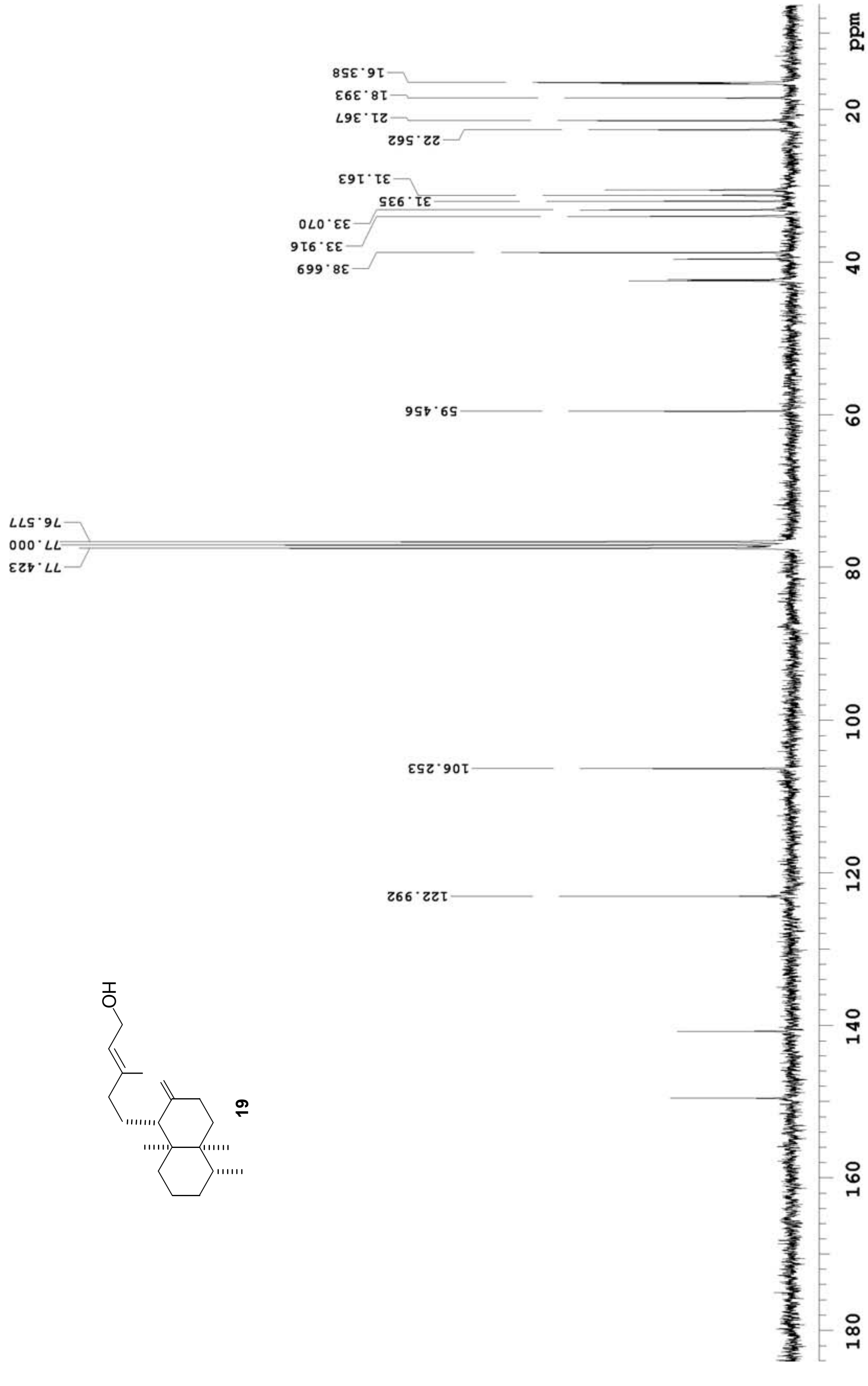
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31.935
33.070
33.916
38.669
59.456
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77.000
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