Supporting Information

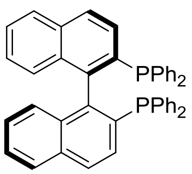
Contents **Page**

PART 1: General experimental details

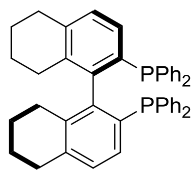
All manipulations were carried out under air unless otherwise noted. TLC plates (UV254 indicator, aluminum backed, thickness 200 mm) and silica gel (standard grade, 230 – 400 mesh) were purchased from EMD Chemicals. Diethyl ether (Fisher) and toluene (Aldrich) were purified over solvent purifier system (SPS). Hexane (Fischer) was purified by distillation from sodium benzophenone ketyl. Dichloromethane (Fischer) was washed with a sequence of concentrated H_2SO_4, deionized water, 5% Na_2CO_3 and deionized water, followed by pre-drying over anhydrous $CaCl_2$, and were then refluxed over and distilled from P_2O_5 under argon. Isopropanol (EMD) and methanol (Burdick & Jackson) was dried over and distilled from activated 4 Å molecular sieves prior to use. Et_3N (Fisher) and benzylamine (Acros) were dried over activated 4 Å molecular sieves and then distilled, degassed, and stored on dried 4 Å sieves under nitrogen. NMR solvents were purchased from Cambridge Isotopes Laboratories. $CDCl_3$ was dried over activated 4 Å molecular sieves and then stored over dried 4 Å sieves. *bis*-(*S*/*R*)-1-Phenylethylamine (Alfa Aesar, 99%, *ee* 98+%) and (*R*)- and (*S*)-[1,1'-binaphthalene]-2,2'-diols (Chem-Impex International, Inc., >99.9%) were used as received after checking optical purity by HPLC. Au(DMS)Cl (DMS = dimethylsufide) was prepared by a literature procedure using chloroauric acid (99.9%, 49% Au) purchased from Strem. Reaction vials (4 mL with green top polypropylene cap and PTFE septa) were purchased from Chemglass Life Sciences, and used as received without further drying. Reaction vials were also recycled and re-used. HPLC grade water was used to prepare surfactant solutions. TPGS-750M was synthesized by a procedure published by our group,[1] and is also commercially available from Sigma-Aldrich. Ligands were either synthesized or generously received from F. Hoffmann-La Roche AG. All other reagents were purchased from Aldrich and Fischer and used as received. Optical rotation data were collected on an Autopol V polarimeter (Rudolph Research Analytical) using the sodium D line (589 nm). Concentrations (*c*) are quoted in grams of analyte per 100 mL. Melting points were determined using a MEL-TEMP II melting point apparatus with samples in

Kimble Kimex 51 capillaries (1.5-1.8 x 90 mm). NMR spectra were recorded at 23 °C on Varian Unity INOVA (400, 500 and 600 MHz) spectrometers. Reported chemical shifts are referenced to residual solvent peaks. IR spectra were acquired on a FTIR Perkin Elmer Spectrum Two: UATR Two spectrometer using 1 cm^{-1} resolution. High resolution mass analyses were obtained using a 5975C Mass Selective Detector, coupled with a 7890A Gas Chromatograph (Agilent Technologies). As capillary column a HP-5MS cross-linked 5% phenylmethylpolysiloxane-diphenyl column (30 m x 0.250 mm, 0.25 micron, Agilent Technologies) was employed. Helium was used as carrier gas at a constant flow of 1 mL/min. Elemental analysis was performed at UCSB. Chiral HPLC data were collected using a Shimadzu SPD-m20a Prominence diode array detector.

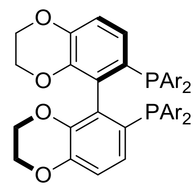
PART 2: Catalyst screening



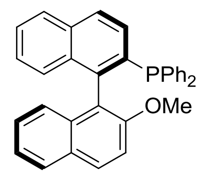
3



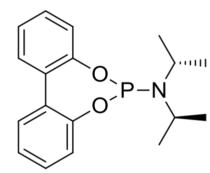
4



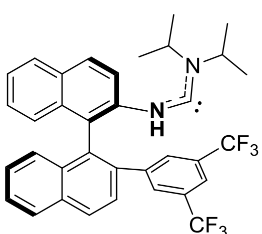
5a (Ar = Ph)
5b [Ar = 3,5(Me)$_2$-C$_6$H$_3$]



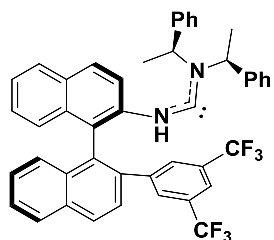
6



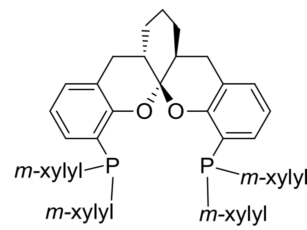
7



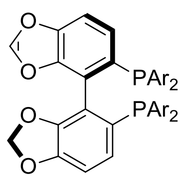
8



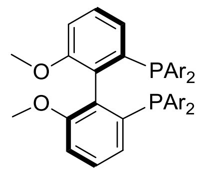
9



10



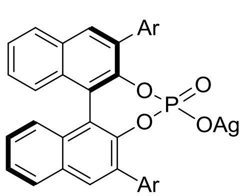
11a (Ar = Ph)
11b [Ar = 3,5-(tBu)$_2$-4-(OMe)-C$_6$H$_2$]
11c [Ar = 3,5-(Me)$_2$-C$_6$H$_3$]
11d (Ar = R = iPr)



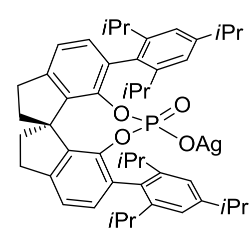
12a (Ar = Ph)
12b [Ar = 3,5-(Me)$_2$-4(NMe$_2$)-C$_6$H$_3$]
12c [Ar = 3,5-(Me)$_2$-C$_6$H$_3$]
12d [Ar = 3,4,5-(Me)$_3$-C$_6$H$_2$]
12e [Ar = 3,5-(tBu)$_2$-C$_6$H$_3$]
12f [Ar = 3,5-(tBu)$_2$-4-(OMe)-C$_6$H$_2$]

nonracemic counterions

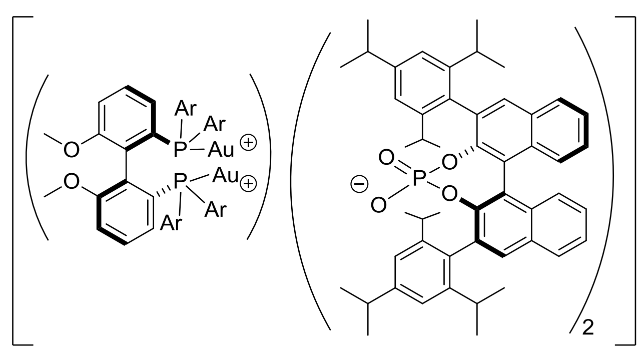
most effective catalyst



***(S)*-13a, *(R)*-13a** [Ar = 4-(CF$_3$)-C$_6$H$_4$]
***(S)*-13b, *(R)*-13b** [Ar = 2,4,6-(iPr)$_3$-C$_6$H$_2$]



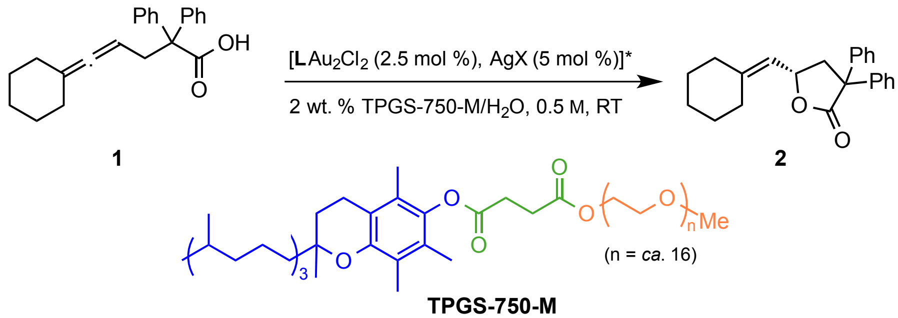
***(S)*-14a, *(R)*-14a**



***(R,R)*-15**

(Ar = 3,5-(tBu)$_2$-4-(OMe)-C$_6$H$_2$)

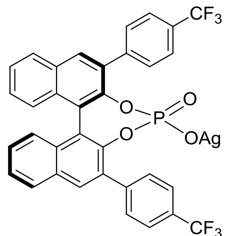
Part 2a: Finding an appropriate ligand



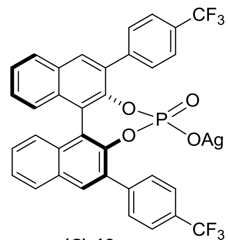
Entry	Ligand (**L**)	**X**⁻	Time (h)	% yield **2**	% ee
1	**3**	BF_4	78	98	3
2	**3**	SbF_6	70	95	1
3	**3**	OTf	68	97	2
4	**4**	SbF_6	74	95	11
5	**5a**	SbF_6	72	95	18
6	**5b**	SbF_6	78	96	30
7	**7**	SbF_6	29	93	1
8	**8**	SbF_6	32	92	7
9	**8**	PMB	56	91	18
10	**9**	PMB	67	67	40
11	**9**	PNB	70	70	50
12	**10**	SbF_6	60	85	29
13	**11a**	SbF_6	70	90	6
14	**11b**	SbF_6	75	91	36
15	**11c**	SbF_6	42	94	7
16	**11d**	SbF_6	78	90	40
17	**11d**	BF_4	78	94	38
18	**11d**	OTf	70	90	22
19	**11d**	PNB	72	95	51
20	**12a**	SbF_6	48	95	12
21	**12b**	SbF_6	49	91	18
22	**12c**	SbF_6	40	85	31
23	**12d**	PNB	30	97	37
24	**12d**	SbF_6	33	97	12
25	**12e**	PNB	38	70	30
26	**12f**	SbF_6	39	98	43
27	**12f**	**PNB**	**48**	**97**	**55**

*$\mathbf{L}Au_2Cl_2$ = **L**AuCl (5 mol %) when **L** = **7**, **8**, and **9**. PNB = *p*-nitrobenzoate, PMB = *p*-methoxybenzoate.

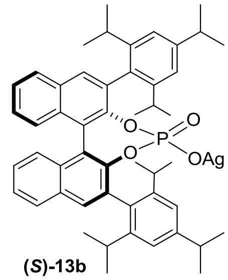
Part 2b: Chiral counterion approach with ligand **12f** – match-mismatch studies



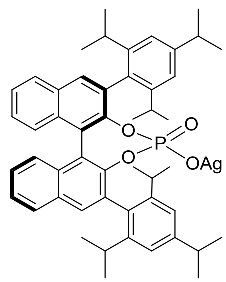
(***R***)**-13a**



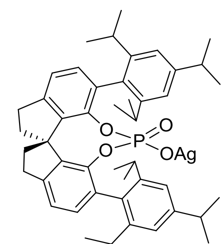
(***S***)**-13a**



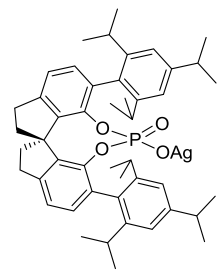
(***S***)**-13b**



(***R***)**-13b**



(***S***)**-14**

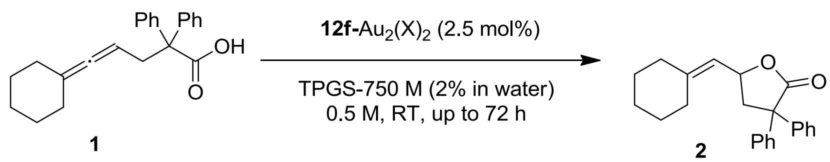


(***R***)**-14**

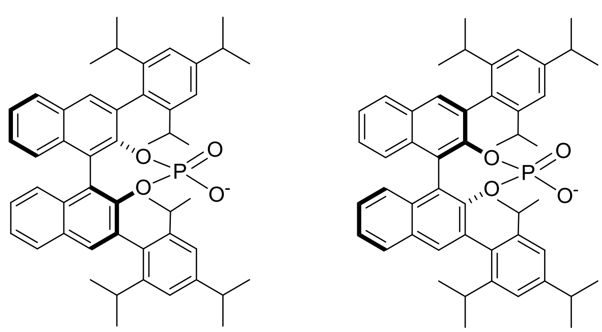
Entry	**12f**-Au_2Cl_2 (2.5 mol%)	Counter-ion (5.0 mol%)	Time (h)	% yield	% ee
1	(*R*)	(*R*)-**13a**	70	97	27
2	(*R*)	(*S*)-**13a**	72	97	51
3	(*R*)	(*R*)-**13b**	72	95	75
4	(*R*)	(*S*)-**13b**	72	96	70
5	(*R*)	(*R*)-**14**	78	96	55
6	(*R*)	(*S*)-**14**	78	96	46
7	(*S*)-	(*R*)-**13a**	66	97	-40
8	(*S*)-	(*S*)-**13a**	70	97	-27
9	(*S*)-	(*R*)-**13b**	72	95	-66
10	(*S*)-	(*S*)-**13b**	72	95	-75
11	(*S*)-	(*R*)-**14**	75	96	-40
12	(*S*)-	(*S*)-**14**	78	96	-55

Part 3: Improved *ee* without silver chloride

A 1:2 ratio of **12f**-Au_2Cl_2 and counterion were dissolved in dry CH_2Cl_2 under argon. The mixture was stirred at RT for 40 min. Silver chloride precipitated and was filtered through Celite and then a 0.25 μm PTFE microfilter. The volatiles were removed under reduced pressure to obtain active catalyst as a solid that was immediately used for the following catalytic reactions.

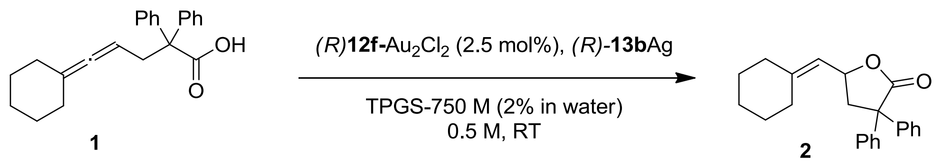


Entry	**12f**	**X**	% yield	% ee
1	*(R)*	*(R)*	92	86
2	*(S)*	*(S)*	*90*	-85
3	*(R)*	*(S)*	90	78
4	*(S)*	*(R)*	91	-78



(*S*)-**X** (*S*)-**X**

Part 4: Improved effect of two cationic gold complexes as catalyst

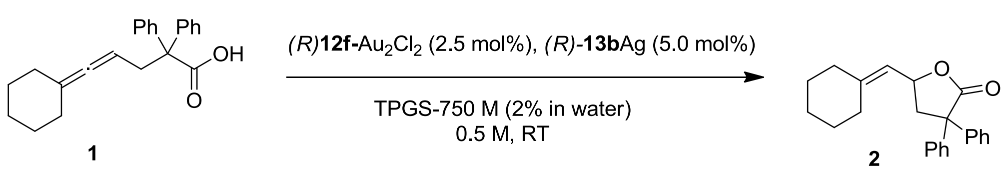


Entry	***(R)*-13b**Ag	Time (h)	% yield	% ee
1	2.5	100	97	49
2	5.0	72	97	75

AgCl precipitates were not removed during catalytic reaction.

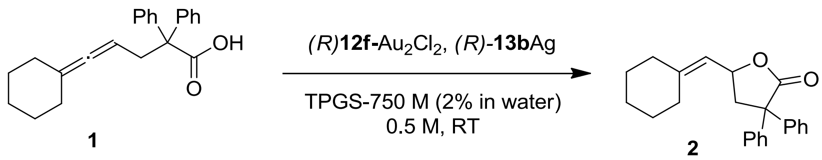
Part 5: Factors affecting *ee*

Part 5a: Acid, base, and nanoparticles



Entry	Additives (5.0 mol%)	Time (h)	% yield	% ee
1	Au nanoparticles	32	90	12
2	Et_3N	9.0	92	33
3	TsOH	5.1	88	18
4	ambient light	100	80	50

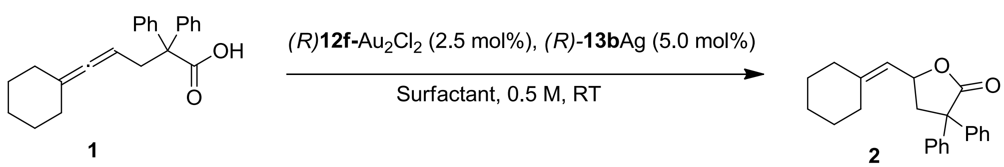
Part 5b. Excess Ligand-AuCl or counterion



Entry	***(R)*-12f**-Au_2Cl_2 (mol%)	***(R)*-13b**Ag (mol%)	Time (h)	% yield	% ee
1	2.5	4.5	80	97	58
2	2.5	5.0	72	97	75
3	2.5	5.5	60	97	60
4	2.5	10.0	32	98	38
5	-	10.0	120	90	27

Part 6: Factors affecting reaction rate

Part 6a: Surfactant (TPGS-750-M) concentration in water

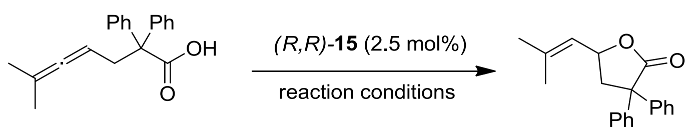


Entry	TPGS-750-M in H_2O	Time (h)	% yield
1	Neat water	100	NR
2	1%	100	67
3	2%	72	97
4	3%	70	98
4	4%	95	97

Part 6b: Surfactants other than TPGS-750M

Entry	Surfactant (2 wt% in water)	Time (h)	% yield
1	Nok	80	68
2	Pluronic	120	50
3	PQS	240	31
4	Reduced PQS	90	89
4	PTS	128	81

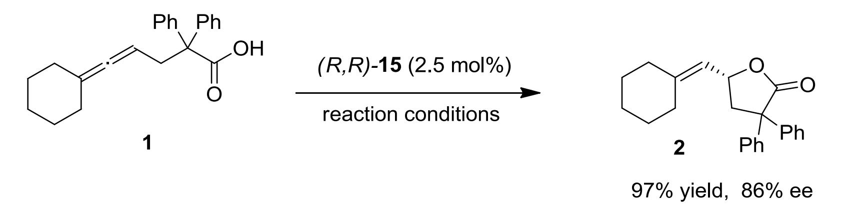
Part 7: Reducing the reaction time by softening solid substrates with solvent additives



Entry	*Reaction conditions	Time (h)	% yield	% ee
1	Mixing solutions of *(R,R)*-**15** in 3 wt. % PTS and **32** in 3 wt. % TPGS-750-M	44	95	80
2	softening all solids in 2-3 drops of DMF followed by slow addition of 3% TPGS-750-M	12	94	83
3	DMF	15	71	23
4	DMSO-TPGS-750-M	12	83	84
5	DMSO	13	69	36
6	toluene-TPGS-750-M	12	98	84
7	Toluene	68	82	70
8	Benzene-TPGS-750-M	13	98	84
9	Benzene	70	80	80

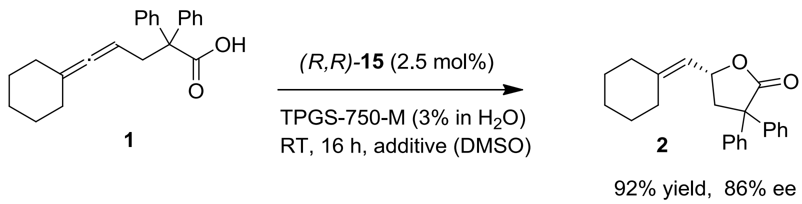
*organic solvent was used only for enhancing the solubility of solid materials, and only few drops of solvent was required to make a homogenous paste of solid. Substrate **32** was chosen due to its excellent crystalline nature.

Part 8: Final optimized conditions



Reaction conditions: 0.06 mmol **1** and 1.5x10^{-3} mmol *(R,R)*-**15** in 3-4 drops of toluene or benzene followed by slow addition of 0.2-0.3 mL 3% TPGS-750-M in water, RT, 16 h.

Part 9: E Factor and recycling studies



$$\text{E Factor} = \frac{\text{Organic waste (Kg)}}{\text{Product (Kg)}}$$

On miligrams scale,

$$= \frac{\text{10\% ether in hexanes (mg) + [crude product (mg) - isolated pure product (mg]}}{\text{Isolated pure product (mg)}}$$

$$= \frac{\text{134 mg + (31 - 28)mg}}{\text{28 mg}} = 4.9$$

Procedure:

Caution: During the entire procedure, the reaction vial was covered with aluminum foil and protected from light. Effective and uniform stirring was the key for these reactions to occur smoothly and reproducibly. Acid **1** (29 mg, 0.09 mmol) and *(R,R)*-**15f** (9.0 mg 0.002 mmol) were placed into a 4.0 mL reaction vial fitted with a cap containing a PTFE septum. The reaction vial was evacuated and purged with argon. Distilled DMSO (3-4 drops) was added to the mixture, which was then stirred for 2-3 min.

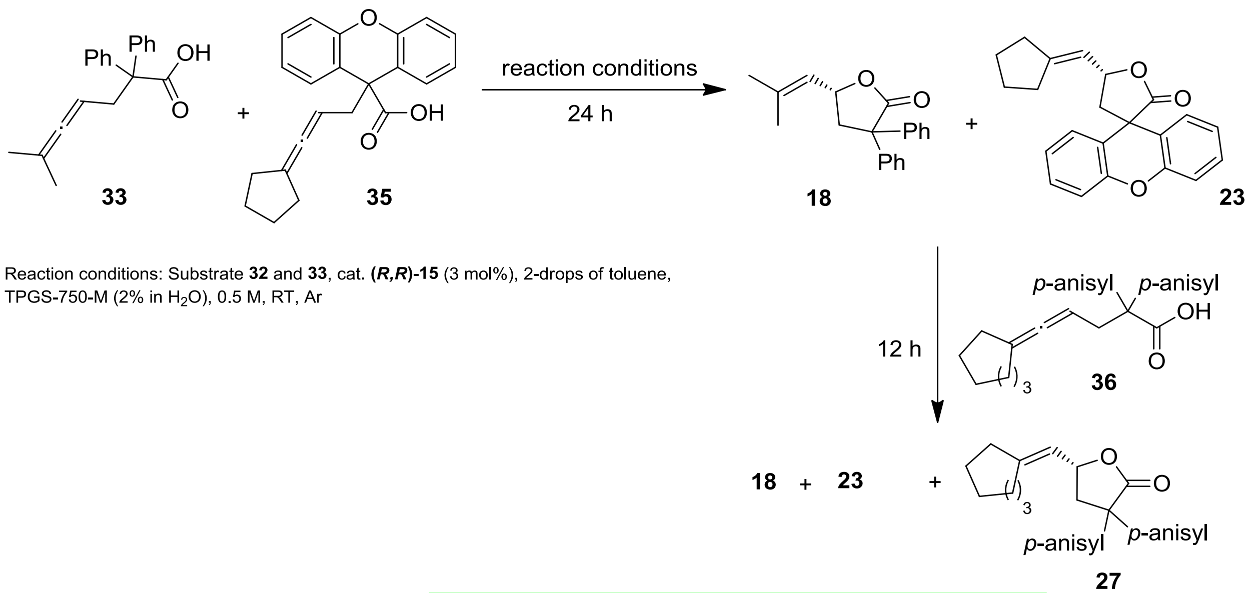
With uniform stirring under an argon atmosphere, 0.2 mL TPGS-750-M (3 wt. % in water) was slowly added to the reaction mixture that was then stirred for 16 h at RT. Approximately 0.2 (weighed 134 mg) mL solution of 10% ether in hexanes was added to the reaction mixture. After stirring for 5 min, the reaction mixture was left undisturbed for 5 min resulting in separation of the organic (containing product) and aqueous (containing surfactant and most of the catalyst) layers. The organic layer was separated, and the volatiles were removed under reduced pressure to obtain a partially pure product as a solid (31.0 mg) which was purified by passing through a silica plug using ether/hexanes (2:3) as eluent. Pure product was obtained as white solid (28.0 mg, 97% yield).

For the recycling studies, to an above aqueous layer (always protected from light), *(R,R)*-**15f** (2.7 mg 0.0009 mmol) was added followed by slow addition of **1** (30 mg, 0.09 mmol). The reaction mixture was vigorously stirred for 16 h at RT after which the same work up procedure was employed. Successive recycling experiments with the same aqueous solution were performed up to 6 times by repeating this procedure (see Table below).

Recycling of the reaction medium

Run	(*R*,*R*)-**15** (mol%)	% Yield **2**	% ee **2**
0	3	97	86
1	1	97	86
2	1	96	86
3	1	97	85
4	1	95	85
5	1	96	85
6	1	96	85

Part 10. Crossover experiment: no side reactions



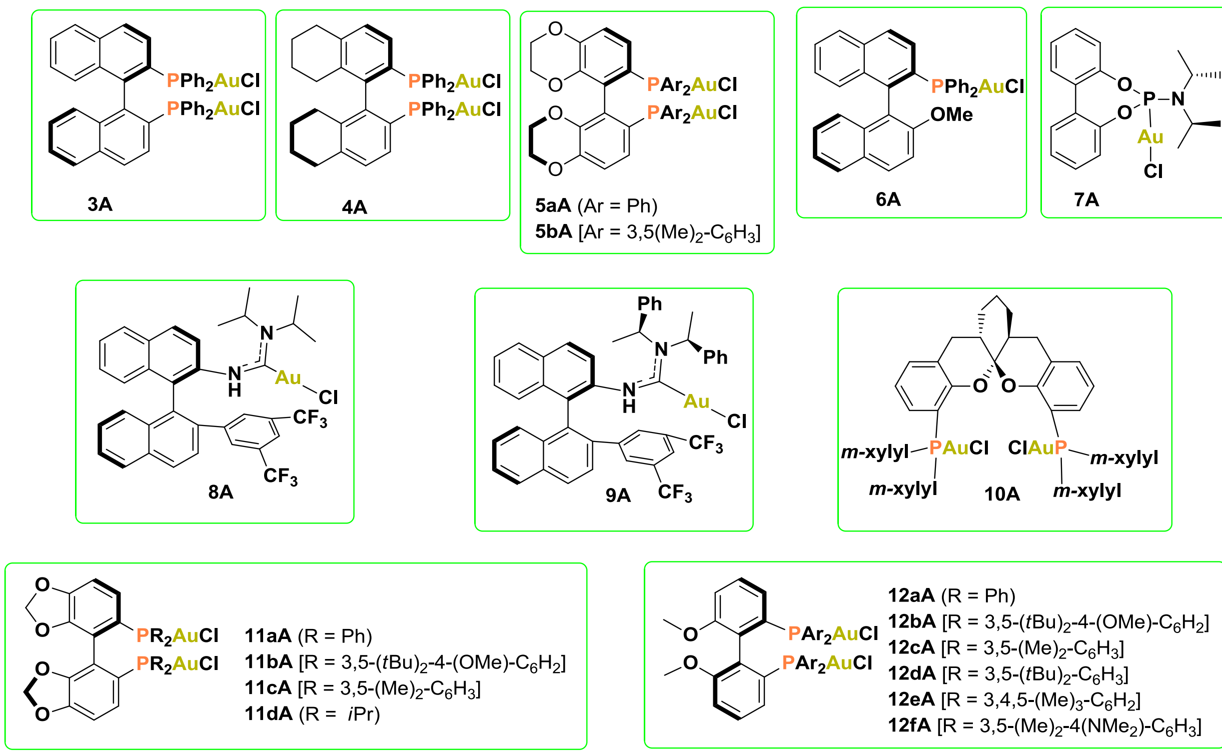
Reaction conditions: Substrate **32** and **33**, cat. **(*R,R*)-15** (3 mol%), 2-drops of toluene, TPGS-750-M (2% in H_2O), 0.5 M, RT, Ar

Separable mixture by column chromatography
(*S*)-18, yield 96%, ee 84%; **(*S*)-23**, yield 95%, ee 97%;
(*S*)-27, yield 96%, ee 81%
-No cross over product, no change in ee, in-flask recycling

Part 11: Synthesis of gold complexes (pre-catalysts)

Complexes **3A**[2], **5aA**[3], **6A**[2], **7A**[4], **8A**[5], **9A**[5], **11aA**[3], **11bA**[3], **12aA**[6], **12bA**[7], **12cA**[8], and **12dA**[9] were synthesized according to literature procedures, with their analytical data in agreement. Complexes **5bA** and **11cA** were generated *in situ* before use. Other complexes **4A**, **10A**, **11dA**, **12eA**, and **12fA** were synthesized according to the general procedure as given below.