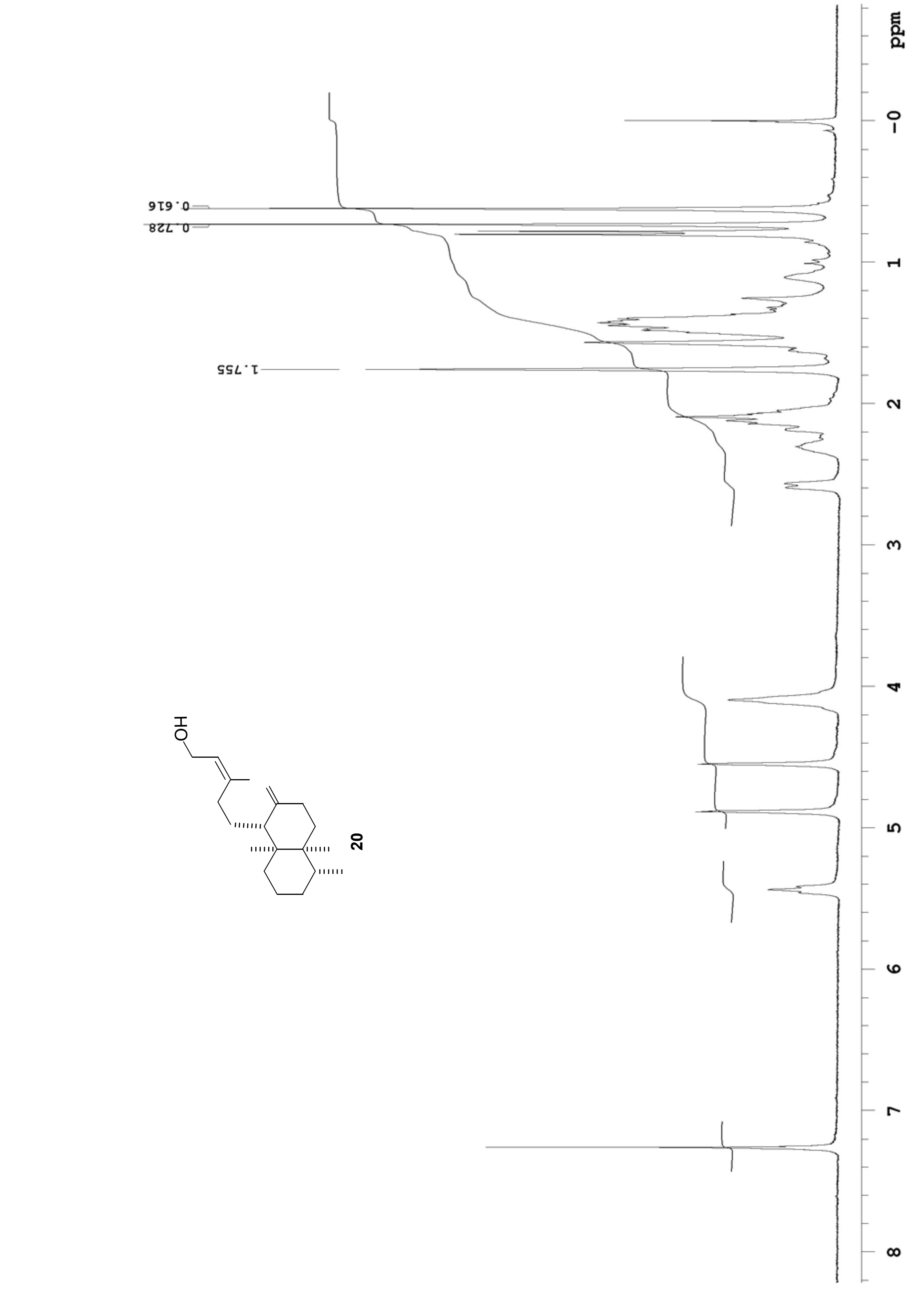
106.253
122.992
OH
19
ppm
20
40
60
80
100
120
140
160
180



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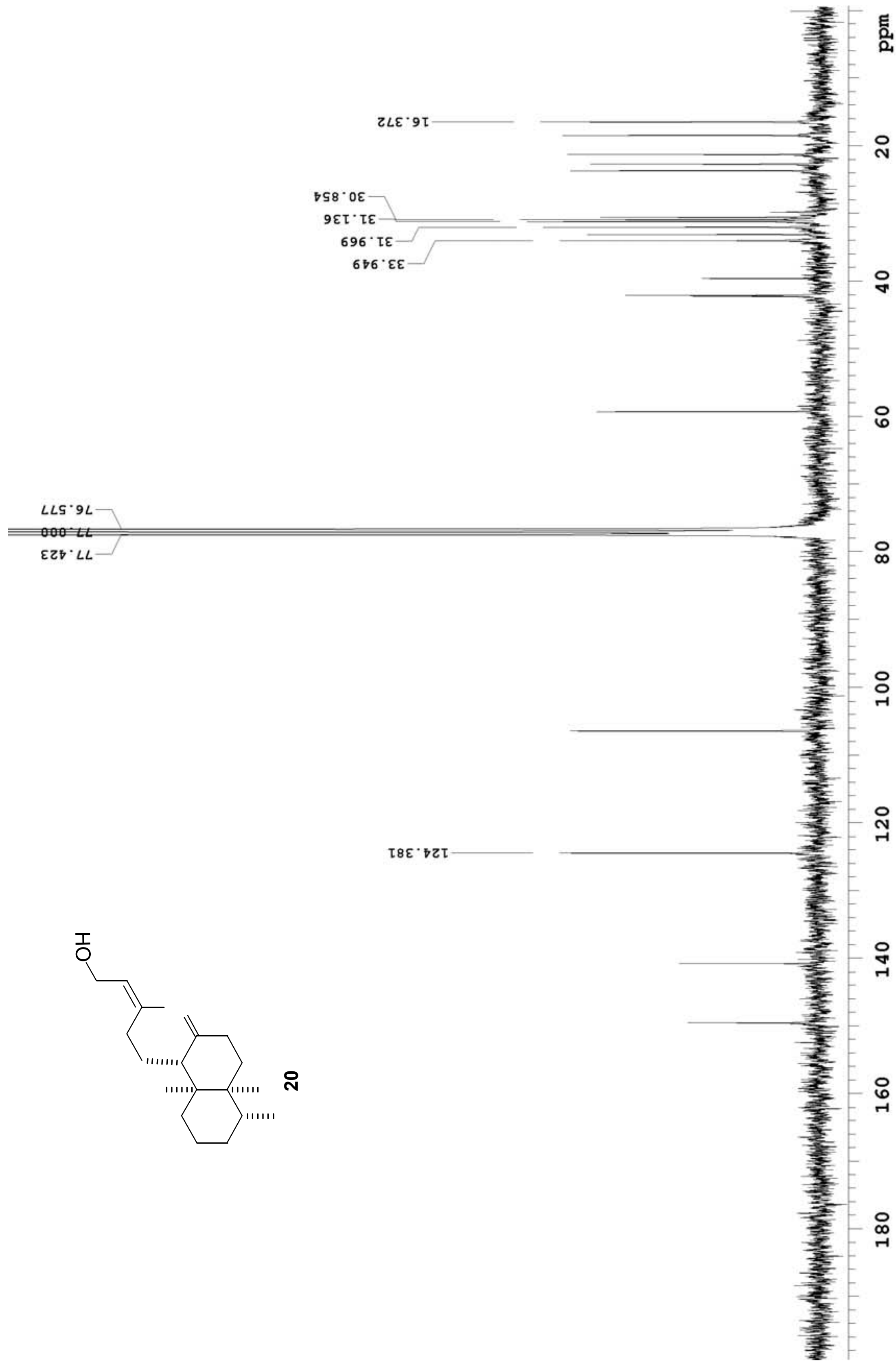
1