In a sealable reaction vessel under an argon atmosphere, the commercially available *bis*(phosphine) ligand (1.0 equiv) was dissolved in 5.0 mL dry CH_2Cl_2 and the mixture stirred at RT until complete dissolution of all solid material. Under a flow of argon, a solution of (DMS)AuCl (0.5 equiv) in 2.0 mL dry CH_2Cl_2 was slowly added to the above solution. The reaction vessel was sealed and the contents stirred overnight at RT. All volatiles were then removed under reduced pressure at RT to obtain the crude complex as a viscous oil. The oil was triturated with dry pentane to obtain a white solid. The pentane was then decanted and the solid redissolved in 0.5 mL dry CH_2Cl_2. After slow addition of dry Et_2O, pure compound was obtained as white crystals. The crystals were filtered through a frit, and dried under reduced pressure.



Analytical data:

***(R)*-H$_8$-BINAP-Au$_2$Cl$_2$ (4aA)**. White solid, yield 81% (282 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.26 (m, 14H), 7.20-7.08 (m, 10H), 3.17-3.10 (m, 2H), 2.86 (t, J = 6.8 Hz, 1H), 2.82 (t, J = 6.8 Hz, 1H), 2.80 (t, J = 6.8 Hz, 1H), 2.34 (t, J = 6.8 Hz, 1H), and 1.99-1.65 (m, 10H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 19.8.

***(5S,8S)*-1,13-bis(bis(3,5-Dimethylphenyl)phosphino)-hexahydro-5*H*-chromeno[3,2-d]xanthenes-Au$_2$Cl$_2$ (10A)**. White solid, yield 78% (32 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.15 (m, 6H), 7.07-7.01 (M, 7H), 6.91-6.87 (M, 3H), 6.27-6.54 (m, 2H), 2.47-2.41 (m, 8H), 1.84-1.82 (m, 1H), 1.68-1.66 (m, 2H), and 1.46-1.44 (m, 1H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 22.9.

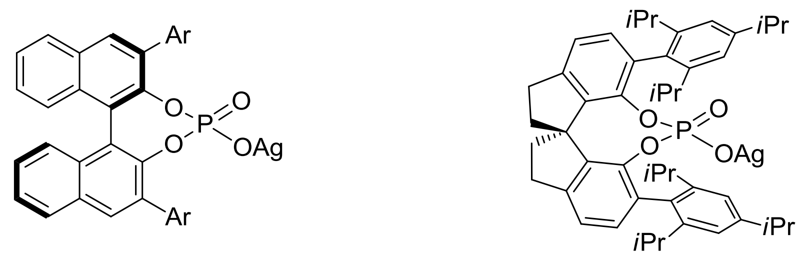
***(R)*-5,5'-bis(Diisopropylphosphino)-4,4'-bibenzo[d][1,3]dioxole-Au_2Cl_2 (11dA).** White solid, yield 93% (184 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.4 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 7.15 (dd, *J* = 8.4, 1.2 Hz, 2H), 6.00 (d, *J* = 2.0 Hz, 4H), 2.65-2.56 (m, 2H), 2.54-2.43 (m, 2H), 1.39 (d, *J* = 6.8 Hz, 3H), 1.35 (d, *J* = 6.8 Hz, 3H), 1.33 (d, *J* = 6.8 Hz, 3H), 1.31 (d, *J* = 6.8 Hz, 3H), 1.29 (d, *J* = 7.2 Hz, 3H), 1.27 (d, *J* = 7.2 Hz, 3H), 1.14 (d, *J* = 7.2 Hz, 3H), and 1.10 (d, *J* = 7.2 Hz, 3H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 43.8.

***(R)*-(6,6'-Dimethoxy-[1,1'-biphenyl]-2,2'-diyl)bis(bis(3,4,5-trimethylphenyl)phosphine)-Au_2Cl_2 (12eA).** White solid, yield 87% (135 mg), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (dt, *J* = 8.4, 3.0 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 1H), 7.03 (d, *J* = 8.0 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.72 (s, 2H), 6.68 (s, 2H), 6.59 (s, 2H), 6.56 (s, 2H), 3.87 (s, 6H), 3.87 (s, 6H), 3.80 (s, 12H), 3.71 (s, 12H), and 3.24 (s, 6H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 26.3.

***(R)*-4,4',4'',4'''-((6,6'-Dimethoxy-[1,1'-biphenyl]-2,2'diyl)bis(phosphinetriyl))tetrakis-(*N*,*N*,2,6-tetramethylaniline)-Au_2Cl_2 (12fA).** White solid, yield 86% (111 mg), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dt, *J* = 8.4, 2.4 Hz, 2H), 7.14 (s, 2H), 7.12 (s, 2H), 7.10 (s, 2H), 7.08 (d, *J* = 8.4, 2.4 Hz, 2H), 7.08 (s, 2H), 6.90 (d, *J* = 8.4 Hz, 2H), 2.97 (s, 6H), 2.82 (s, 12H), 2.79 (s, 12H), 2.24 (s, 12H), and 2,.22 (s, 12H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 20.1.

Part 12: Synthesis of nonracemic silver phosphates

Chiral silver phosphates

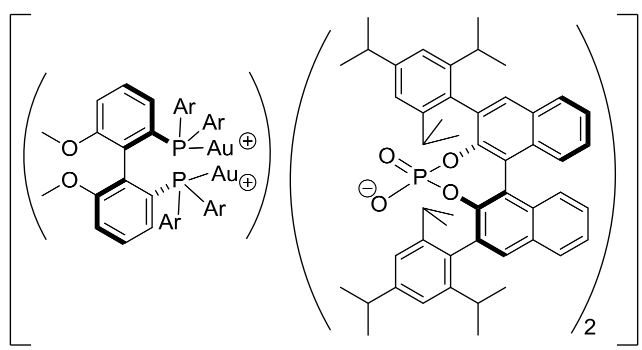


***(S)*-13a, *(R)*-13a** [Ar = 4-(CF_3)-C_6H_4]
***(S)*-13b, *(R)*-13b** [Ar = 2,4,6-(*i*Pr)$_3$-C_6H_2]

***(S)*-14a, *(R)*-14a**

Chiral phosphoric acids and their silver salts were synthesized according to a literature procedure;[10] analytical data were in agreement.

Part 13: Synthesis of catalyst *(R,R)*-**15**



***(R,R)*-15**

In a sealable reaction vessel, *(R)-(*6,6'-dimethoxy-[1,1'-biphenyl]-2,2'-diyl)bis(bis(3,5-di-*t*-butyl-4-methoxyphenyl)phosphine)-*bis*(gold chloride) (80.0 mg, 0.0495) was dissolved in 10.0 mL dry CH_2Cl_2. The reaction vessel was sealed and stirring maintained for 5 min at RT. After 5 min, a solution of *(R)*-silver-3,3'-bis(2,4,6-triisopropylphenyl)-1,1-binaphthyl-2,2'-phosphate (85.1 mg, 0.099 mmol) in dry

CH_2Cl_2 was slowly added *via* glass pipette. The reaction vessel was sealed, wrapped with aluminum foil, and stirred for 4 h at RT. The mixture was then filtered though Celite using additional CH_2Cl_2 (20 mL). The solvent was then evaporated under reduced pressure at RT to obtain crude product as a solid material. The solid was dissolved in 10.0 mL CH_2Cl_2 and repeatedly filtered through Celite (3 times with a fresh Celite pad). The solvent was evaporated under reduced pressure to obtain solid material which was recrystallized in toluene/isopropanol (with 2 drops of dry DMF) to obtain pure product as a shinning white crystalline solid (110 mg, 73%). ^1H NMR (400 MHz, $CDCl_3$) δ 7 82-7.77 (m, 4H), 7.68 (d, *J* = 13.6 Hz, 4H), 7.39-7.30 (m, 6H), 7.26-7.00 (m, 13H), 6.92-6.88 (m, 7H), 6.62 (br. s, 2H), 6.56 (d, *J* = 8.4 Hz, 2H), 6.37 (dd, *J* = 10.8, 8.4 Hz, 2H), 5.68 (dt, *J* = 8.0, 2.8 Hz, 2H), 3.63 (s, 6H), 3.83 (s, 6H), 3.07-2.97 (m, 4H), 2.82-2.77 (m, 2H), 2.74-2.69 (m, 2H), 2.61-2.55 (m, 2H), 2.55 (s, 6H), 2.42-2.35 (m, 2H), 1.59 (br. s, 6H), 1.39 (d, *J* = 6.0 Hz, 6H), 1.31-0.96 (m, 90 H), 0.95-.078 (m, 18H), 0.71 (d, *J* = 6.0 Hz, 18H), and 0.54 (d, *J* = 6.0 Hz, 6H). ^{31}P NMR (400 MHz, $CDCl_3$) δ 14.8, and 6.14. Anal Calcd for $C_{174}H_{216}Au_2O_{14}P_4$ + 0.4 DMF (solvent content by ^1H NMR): C, 68.55; H, 7.12 %. Found: C, 68.60; H, 7.13%. HRMS [ESI, $(C_{74}H_{104}Au_2O_6P_2)^{2+}$] Calcd: 772.3319, Found: *m/z* 772.3361.

Part 14: General procedure for catalytic reactions

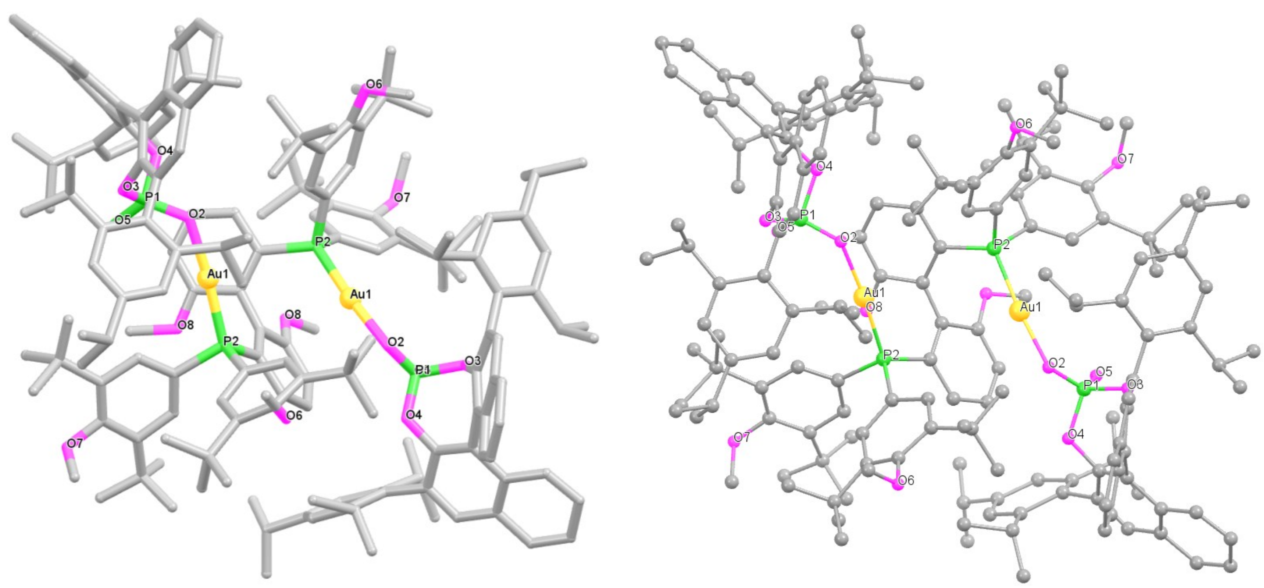
Asymmetric intramolecular hydrocarboxylation reactions. Under oxygen-free conditions, enantiomerically and diastereromerically pure chiral gold catalyst *(R,R)*-**15** (2.5 mol %) and pure allenoic acid (1.0 equiv) were taken up in a 4.0 mL screw-cap vial fitted with a PTFE/silicone septum. The vial was wrapped with aluminum foil, and a few drops (3-4) of either benzene or toluene were added. The reaction mixture was stirred for 2-3 min to obtain a uniform pasty solid. With uniform stirring, 0.2-0.3 mL of an aqueous solution of freshly prepared TPGS-750-M (3 wt % in water) was slowly added *via* syringe. The septum was wrapped with Parafilm and reaction mixture was effectively stirred at RT until complete consumption of starting allenoic acid. Reaction progress was monitored by

TLC using Et_2O:hexanes as eluent. After complete consumption of starting material, a minimum amount of organic solvent (8-10% ether in hexanes) was added *via* syringe, and the reaction mixture was stirred for 5 min. Stirring was stopped, and reaction mixture was left undisturbed for 5 min resulting in separation of organic (containing product) and aqueous (containing surfactant and most of catalyst) layers. The organic layer was separated, and all volatiles were removed under reduced pressure to obtain a partially pure product. Compounds were purified by flash chromatography and then analyzed by polarimetry, chiral HPLC, and NMR.

Preparation of racemic material for chiral HPLC analysis. $(PPh_3)AuCl$ (5.0 mol %) and $AgBF_4$ (5.0 mol %) were taken up in a 4.0 mL screw-cap reaction vial fitted with a PTFE/silicone septum. The vial was wrapped with aluminum foil, and CH_2Cl_2 (2.0 mL) was added to the reaction mixture. The mixture was stirred for 15 min at RT. After 15 min, the solvent was evaporated under reduced pressure to obtain active catalyst as a solid material. To the vial containing active catalyst, a few drops (3-4) of either DMSO or toluene were added. The reaction mixture was stirred for 2-3 min to obtain a uniform pasty solid. With uniform stirring, Et_3N (10 mol %) and 0.2-0.3 mL aqueous solution of freshly prepared TPGS-750-M (3 wt % in water) was slowly added *via* syringe. The reaction mixture was effectively stirred at RT until complete consumption of starting allenoic acid. Reaction progress was monitored by TLC using Et_2O:hexanes as eluent. After complete consumption of starting material, a minimum amount of organic solvent (8-10% ether in hexanes) was added *via* syringe, and the reaction mixture was stirred for 5 min. Stirring was stopped, and the reaction mixture was left undisturbed for 5 min resulting in separation of organic (containing product) and aqueous (containing surfactant and most of catalyst) layers. The organic layer was separated, and all volatiles were removed under reduced pressure to obtain a partially pure product.

Part 15: X-Ray crystallographic data and procedures

X-ray Crystallographic Analysis of *(R,R)*-15. Colorless blocks were obtained by slow diffusion of methanol into a solution of *(R,R)*-15 in toluene. A sample measuring 0.30 x 0.30 x 0.20 mm was cut from a larger plate for diffraction analysis. The asymmetric unit consists of two crystallographically nonequivalent *(R,R)*-15. The crystal was mounted on a glass fiber and transferred to a Bruker Kappa Apex II diffractometer. The APEX program was used to determine the unite cell parameters and data collection (10 sec / frame, 0.3 deg. /frame for a sphere of diffraction data). The data were collected at 100K using Oxford nitrogen gas cryostream system. The raw frame data were processed using SAINT program. The absorption correction was applied using program SADABS. Subsequent calculations were carried out using SHELXTL program. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques.

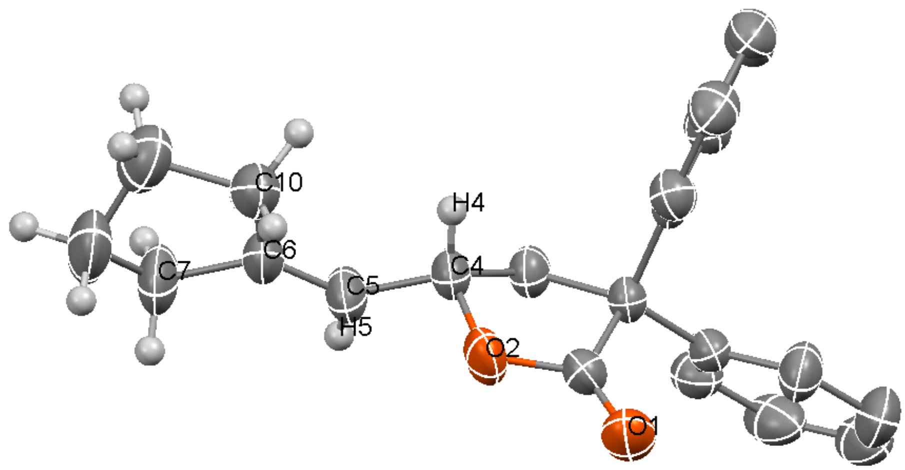


X-ray crystal structure of ***(R,R)*-15** (different views)

Table 1. Crystal data and structure refinement for ***(R,R)*-15**

Empirical formula	C174 H216 Au2 O14 P4	
Formula weight	3049.28	
Temperature	100(2) K	
Wavelength	71.073 pm	
Crystal system	Orthorhombic	
Space group	I222	
Unit cell dimensions	a = 1778.49(3) pm	α= 90°.
	b = 4415.51(8) pm	β= 90°.
	c = 4521.47(10) pm	γ = 90°.
Volume	35.5068(12) nm^3	
Z	8	
Density (calculated)	1.141 Mg/m^3	
Absorption coefficient	1.740 mm^{-1}	
F(000)	12720	
Crystal size	0.25 x 0.2 x 0.05 mm^3	
Theta range for data collection	0.64 to 28.28°.	
Index ranges	-23<=h<=21, -55<=k<=58, -60<=l<=42	
Reflections collected	108855	
Independent reflections	44076 [R(int) = 0.0685]	
Completeness to theta = 28.28°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6208	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	44076 / 204 / 852	
Goodness-of-fit on F^2	1.785	
Final R indices [I>2sigma(I)]	R1 = 0.0853, wR2 = 0.1902	
R indices (all data)	R1 = 0.1176, wR2 = 0.1991	
Absolute structure parameter	0.010(8)	
Largest diff. peak and hole	2.279 and -1.556 e.Å^{-3}	

X-ray Crystallographic Analysis of (*S*)-19. Colorless blocks were obtained by slow diffusion of pentane into a solution of **3a** in CH_2Cl_2/Et_2O (1:1). A sample measuring 0.30 x 0.30 x 0.20 mm was cut from a larger plate for diffraction analysis. The asymmetric unit consists of two crystallographically non-equivalent **19**. $C_{22}H_{22}O_2$, Mr = 318.4 g mol^{-1}, monoclinic, space group P2(1), a = 860.24(4), b = 1027.07(4), c = 1012.34(4) pm, β = 98.437(2)°., 0.88475(6) nm^3, Z = 2, ρcalcd = 1.195 Mg/m^3, μ = 0.588 mm^{-1}, T = 296(2) K, 2θmax = 65.14°, 6215 total reflections, 2735 independent [R(int) = 0.0477]. Final R1 indices[I>2σ(I)] = R1 = 0.0616, wR2 = 0.1736.

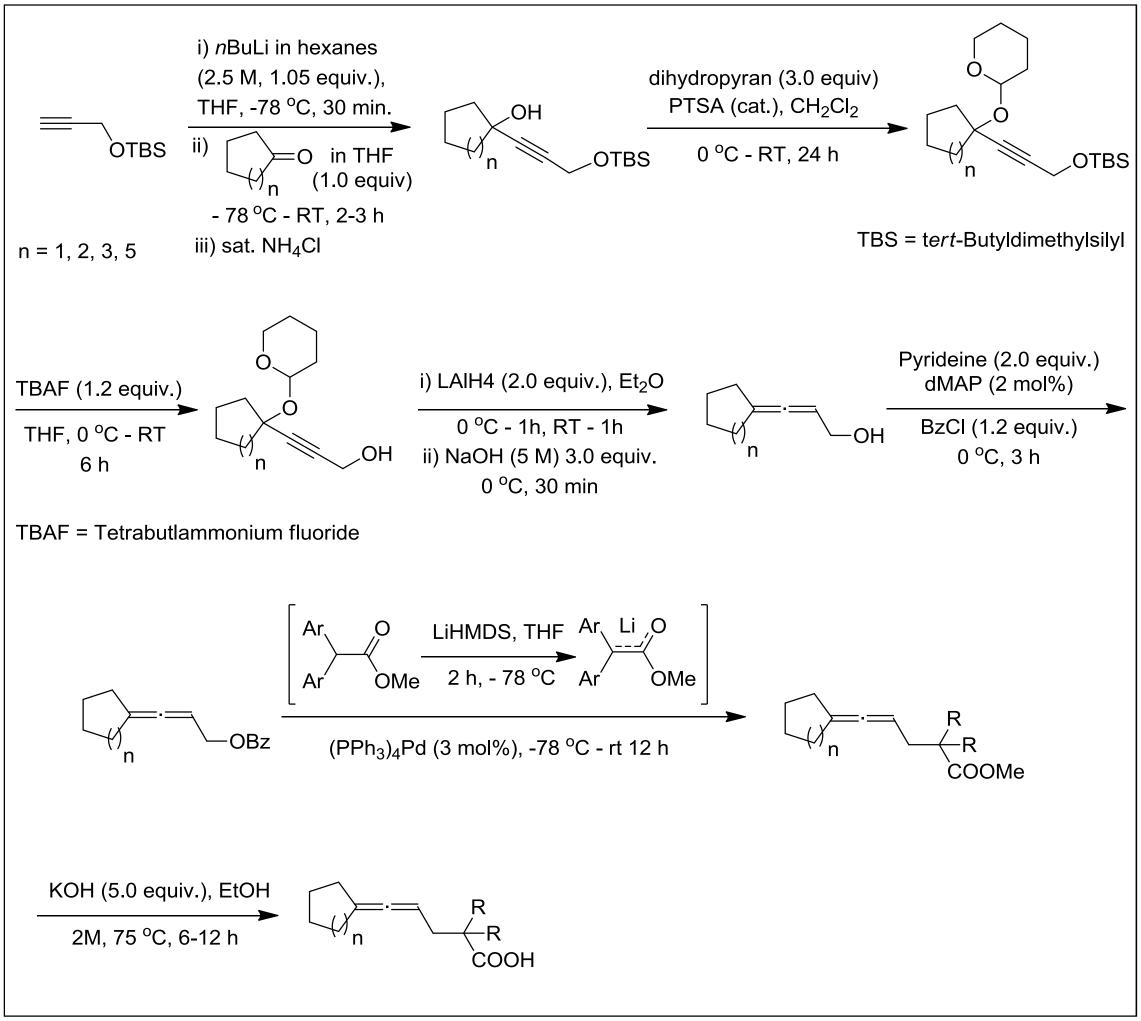


X-ray structure of **(*S*)-19**

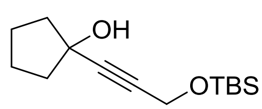
Table 2. Crystal data and structure refinement for **(*S*)-19**.

Empirical formula	C22 H22 O2	
Formula weight	318.40	
Temperature	296(2) K	
Wavelength	154.178 pm	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 860.24(4) pm	α= 90°.
	b = 1027.07(4) pm	β= 98.437(2)°.
	c = 1012.34(4) pm	γ = 90°.
Volume	0.88475(6) nm^3	
Z	2	
Density (calculated)	1.195 Mg/m^3	
Absorption coefficient	0.588 mm^{-1}	
F(000)	340	
Crystal size	0.30 x 0.30 x 0.20 mm^3	
Theta range for data collection	4.42 to 65.14°.	
Index ranges	-9<=h<=8, -12<=k<=11, -11<=l<=11	
Reflections collected	6215	
Independent reflections	2735 [R(int) = 0.0477]	
Completeness to theta = 65.14°	97.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.75264 and 0.4409	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2735 / 1 / 218	
Goodness-of-fit on F^2	1.069	
Final R indices [I>2sigma(I)]	R1 = 0.0616, wR2 = 0.1736	
R indices (all data)	R1 = 0.0619, wR2 = 0.1741	
Absolute structure parameter	-0.4(4)	
Extinction coefficient	0.008(2)	
Largest diff. peak and hole	0.228 and -0.172 e.$Å^{-3}$	

Part 16: General scheme for the syntheses of substrates[11]

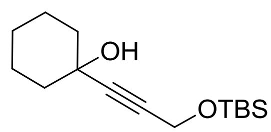


1-[3-((*t*-Butldimethylsilyl)oxy)prop-1-yn-1-yl)]cyclopentanol



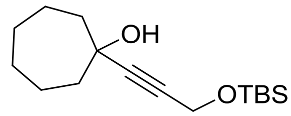
To a well dried 500 mL two neck round-bottom flask equipped with a septum and air condenser having an argon balloon atop, a solution of *t*-butyldimethyl(prop-2-yn-1-yloxy)silane (10.0 g, 58.78 mmol) in 100 mL dry THF was added. The reaction mixture was cooled to -78 °C, and then 22.4 mL *n*-BuLi (2.5 M in hexanes) was very slowly added *via* syringe. The reaction mixture was stirred for 45 min at -78 °C. After 45 min, a solution of cyclopentanone (5.2 mL, 58.78 mmol) in 10 mL dry THF was slowly added to the reaction mixture. After addition, the reaction mixture was stirred for 50 min at -78 °C, and an additional 2 h at RT. The reaction mixture was quenched with 60 mL of 0.5 M aqueous NH_4Cl. The organic layer was separated, and aqueous layer was extracted with diethyl ether (50 x 2). The combined organic extracts were washed with brine and dried over anhydrous $MgSO_4$. Volatiles were removed *via* rotary evaporation and then high vacuum to obtain pure compound as colorless oil. Yield 14.5 g (97%), R_f = 0.45 (1:9, Et_2O/hexanes). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.35 (s, 2H), 2.04 (br. s, 1H, OH), 1.89-1.82 (m, 2H), 1.72-1.59 (m, 2H), 1.58-1.46 (m, 4H), 0.90 (s, 9H), and 0.12 (s, 6H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ 88.6, 81.9, 74.6, 51.9, 42.4, 26.0, 23.5, and - 4.9. IR (neat) ν = 3275, 2357, 1103, 1070 cm^{-1}. HRMS [ESI, $(C_{14}H_{26}O_2Si+H)^+$] Calcd: 255.1780, Found: *m/z* 255.1789.