-0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30.854
31.136
31.969
33.949
76.577
77.000
77.423
124.381
OH
20
ppm
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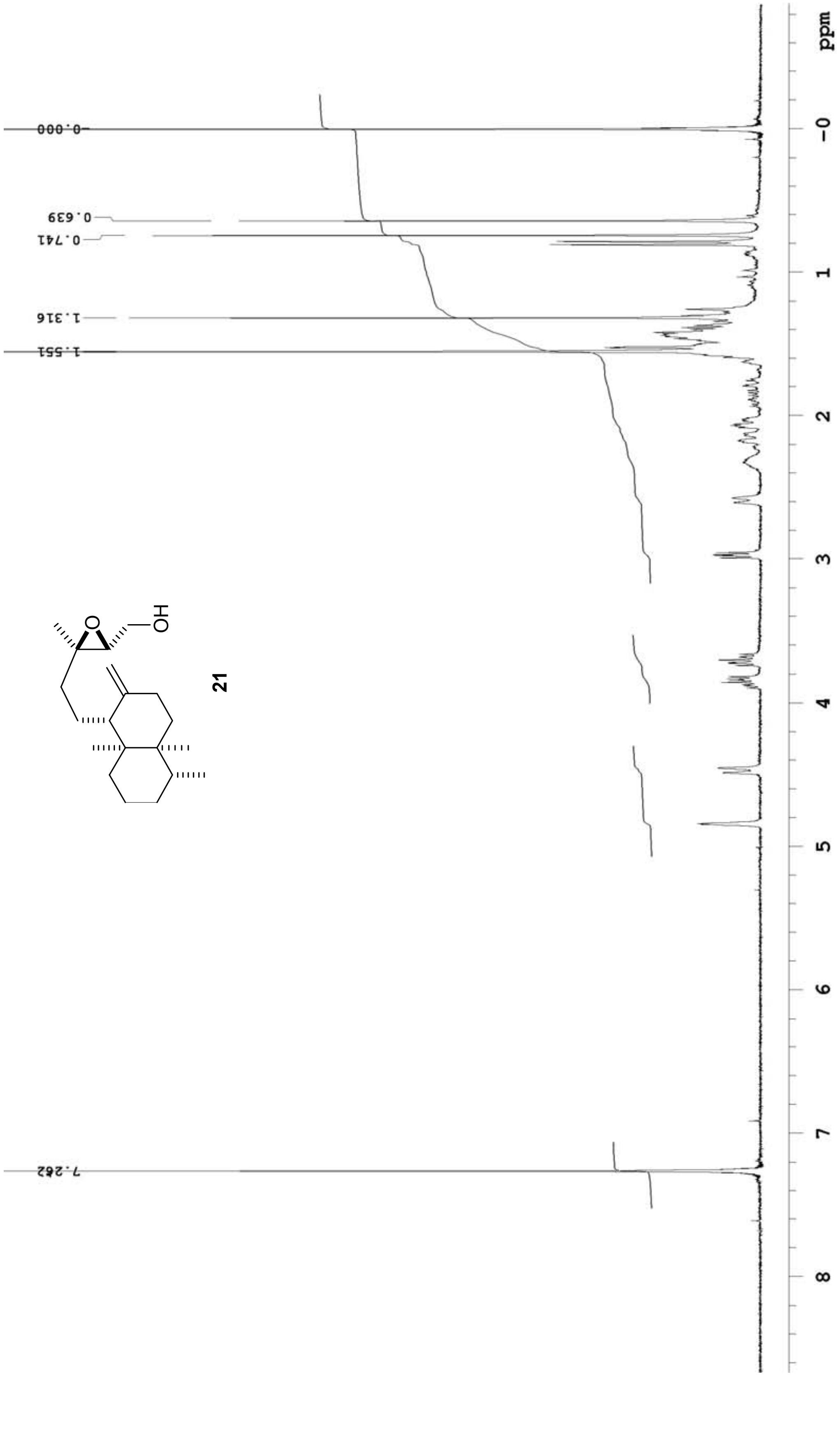
40
60
80
100
120
140