1-[3-((*t*-Butldimethylsilyl)oxy)prop-1-yn-1-yl)]cyclohexanol[11]



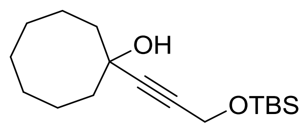
Viscous oil, yield 12.9 g (89%), R_f = 0.66 (1:19, Et_2O/hexanes).^{1}H NMR (400 MHz, $CDCl_3$) δ 5.07 (dd, *J* = 5.2, 1.2 Hz, 1H), 4.36 (s, 2H), 3.96-3.90(m, 1H), 3.49-3.44 (m, 1H), 2.00-1.97 (m, 1H), 1.85-1.80 (m, 2H), 1.72-1.56 (m, 6H),1.55-1.46 (m, 6H), 1.28-1.20 (m, 1H), 0.89 (s, 1H), and 0.11 (s, 6H). ^{13}C NMR (101MHz, $CDCl_3$) δ 96.0, 86.2, 84.7, 75.2, 63.8, 51.9, 38.9, 38.5, 32.3, 29.9, 25.6, 25.4,20.8, 18.4, and -4.9. IR (neat) ν 3279, 2358, 1059, 1071 cm^{-1}. HRMS [ESI,$(C_{20}H_{36}O_3Si+H)^+$] Calcd: 353.2511, Found: *m/z* 353.2516.

1-[3-((*t*-Butyldimethylsilyl)oxy)prop-1-yn-1-yl]cycloheptanol



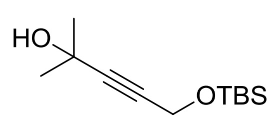
White solid (mp 62-63 °C), yield 13.2g (91%), R_f = 0.41 (1:9, Et_2O/hexanes). ^1H NMR (400 MHz, $CDCl_3$) δ 4.35 (s, 2H),2.01 (d, J = 8.0 Hz, 1H), 1.98 (d, J = 8.0 Hz, 1H), 1.85-1.77 (m, 3H), 1.67-1.49 (m, 7H),0.91 (s, 9H), and 0.12 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 89.7, 82.1, 71.8, 51.9,43.1, 28.3, 25.9, 22.3, and - 4.9. IR (neat) ν 3271, 2357, 1103, 1071 cm^{-1}. HRMS[ESI, $(C_{16}H_{30}O_2Si+H)^+$] Calcd: 283.2093, Found: *m/z* 283.2090.

1-[3-((*t*-Butyldimethylsilyl)oxy)prop-1-yn-1-yl]cyclooctanol



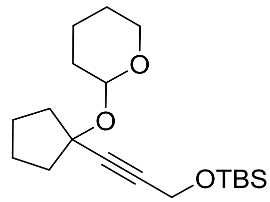
Oil, yield 13.2 g (91%), R_f = 0.44 (1:9, Et_2O/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 4.34 (s, 2H), 2.42-2.39 (m, 1H), 1.97-1.84 (m, 5H), 1.62-1.46 (m, 9H),0.90 (s, 9H), and 0.12 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 89.3, 81.9, 71.3, 51.8, 41.9, 38.1, 27.9, 27.2, 25.8, 24.5, and – 5.1. IR (neat) ν 3278, 2355, 1101, 1075. HRMS [ESI, $(C_{17}H_{32}O_2Si+H)^+$] Calcd: 297.2250, Found: *m/z* 297.2251.

5-[(*t*-Butyldimethylsilyl)oxy]-2-methylpent-3-yn-2-ol[12]



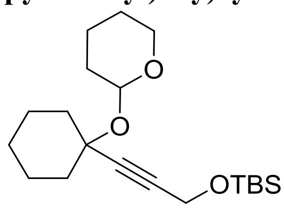
Viscous oil, yield 5.7 g (90%), R_f = 0.48 (1:9, Et_2O/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 4.33 (s, 2H), 1.88 (br. s, 1H), 1.51 (s, 6H), 0.91 (s, 9H), and 0.13 (s, 6H).

***t*-Butyldimethyl[(3-(1-((tetrahydro-2*H*-pyran-2-yl)oxy)cyclopentyl)prop-2-yn-1-yl)oxy]silane**



p-Toluenesulfonic acid monohydrate (37.5 mg, 0.197 mmol) was added to a solution of 1-(3-((*t*-butyldimethylsilyl)oxy)prop-1-yn-1-yl)cyclopentanol (10 g, 39.30 mmol) in 50 mL dry dichloromethane, and the reaction mixture was stirred for 10 min at 0 °C. After 10 min, dihydrpyran (10 mL, 117.9 mmol) was added and the mixture stirred at 0 °C for 6 h followed by 18 h stirring at RT. It was then quenched with 5 mL of triethylamine and stirred for additional 20 min at RT. The DCM was evaporated *in vacuo* to obtain crude compound as a yellow viscous oil. The material was dissolved in 200 mL diethyl ether and washed sequentially with 0.5 N $NaHCO_3$, water, and brine. The organic layer was separated and dried over anhydrous $MgSO_4$. Volatiles were evacuated by rotary evaporation to obtain crude product as a viscous oil. Pure product was obtained by flash chromatography over the silica using ether:hexanes (2:98, 5:95) as eluent. Viscous oil, yield 11.9 g (90%), R_f = 0.55 (1:9, Et_2O/hexanes). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.04 (dd, *J* = 5.6, 3.2 Hz, 1H), 4.35 (s, 2H), 3.94-3.89 (m, 1H), 3.53-3.47 (m, 1H), 2.24-2.18 (m, 1H), 2.00-1.47 (m, 13H), 0.91 (s, 9H), and0.12 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 96.7, 86.6, 83.3, 81.0, 63.6, 52.0, 41.4,40.0, 32.1, 25.9, 25.6, 23.4, 23.0, 20.5, 18.4, and - 4.9.

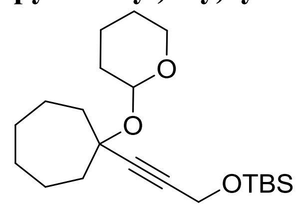
***t*-Butyldimethyl[(3-(1-((tetrahydro-2*H*-pyran-2-yl)oxy)cyclohexyl)prop-2-yn-1-yl)oxy]silane**



Viscous oil, yield 9.84 g (78%), R_f = 0.51 (1:9, Et_2O/hexanes). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.07 (dd, *J* = 5.2, 1.2 Hz, 1H), 4.36 (s, 2H), 3.96-3.90(m, 1H), 3.49-3.44 (m, 1H), 2.00-1.97 (m, 1H), 1.85-

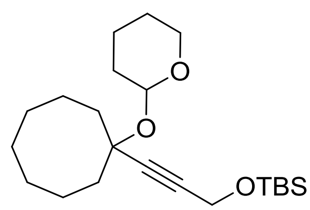
1.80 (m, 2H), 1.72-1.56 (m, 6H),1.55-1.46 (m, 6H), 1.28-1.20 (m, 1H), 0.89 (s, 1H), and 0.11 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 96.0, 86.2, 84.7, 75.2, 63.8, 51.9, 38.9, 38.5, 32.3, 29.9, 25.6, 25.4,20.8, 18.4, and -4.9.

***t*-Butyldimethyl[(3-(1-((tetrahydro-2*H*-pyran-2-yl)oxy)cycloheptyl)prop-2-yn-1-yl)oxy]silane**



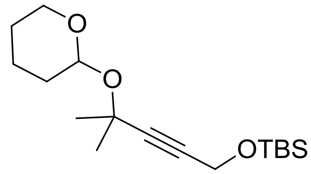
Viscous oil, yield 9.8 g (70%), R_f = 0.57 (1:9, Et_2O/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.07-5.05 (m, 1H), 4.37 (s, 2H), 3.97-3.92 (m, 1H), 3.51-3.45 (m, 1H), 2.02-1.96 (m, 3H), 1.88-1.82 (m, 2H), 1.73-1.49 (m, 13H), 0.91 (s, 9H), and 0.13 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 96.1, 87.5, 83.8, 78.4, 63.8, 52.0, 42.2, 40.9, 32.4, 28.8, 25.9, 25.6, 22.2, 22.0, 20.8, 18.4, and - 4.9. IR (neat) ν = 3275, 2355, 1102, 1075 cm^{-1}. HRMS [ESI, $(C_{21}H_{38}O_3Si+H)^+$] Calcd: 367.2668, Found: *m/z* 367.2671.

***t*-Butyldimethyl[(3-(1-((tetrahydro-2*H*-pyran-2-yl)oxy)cyclooctyl)prop-2-yn-1-yl)oxy]silane**



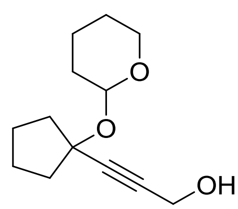
Viscous oil, yield 5.7 g (89%), R_f = 0.60 (1:9, Et_2O/hexanes). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.07-5.06 (m, 1H), 4.36 (s, 2H), 3.97-3.92 (m, 1H), 3.51-3.46 (m, 1H), 2.01-1.96 (m, 1H), 1.96-1.81 (m, 4H), 1.68-1.46 (m, 15H), 0.91 (s, 9H), and 0.13 (s, 6H). IR (neat) ν 3270, 2350, 1102, 1078 cm^{-1}. HRMS [ESI, $(C_{22}H_{40}O_3Si+H)^+$] Calcd: 381.2825, Found: *m/z* 381.2831.

t-Butyldimethyl[(4-methyl-4-((tetrahydro-2*H*-pyran-2-yl)oxy)pent-2-yn-1-yl]silane[13]



Viscous oil, yield 5.9 g (67%), R_f = 0.46 (1: 9, Et_2O/hexanes). ^1H NMR (600 MHz, $CDCl_3$) δ 5.04-5.03 (m, 1H), 4.34 (s, 2H), 3.95-3.92 (m, 1H), 3.50-3.47 (m, 1H), 1.85-1.83 (m, 1H), 1.71 1.67 (m, 1H), 1.52 (s, 6H), 1.48 (s, 4H), 0.91 (s, 9H), and 0.12 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 96.4, 87.3, 82.8, 71.3, 63.6, 51.9, 32.1, 30.8, 29.8, 25.9, 25.5, 20.8, and - 4.9. IR (neat) ν 3275, 2368, 1110, 1079 cm^{-1}. HRMS [ESI, $(C_{17}H_{32}O_3Si+H)+$] Calcd: 313.2199, Found: *m/z* 313.2198.

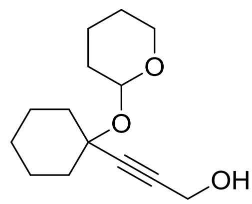
3-[1-((Tetrahydro-2*H*-pyran-2-yl)oxy)cyclopentyl]prop-2-yn-1-ol



Tetrabutylammonium fluoride (9.52 g, 36.41 mmol) was added to a solution of *tert*-butyldimethyl[(3-(1-((tetrahydro-2*H*-pyran-2-yl)oxy)cyclopenttyl)prop-2-yn-1-yl)oxy]silane (10.0 g, 30.34 mmol) in 50 mL THF at 0 °C, and reaction mixture was stirred for overnight at RT. After complete consumption of the starting material as monitored by TLC, the reaction mixture was diluted with 100 mL EtOAc, and washed thoroughly with water. The organic layer was separated and dried over anhydrous $MgSO_4$. The solvent was evacuated *via* rotary evaporation to obtain crude compound as a yellow oil. The crude compound was purified by column chromatography over silica, using ether/hexanes as eluent (1:4). Viscous oil, yield 5.1 g (76%), R_f = 0.44 (2:3, ether/hexanes). ^1H NMR

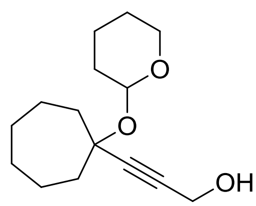
(400 MHz, $CDCl_3$) δ 5.05 (dd, J = 4.8, 3.2 Hz, 1H), 4.28 (d, J = 6.4 Hz, 2H), 3.95-3.89 (m, 1H), 3.54-3.49 (m, 1H), 2.37-2.30 (m, 1H), 2.22-2.15 (m, 1H), 2.01-1.88 (m, 2H), 1.85-1.75 (m, 4H), 1.74-1.64 (m, 3H), and 1.58-1.48 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 96.3, 87.4, 83.0, 80.7, 63.3, 51.2, 41.2, 40.3, 32.0, 25.5, 23.4, 23.0, and 20.1.

3-[1-((Tetrahydro-2*H*-pyran-2-yl)oxy)cyclohexyl]prop-2-yn-1-ol[14]



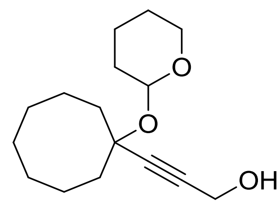
Viscous oil, yield 4.5 g (75%), R_f = 0.41 (2:3, ether/hexanes). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.13-5.11 (m, 1H), 4.32 (d, J = 6.4 Hz, 2H), 3.99-3.93 (m, 1H), 3.53-3.45 (m, 1H), 2.01-1.99 (m, 2H), 1.87-1.71 (m, 2H), 1.70-1.51 (m, 12H).

3-[1-((Tetrahydro-2*H*-pyran-2-yl)oxy)cycloheptyl]prop-2-yn-1-ol



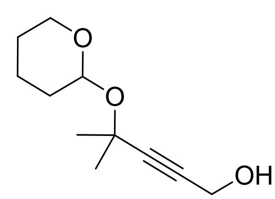
Viscous oil, yield 7.2 g (77%), R_f = 0.55 (1:4, EtOAc/hexanes). ^{1}H NMR (600 MHz, $CDCl_3$) δ 5.08 (dd, J = 5.2, 3.6 Hz, 1H), 4.30 (d, J = 5.4 Hz, 2H), 3.97-3.93 (m, 1H), 3.52-3.48 (m, 1H), 2.09 (br. s, 1H, OH), 2.08-1.95 (m, 2H), 1.96 (d, J = 7.6 Hz, 1H), 1.90-1.79 (m, 2H), 1.72-1.57 (m, 3H), and 1.56-1.46 (m, 10H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 95.6, 88.5, 83.5, 78.1, 63.3, 51.3, 41.9, 41.2, 32.3, 28.7, 28.2, 25.7, 22.3, 22.0, and 20.4. IR (neat) ν 3311, 3258, 2358, 1101, 1066 cm^{-1}. HRMS [ESI, (C15H24O3+Na)+] Calcd: 275.1623, Found: *m/z* 275.1632.

3-[1-((Tetrahydro-2*H*-pyran-2-yl)oxy)cyclooctyl]prop-2-yn-1-ol



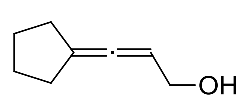
Viscous oil, yield 4.7 g (81%), R_f = 0.56 (1:4, EtOAc/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.08 (dd, J = 5.2, 3.6 Hz, 1H), 4.30 (d, J = 6.0 Hz, 2H), 3.97-3.93 (m, 1H), 3.52-3.48 (m, 1H), 2.11-2.04 (m, 1H), 1.99-1.96 (m, 2H), 1.91-1.85 (m, 1H), 1.84-1.80 (m, 2H), and 1.73-1.26 (m, 14H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 95.4, 88.2, 83.3, 77.8, 63.3, 51.3, 36.5, 35.9, 32.3, 28.4, 28.0, 25.6, 24.7, 22.1, 21.9, and 20.4. IR (neat) ν = 3319, 3261, 2357, 1105, 1066 cm^{-1}. HRMS [ESI, $(C_{16}H_{26}O_3+Na)^+$] Calcd: 289.1780, Found: *m/z* 289.1788.

4-Methyl-4-[(tetrahydro-2H-pyran-2-yl)oxy]pent-2-yn-1-ol[13]



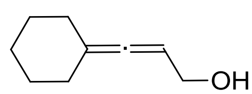
Clear oil, yield 2.9 g (78%), R_f = 0.41 (1:4, EtOAc/hexanes). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 5.04-5.06 (m, 1H), 4.25 (d, J = 6.0 Hz, 2H), 3.91-3.95 (m, 1H), 3.46-3.52 (m, 1H), 3.26 (t, J = 6.0 Hz, 1H), 1.45-1.85 (m, 12H).

3-Cyclopentylideneprop-2-en-1-ol[15]



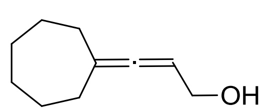
To a well-dried 250 mL two-neck round bottom flask with rubber septum and reflux condenser having a argon balloon atop, 100 mL dry diethyl ether was added *via* syringe. The contents were cooled to 0 °C under an inert atmosphere, and $LiAlH_4$ (1.7 g, 44.6 mmol) was added by opening the septum under a slow flow of argon. The septum was closed, and the contents of the round bottom flask were stirred for 5 min under argon. To this slurry, a solution of 3-[1-((tetrahydro-2*H*-pyran-2-yl)oxy)cyclopentyl]prop-2-yn-1-ol (5.0 g, 22.29 mmol) in 10 mL dry diethyl ether was slowly added *via* syringe. The reaction mixture was allowed to reach RT, and then stirred for 2 h. After 2 h, the mixture was cooled to 0 °C, and the excess LAH was quenched with 5.0 mL 5.0 M NaOH. The reaction mixture was then stirred for 30 min at RT. After 30 min, it was diluted with 100 mL diethyl ether, and then filtered through Celite. The organic layer was dried over anhydrous sodium sulfate. Solvent was evacuated *via* rotary evaporation to obtain pure compound as a transparent oil. Yield 2.11 g (76%), R_f = 0.30 (1:4, EtOAc/hexanes). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.33-5.26 (m, 1H), 4.08 (d, J = 5.2 Hz, 2H), 2.40-2.36 (m,4H), 1.71-1.65 (m, 4H), and 1.55 (br., s, 1H, OH). ^{13}C NMR (151 MHz, CD_2Cl_2): 196.4,107.1, 92.7, 61.3, 31.7, and 27.4.

3-Cyclohexylideneprop-2-en-1-ol[14]



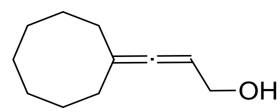
Transparent oil, yield 2.8 g (85%), R_f = 0.33 (1:4, EtOAc/hexanes). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.23-5.19 (m, 1H), 4.07 (t, J = 5.6 Hz, 2H), 2.15-2.12 (m, 4H), and 1.63-1.51 (m, 6H).

3-Cyclooctylideneprop-2-en-1-ol



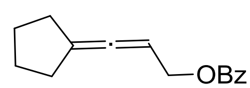
Transparent oil, yield 3.1 g (70%), R_f = 0.35 (1:4, EtOAc/hexanes). ^{1}H NMR (600 MHz, $CDCl_3$) δ 5.19-5.17 (m, 1H), 4.05 (t, J = 6.0 Hz, 2H), 2.29-2.21 (m, 4H), and 1.62-1.57 (m, 4H), 1.56-1.52 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 200.6, 108.2, 89.7, 61.2, 32.6, 29.5, and 28.6. HRMS [ESI, $(C_{10}H_{16}O+Na)^+$] Calcd: 175.1099, Found: m/z 175.1091.

3-Cyclooctylideneprop-2-en-1-ol



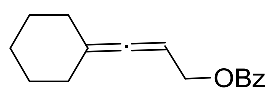
Transparent oil, yield 2.9 g (78%), R_f = 0.36 (1:4, EtOAc/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.24-5.20 (m, 1H), 4.09 (t, J = 5.5 Hz, 2H), 2.22-2.15 (m, 4H), and 1.70-1.56 (m, 6H), 1.55-1.52 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.1, 107.9, 90.3, 61.2, 31.8, 27.1, 26.9, and 26.3. HRMS [ESI, $(C_{11}H_{18}O+Na)^+$] Calcd: 189.1255, Found: m/z 189.1251.

3-Cyclopentylideneallyl benzoate



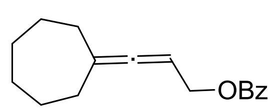
This compound was prepared by a modified literature procedure. Under an argon atmosphere, a solution of 3-cyclopentylideneprop-2-en-1-ol (2.0 g, 16.10 mmol) in 30.0 mL dry CH_2Cl_2 was transferred into oven dried two-neck round bottom flask. The reaction mixture was cooled to 0 °C, and pyridine (2.73 mL, 33.8 mmol) and a catalytic amount of DMAP were added. The reaction mixture was stirred at 0 ^{o}C for 5 min. followed by slow syringe addition of freshly distilled dry benzoyl chloride (1.46 mL, 16.9 mmol). After the addition the reaction mixture was warmed to RT and stirred for an additional 3-4 h. After complete consumption of starting material as monitored by TLC, CH_2Cl_2 was evaporated under reduced pressure to obtain the crude product as a light yellow oil. The material was dissolved in 50.0 mL diethyl ether and then sequentially washed with 0.5 N cold HCl (50 mL), aqueous $NaHCO_3$, and brine. The organic layer was separated and dried over anhydrous $MgSO_4$. Solvent was evaporated under reduced pressure to obtain crude product as an oil which was purified by flash column chromatography using silica gel and ether/hexanes as eluent (1:15) to obtain pure product as a transparent oil. *Caution*: All allenyl benzoates are unstable on silica gel, and therefore, purification should be achieved with minimal silica and done very quickly to minimize decomposition. Transparent oil, yield 3.20 g (89%), R_f = 0.41 (1:15, Et_2O/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08-8.05 (m, 2H), 7.57-7.53 (m, 1H), 7.35 (m, 2H), 5.35- 5.28 (m, 1H), 4.79 (d, J = 6.8 Hz, 2H), 2.40-2.36 (m, 4H), and 1.67-1.61 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.8, 166.5, 133.0, 130.1, 129.7, 128.4, 106.1, 87.4, 63.8, 31.3, and 27.1. HRMS [ESI, $(C_{15}H_{16}O_2+H)^+$] Calcd: 229.1228, Found: *m/z* 229.1225.

3-Cyclohexylideneallyl benzoate[14]



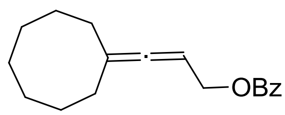
Transparent oil, yield 2.5 g (89%), R_f = 0.40 (1:15, ether/hexanes). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08- 8.06 (m, 2H), 7.58-7.53 (m, 1H), 7.44 (t, J = 8.0 Hz, 2H), 5.25-5.21 (m, 1H), 4.78 (d, J = 6.4 Hz, 2H), 2.14-2.11 (m, 4H), 1.62-1.45 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.0, 166.5, 133.0, 13,6, 129.8, 128.4, 104.9, 104.8, 84.8, 64.0, 31.2, 27.3, 26.1. HRMS [ESI, $(C_{16}H_{18}O_2+H)^+$] Calcd: 243.1385, Found: *m/z* 243.1381.

3-Cycloheptylideneallyl benzoate



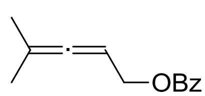
Transparent oil, yield 3.35 g (85%), R_f = 0.44 (1:15, Et_2O/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08-8.06 (m, 2H), 7.57-7.53 (m, 1H), 7.43 (dt, J = 8.0, 1.6 Hz, 2H), 5.23-5.19 (m, 1H), 4.77 (d, J = 6.5 Hz, 2H), 2.29-2.23 (m, 4H), 1.64-1.58 (m, 4H), and 1.54-1.49 (m, 4). ^{13}C NMR (126 MHz, $CDCl_3$) δ 203.3, 166.5, 132.9, 130.6, 129.8, 128.4, 106.9, 84.7, 63.9, 32.3, 29.4, and 28.5. HRMS [ESI, $(C_{17}H_{20}O_2+H)^+$] Calcd: 257.1541, Found: m/z 257.1547.

3-Cyclooctylideneallyl benzoate



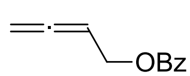
Transparent oil, yield 4.50 g (89%), R_f = 0.46 (1:15, Et_2O/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08-8.05 (m, 2H), 7.57-7.53 (m, 1H), 7.45 (dt, J = 8.0, 1.6 Hz, 2H), 5.27-5.24 (m, 1H), 4.78 (d, J = 6.5 Hz, 2H), 2.29-2.14 (m, 4H), and 1.68-1.48 (m, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 203.7, 166.6, 133.0, 130.6, 129.8, 128.4, 106.9, 85.3, 63.7, 31.5, 26.9, 26.8, and 26.2. HRMS [ESI, $(C_{18}H_{23}O_2+H)^+$] Calcd: 271.1698, Found: m/z 271.1701.

4-Methylpenta-2,3-dien-1-yl-benzoate[16]



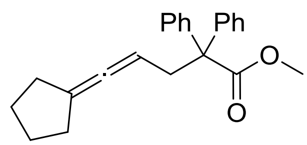
Transparent oil, yield 5.2 g (84%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07-8.05 (m, 2H), 7.57-7.53 (m, 1H), 7.45-7.42 (m, 2H), 5.24-5.21 (m, 1H), 7.77 (d, J = 6.5 Hz, 2H), 1.71 (s, 3H), 1.70 and (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 203.4, 166.5, 132.9, 130.6, 129.7, 128.4, 97.6, 85.0, 63.8, and 20.3.

Buta-2,3-dien-1-yl benzoate[17]



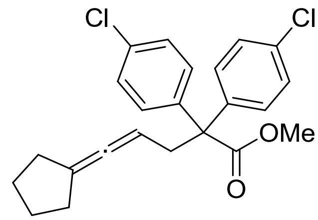
Transparent oil, yield 0.89 g (77%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07-8.05 (m, 2H), 7.58-7.54 (m, 1H), 7.45-7.42 (m, 2H), 5.42 (quin, *J* = 7.0 Hz, 1H), 4.90-4.87 (m, 2H), and 4.84-4.82 (m, 2H),. ^{13}C NMR (126 MHz, $CDCl_3$) δ 210.0, 166.5, 133.1, 130.3, 129.8, 128.5, 86.6, 76.9, and 62.8. HRMS [ESI, $(C_{11}H_{10}O_2+H)^{+}$] Calcd: 175.0759, Found: *m/z* 175.0760.