160
180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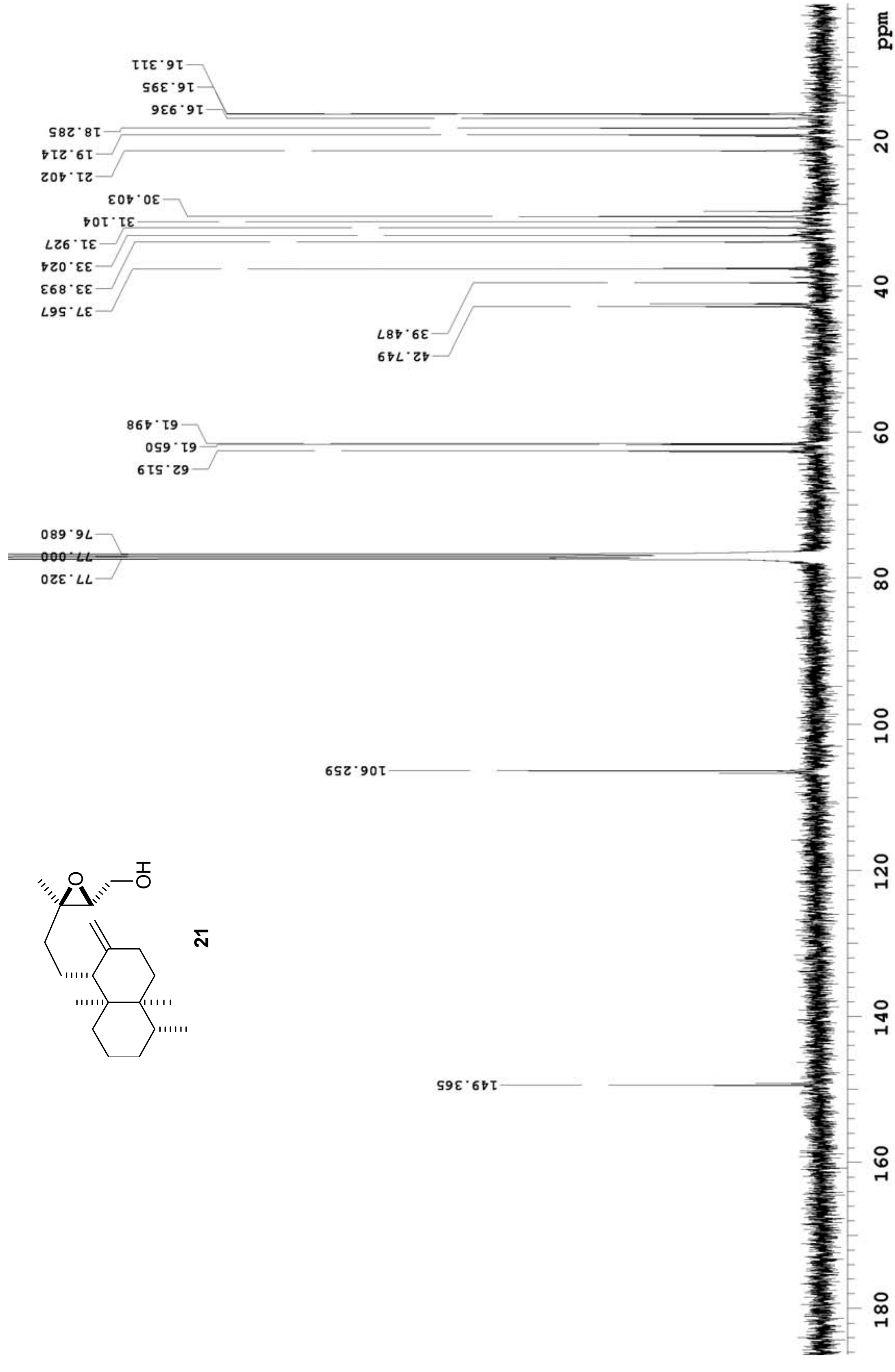
ppm
HO
O
21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16.936
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19.214