Methyl-5-cyclohexylidene-2,2-diphenylpent-4-enoate[18]



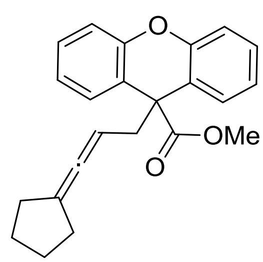
Under an inert and dry atmosphere, a solution of methydiphenyl acetate (3.20 g, 14.14 mmol) in 60.0 mL dry THF was added to an oven dried 100 mL two-neck round bottom flask. The mixture was cooled to -78 °C and lithium hexamethyldisilazide (2.60 g, 15.55 mmol) was added under a flow of dry argon. The reaction mixture was allowed to stir for 2 h at - 78 °C under argon. Appearance of a yellow coloration indicates the lithiation process. In another oven dried 250 mL two neck round bottom flask under argon, a solution of 3-cyclopentylideneallyl benzoate (3.23 g, 14.14 mmol) in dry 50 mL dry THF was added *via* syringe followed by addition of tetrakis-(triphenylphosphine)palladium (0.41 g, 0.354 mmol). The reaction mixture was stirred for 1 h, and then the lithiated solution of methyldiphenyl acetate was added *via* cannula. After the addition, the reaction mixture was stirred for 6 h at RT after which it was diluted with 50 mL diethyl ether, and sequentially washed with 0.5 N $NaHCO_3$, and water. The aqueous layer was extracted with an additional 50 mL diethyl ether. The combined organic layer was dried over anhydrous sodium sulfate, and the solvent was evaporated under reduced pressure to give crude product as a light yellow oil. This material was further purified by flash chromatography using silica gel and ether/hexanes as eluent (1:15, 1:9) to obtain pure compound as a transparent viscous oil, yield 3.90 g (81%), R_f = 0.53 (1:4, Et_2O/hexanes). ^1H NMR (400 MHz, $CDCl_3$) δ 7.34-7.23 (m, 10H), 7.87-7.79 (m, 1H), 3.70 (s, 3H), 3.10 (d, J = 7.2 Hz, 2H), 2.15-2.11 (m, 4H), and 1.59-1.54 (m, 4H).

Methyl 2,2-bis(4-chlorophenyl)-5-cyclopentylidenepent-4-enoate



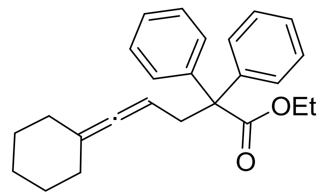
Viscous oil, yield 0.82 g (79%), R_f = 0.49 (1:4, Et_2O/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 7.27-7.25 (m, 4H), 7.19-7.18 (m, 4H), 4.79-4.75 (m, 1H), 3.69 (s, 3H), 3.03 (d, J = 7.5 Hz, 2H), 2.18-2.09 (m, 4H), and 1.60-1.55 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.5, 173.8, 140.6, 132.9, 130.4, 128.0, 103.5, 86.4, 59.7, 52.6, 39.1, 30.8, and 26.9. HRMS [ESI, $(C_{23}H_{22}Cl_2O_2+H)^+$] Calcd: 401.1075, Found: *m/z* 401.1072.

Methyl-9-(3-cyclopentylideneallyl)-9*H*-xanthene-9-carboxylate



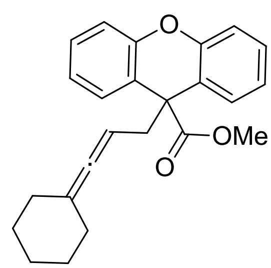
Viscous oil, yield 1.52 g (81%), R_f = 0.41 (1:4, Et_2O/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 7.25-7.18 (m, 4H), 7.08-7.03 (m, 4H), 4.61-4.55 (m, 1H), 3.60 (s, 3H), 3.00 (d, J = 7.5 Hz, 2H), 1.91-1.86 (m, 2H), 1.70-1.65 (m, 2H), and 1.46-1.43 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.5, 174.3, 150.7, 128.5, 127.1, 123.1, 121.3, 116.5, 103.6, 85.1, 52.8, 50.1, 40.9, 30.6, and 26.8. HRMS [ESI, $(C_{23}H_{22}O_3+H)^+$] Calcd: 347.1647, Found: *m/z* 347.1648.

Ethyl-5-cyclohexylidene-2,2-diphenyl-4-enaoate[18]



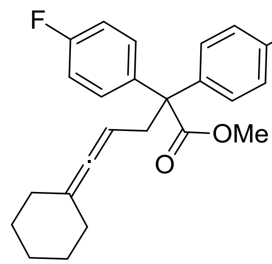
Transparent viscous oil (yield 1.23 g (80%), R_f = 0.49 (1:4, Et_2O/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.23 (m, 10H), 4.78-4.75 (m, 1H), 4.20 (q, J = 7.5 Hz, 2H), 3.14 (d, J = 7.5 Hz, 2H), 1.91-1.88 (m, 4H), 1.51-1.46 (m, 6H), and 1.20 (t, J = 7.5 Hz, 3H).

Methyl-9-(3-cyclohexylideneallyl)-9*H*-xanthane-9-carboxylate



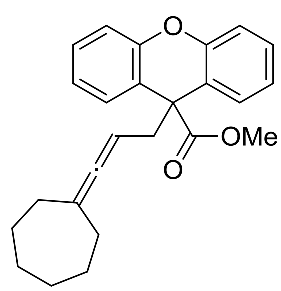
Viscous oil, yield 1.22 g (87%), R_f = 0.39 (1:4, Et_2O/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26-7.23 (m, 2H), 7.18 (dd, J = 8.0, 2.0 Hz, 2H), 7.09-7.04 (m, 4H), 4.44-4.40 (m, 1H), 3.62 (s, 3H), 2.98 (d, J = 7.5 Hz, 2H), 1.64-1.56 (m, 4H), and 1.39-1.28 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.2, 174.5, 150.8, 128.6, 127.3, 123.2, 121.4, 116.7, 101.9, 82.5, 52.9, 50.5, 42.1, 31.0, 27.3, and 26.1. HRMS [ESI, $(C_{24}H_{24}O_3+H)^+$] Calcd: 361.1804, Found: *m/z* 361.1809.

Methyl-5-cyclohexylidene-2,2-bis(4-fluorophenyl)pent-4-enoate



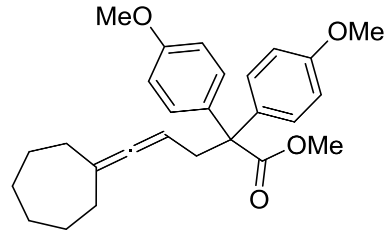
Viscous oil, yield 0.79 g (71%), R_f = 0.43 (1:4, Et_2O/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27-7.21 (m, 4H), 7.05-6.95 (m, 4H), 4.69-4.65 (m, 1H), 3.69 (s, 3H), 3.03 (d, J = 7.0 Hz, 2H), 1.89-1.87 (m, 4H), and 1.52-1.43 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.7, 174.4, 162.7, 138.3 (d, $^3J_{(C,F)}$ = 3.5 Hz), 130.8 (d, $^2J_{(C,F)}$ = 7.9 Hz), 114.7 (d, $^1J_{(C,F)}$ = 21.3 Hz), 102.2, 84.1, 59.6, 52.6, 39.8, 31.2, 27.4. and 26.2. HRMS [ESI, $(C_{24}H_{24}F_2O_2+H)^+$] Calcd: 383.1823, Found: *m/z* 383.1819.

Methyl-9-(3-cycloheptylideneallyl)-9*H*-xanthane-9-carboxylate



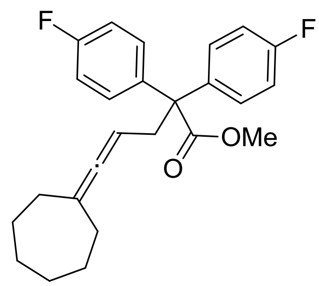
Viscous oil, yield 1.89 g (83%), R_f = 0.40 (1:4, Et_2O/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25-7.22 (m, 2H), 7.17 (dd, J = 8.0, 1.5 Hz, 2H), 7.08-7.03 (m, 4H), 4.42-4.37 (m, 1H), 3.62 (s, 3H), 2.95 (d, J = 7.5 Hz, 2H), 1.77-166 (m, 4H), and 1.38-1.34 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 204.3, 174.5, 150.8, 128.6, 127.3, 123.3, 121.5, 116.7, 103.9, 82.3, 52.9, 50.5, 42.3, 32.0, 29.5, and 28.4. HRMS [ESI, $(C_{25}H_{26}O_3+H)^+$] Calcd: 375.1960, Found: *m/z* 375.1952.

Methyl-5-cycloheptylidene-2,2-bis(4-methoxyphenyl)pent-4-enoate



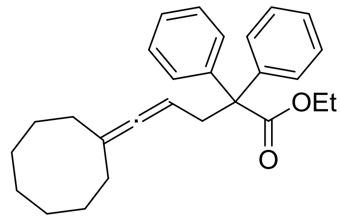
Viscous oil, yield 1.74 g (73%), R_f = 0.40 (2:3, Et_2O/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 7.21-7.14 (m, 4H), 6.82 (d, *J*= 9.0 Hz, 4H), 4.70-4.67 (m, 1H), 3.79 (s, 6H), 3.68 (s, 3H), 3.02 (d, *J* = 7.5 Hz, 2H), 2.15-2.01 (m, 4H), and 1.53-1.42 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 203.7, 175.0, 158.2, 134.8, 130.1, 130.0, 113.1, 103.7, 84.2, 59.2, 55.2, 52.3, 39.6, 33.0. and 29.3. HRMS [ESI, $(C_{27}H_{32}O_4+H)^+$] Calcd: 421.2379, Found: *m/z* 421.2377.

Methyl-5-cycloheptylidene-2,2-bis(4-fluorophenyl)pent-4-enoate



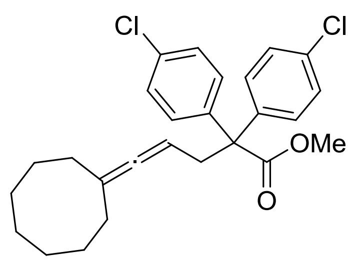
Viscous oil, yield 1.50 g (77%), R_f = 0.45 (1:4, Et_2O/hexanes). ^1H NMR (400 MHz, $CDCl_3$) δ 7.26-7.21 (m, 4H), 7.03-6.96 (m, 4H), 4.68-4.64 (m, 1H), 3.70 (s, 3H), 3.03 (d, *J* = 7.2 Hz, 2H), 2.02.2.00 (m, 4H), and 1.54-1.46 (m, 8H). ^{19}F NMR (376 MHz, $CDCl_3$) δ –115.9. ^{13}C NMR (126 MHz, $CDCl_3$) δ 204.1, 174.4, 162.7, 160.8, 138.3 (d, $^3J_{(C,F)}$ = 3.5 Hz), 130.8 (d, $^2J_{(C,F)}$ = 7.9 Hz), 114.8 (d, $^1J_{(C,F)}$ = 21.3 Hz), 104.2, 83.8, 59.6, 52.7, 39.8, 32.2, 29.4. and 28.5. HRMS [ESI, $(C_{25}H_{26}F_2O_2+H)^+$] Calcd: 397.1979, Found: *m/z* 397.1987.

Ethyl-5-cyclooctylidene-2,2-diphenylpent-4-enoate



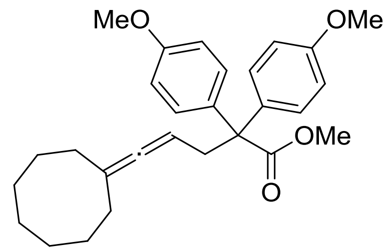
Viscous oil, yield 1.12 g (83%), R_f = 0.47 (1:4, Et_2O/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 7.33-7.21 (m, 10H), 4.79-4.75 (m, 1H), 4.17 (q, J = 9.0 Hz, 2H), 3.09 (d, J = 7.5 Hz, 2H), 1.90-1.85 (m, 4H), 1.54-1.42 (m, 10H), and 1.17 (t, J = 9.0 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 203.9, 174.2, 142.7, 129.3, 127.8, 126.8, 103.7, 85.0, 61.3, 60.7, 39.0, 31.7, 31.3, 26.9, 26.8, and 14.1. HRMS [ESI, $(C_{27}H_{32}O_2+H)^+$] Calcd: 389.2481, Found: *m/z* 389.2489.

Methyl-2,2-bis(4-chlorophenyl)-5-cyclooctylidenepent-4-enoate



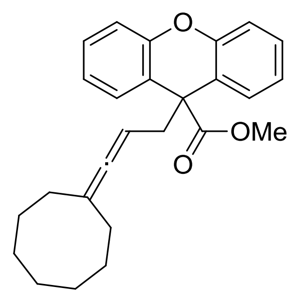
Viscous oil, yield 2.22 g (86%), R_f = 0.42 (1:4, Et_2O/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 7.27 (d, J = 9.0 Hz, 4H), 7.19 (d, J = 9.0 Hz, 4H), 4.72-4.69 (m, 1H), 3.70 (s, 3H), 3.02 (d, J = 7.5 Hz, 2H), 1.92-1.89 (m, 4H), and 1.49-1.44 (m, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 204.0, 173.8, 140.6, 133.0, 130.4, 128.0, 104.1, 84.1, 59.8, 52.6, 38.9, 31.2, 26.7, and 26.1. HRMS [ESI, $(C_{26}H_{28}Cl_2O_2+H)^+$] Calcd: 443.1545, Found: *m/z* 443.1539.

Methyl-2,2-bis(4-methoxyphenyl)-5-cyclooctylidenepent-4-enoate



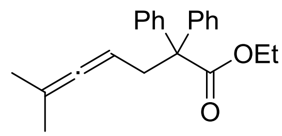
Viscous oil, yield 1.35 g (79%), R_f = 0.38 (2:3, Et_2O/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 7.20 (d, J = 9.0 Hz, 4H), 6.82 (d, J = 9.0 Hz, 4H), 4.76-4.72 (m, 1H), 3.80 (s, 6H), 3.69 (s, 3H), 3.03 (d, J = 7.5 Hz, 2H), 1.95-1.92 (m, 4H), and 1.56-1.43 (m, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 203.9, 175.2, 158.3, 134.9, 130.3, 113.2, 103.7, 85.1, 59.4, 55.4, 52.5, 39.3, 31.4, 26.9, and 26.3. HRMS [ESI, $(C_{28}H_{34}O_4+H)^+$] Calcd: 435.2535, Found: *m/z* 435.2540.