21.402
30.403
31.104
31.927
33.024
33.893
37.567
39.487
42.749
61.498
61.650
62.519
76.680
77.000
77.320
106.259
149.365
HO
O
ppm
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40
60
80
100
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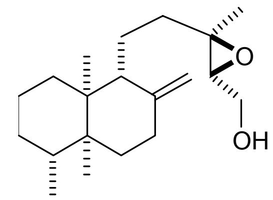
140
160
180

21



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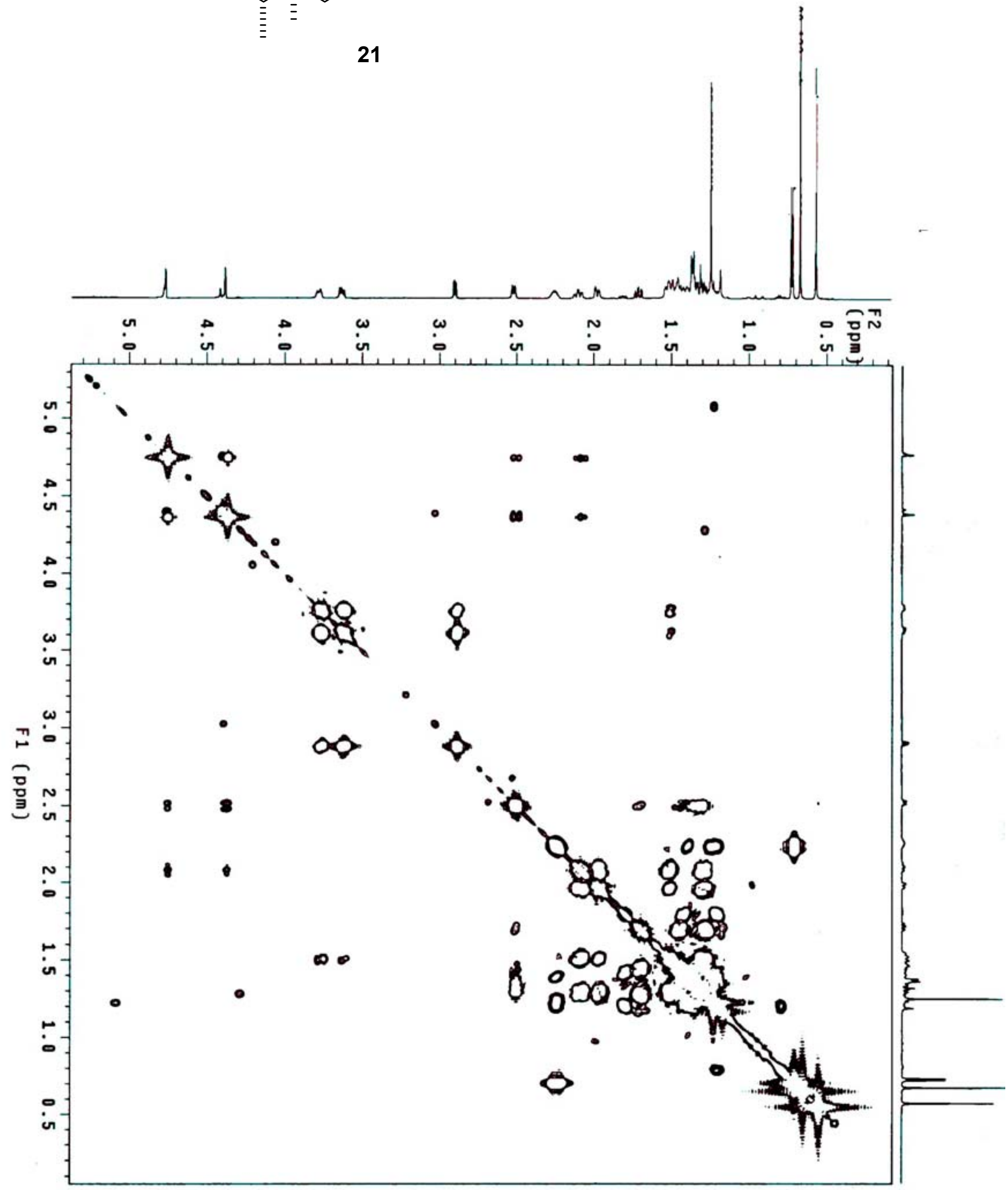

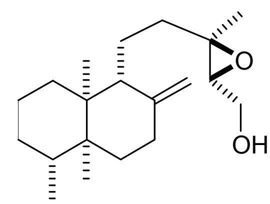

21