Methyl-9-(3-cyclooctylideneallyl)-9*H*-xanthane-9-carboxylate



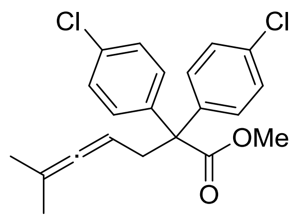
Viscous oil, yield 1.89 g (85%), R_f = 0.42 (1:4, Et_2O/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 7.23-7.23 (m, 2H), 7.16 (dd, J = 7.5, 1.5 Hz, 2H), 7.09-7.03 (m, 4H), 4.44-4.40 (m, 1H), 3.63 (s, 3H), 2.94 (d, J = 7.5 Hz, 2H), 1.70-166 (m, 4H), and 1.43-1.32 (m, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 204.3, 174.5, 150.9, 128.7, 127.3, 123.4, 121.5, 116.7, 103.9, 83.0, 52.9, 50.6, 42.1, 31.2, 26.8, 26.7, and 26.1. HRMS [ESI, $(C_{26}H_{28}O_3+H)^+$] Calcd: 389.2117, Found: *m/z* 389.2120.

6-Ethyl 6-methyl-2,2-diphenylhepta-4,5-dienoate



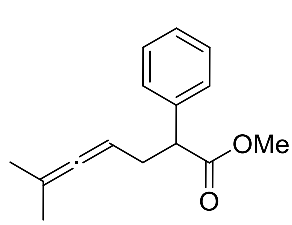
Viscous oil, yield 1.12 g (73%), R_f = 0.49 (1:4, Et_2O/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 7.31-7.22 (m, 10H), 4.76-4.70 (m, 1H), 4.18 (q, J = 7.0 Hz, 2H), 3.09 (d, J = 7.5 Hz, 2H), 1.48 (s, 3H), 1.47 (s, 3H), and 1.18 (t, J = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 203.9, 174.1, 142.7, 129.3, 127.8, 126.8, 94.5, 84.8, 61.3, 60.6, 39.2, 20.2, and 14.1.

Methyl 2,2-bis(4-chlorophenyl)-6-methylhepta-4,5-dienoate



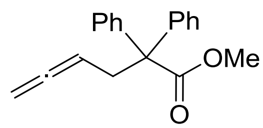
Viscous oil, yield 0.87 g (78 %), R_f = 0.49 (1:4, Et_2O/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 7.28-7.25 (m, 4H), 7.20-7.18 (m, 4H), 4.68-4.63 (m, 1H), 3.02 (d, J = 7.5 Hz, 2H), 1.49 (s, 3H), and 1.48 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 203.9, 173.8, 140.6, 132.9, 130.4, 128.0, 94.9, 83.9, 59.6, 52.3, and 38.9, 20.1. HRMS [ESI, $(C_{21}H_{20}Cl_2O_2+H)^+$] Calcd: 375.0919, Found: *m/z* 375.0931.

Methyl 6-methyl-2-phenylhepta-4,5-dienoate



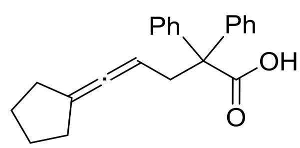
Viscous oil, yield 0.23 g (69%), R_f = 0.39 (1:4, Et_2O/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 7.31-7.23 (m, 5H), 4.96-4.92 (m, 1H), 3.68-3.64 (m, 1H), 3.65 (s, 3H), 2.78-2.71 (m, 1H), 2.41-2.37 (m, 1H), 1.60 (s, 3H), and 1.58 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 202.3, 174.0, 138.7, 128.6, 128.0, 127.2, 96.6, 86.3, 52.0, 51.2, 32.9, 20.6, and 20.5. HRMS [ESI, $(C_{215}H_{18}O_2+H)^+$] Calcd: 231.1385, Found: *m/z* 231.1389.

Methyl 2,2-diphenylhexa-4,5-dienoate[14, 18]



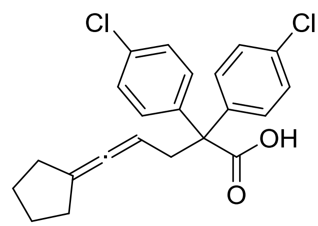
This compound was prepared according to the literature,[18] and analytical data was in agreement.

5-Cyclopentylidene-2,2-diphenylpent-4-enoic acid[18]



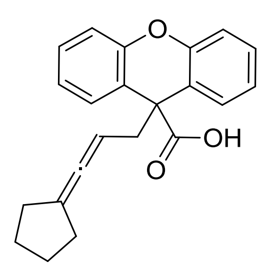
Into a 100 mL two neck round bottom flask fitted with a reflux condenser, methyl-5-cyclohexylidene-2,2-diphenylpent-4-enoate (1.5 g, 4.51 mmol) was dissolved in 10 mL ethanol. KOH (1.26 g, 22.55 mmol) was added to the reaction mixture followed by addition of 0.2 mL water. The mixture was refluxed for 6 h after which it was cooled to RT and diluted with 20 mL water and 50 mL hexanes. The aqueous layer was separated and washed twice with 10 mL hexanes. It was then neutralized with 0.5 N HCl to obtain a turbid mixture containing the desired compound. The aqueous layer was extracted twice with CH_2Cl_2 (15 mL). The organic layer was separated, dried over anhydrous sodium sulfate and the solvent evaporated under reduced pressure to obtain a moderately pure product as an off white solid. Pure product was obtained by flash chromatography over silica gel and ether/hexanes as eluent (1:3). White crystalline solid (mp = 162-163 °C), yield 1.35 g (94%), R_f = 0.38 (1:4, EtOAc/hexanes). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.2 (br. s, 1H, COOH), 7,32-7.21 (m, 10H), 4.72-4.67 (m, 1H), 3.07 (d, J = 7.6 Hz, 2H), 1.85-1.83 (m, 4H), and 1.44-1.40 (m, 4H). ^{13}C NMR (101 MHz, CDCl3) δ 200.8, 179.4, 142.1, 129.3, 128.0, 127.1, 102.1, 84.2, 60.5, 39.4, 31.1, 27.4, and 26.2. IR (neat) ν 3052 (br), 2971 (m), 2952 (m), 2851 (w), 1964 (w), 1695 (s), 1491 (m) cm^{-1}.

2,2-Bis(4-chlorophenyl)-5-cyclopentylienepent-4-enoic acid



White crystalline solid (mp = 126-127 °C), yield 0.81 g (89%), R_f = 0.53 (1:4, EtOAc/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.1 (br. s, 1H, COOH), 7.29-7.19 (m, 8H), 4.79-4.73 (m, 1H), 3.00 (d, J = 7.2 Hz, 2H), 2.14-2.05 (m, 4H), and 1.57-1.51 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.8, 178.7, 140.2, 133.4, 130.6, 128.3, 103.9, 86.3, 59.7, 39.1, 30.9, and 27.0. IR (neat) ν 3060 (br), 2917 (m), 2853 (w), 1962 (w), 1691 (s), 1491 (s) cm-^{1}. HRMS [ESI, ($C_{22}H_{20}Cl_2O_2$+Na)+] Calcd: 409.0738, Found: *m/z* 409.0738.

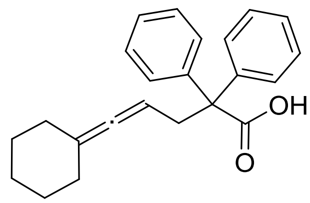
9-(3-Cyclopentylideneallyl)-9H-xanthene-9-carboxylic acid



White solid (mp = 62-63 °C), yield 0.48 g (78%), R_f = 0.51 (1:4, EtOAc/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.8 (br. s, 1H, COOH), 7.27-7.21 (m, 4H), 7.07-7.03 (m, 4H), 4.61-4.54 (m, 1H), 2.99 (d, J = 6.8 Hz, 2H), 1.88-1.82 (m, 2H), 1.63-1.57 (m, 2H), and 1.45-1.40 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.8, 178.5, 150.9, 129.0, 127.4, 123.3, 120.7, 116.8, 104.1, 85.2, 49.9, 39.5, 30.7, and 26.9.

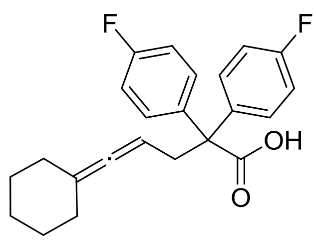
IR (neat) ν 3053 (br), 2970 (m), 2921 (m), 2866 (w), 1961 (w), 1901 (w) 1696 (s), 1480 (m) cm^{-1}. HRMS [ESI, $(C_{22}H_{20}O_3+Na)^+$] Calcd: 355.1310, Found: *m/z* 355.1317.

5-Cyclohexylidene-2,2-diphenylpent-4-enoic acid[18]



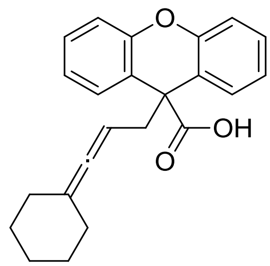
White crystalline solid (mp = 162-163 °C, reported 156-160 °C), yield 0.82 g (97%), R_f = 0.35 (1:4, EtOAc/hexanes). ^1H NMR (400 MHz, $CDCl_3$) δ 11.2 (br. s, 1H, COOH), 7,32-7.21 (m, 10H), 4.72-4.67 (m, 1H), 3.07 (d, J = 7.6 Hz, 2H), 1.85-1.83 (m, 4H), and 1.44-1.40 (m, 4H).

2,2-bis(4-Fluorophenyl)-5-cyclohexylienepent-4-enoic acid



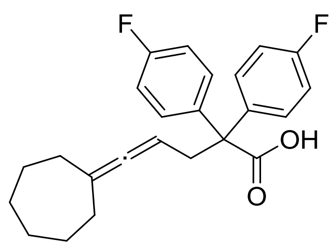
White solid (mp = 135-136 °C), yield 0.33 g (89%), R_f = 0.50 (1:4, EtOAc/hexanes). ^1H NMR (500 MHz, $CDCl_3$) δ 10.6 (br. s, 1H, COOH), 7.29-7.25 (m, 4H), 7.01-6.96 (m, 4H), 4.69-4.66 (m, 1H), 3.03 (d, J = 7.5 Hz, 2H), 1.90-1.85 (m, 4H), and 1.49-1.43 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.9, 179.7, 162.0 (d, $^1J_{(C,F)}$ = 248 Hz), 137.7 (d, $^4J_{(C,F)}$ = 3.2 Hz), 130.9 (d, $^3J_{(C,F)}$ = 7.8 Hz), 114.9 (d, $^2J_{(C,F)}$ = 21.2 Hz), 102.4, 83.8, 59.5, 39.6, 31.1, 27.3, 26.1. IR (neat) ν = 3057 (br), 2973 (m), 2922 (m), 2867 (w), 1962 (w), 1901 (w) 1696 (s), 1482 (m) cm^{-1}. HRMS [ESI, $(C_{23}H_{22}F_2O_2+Na)^+$] Calcd: 391.1486, Found: *m/z* 391.1480.

9-(3-Cyclohexylideneallyl)-9H-xanthene-9-carboxylic acid



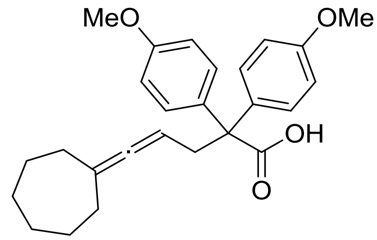
White solid (mp = 64-65 °C), yield 0.4 g (88%), R_f = 0.51 (1:4, EtOAc/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.2 (br. s, 1H, COOH), 7.29-7.26 (m, 4H), 7.09-7.06 (m, 4H), 4.44-4.31 (m, 1H), 2.99 (d, J = 7.5 Hz, 2H), 1.61-1.57 (m, 4H), and 1.36-1.31 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 201.2, 179.0, 150.9, 128.9, 127.5, 123.3, 120.6, 116.8, 102.2, 82.4, 50.1, 40.6, 31.0, 27.2, and 26.1. IR (neat) ν 3056 (br), 2972(m), 2918 (m), 2864 (w), 1963 (w), 1903(w) 1698 (s), 1482 (m) cm^{-1}. HRMS [ESI, $(C_{23}H_{22}O_3+Na)^+$] Calcd: 369.1467, Found: *m/z* 369.1469.

2,2-bis(4-Fluorophenyl)-5-cycloheptylienepent-4-enoic acid



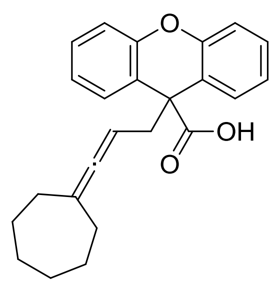
White solid (mp = 142-143 °C), yield 0.66 g (93%), R_f = 0.48 (1:4, EtOAc/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.5 (br. s, 1H, COOH), 7.29-7.26 (m, 4H), 7.01-6.97 (m, 4H), 4.69-4.66 (m, 1H), 3.02 (d, J = 7.5 Hz, 2H), 1.99-1.93 (m, 4H), and 1.47-1.44 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 204.2, 179.9, 162.9 (d, $^1J_{(C,F)}$ = 247 Hz), 137.7 (d, $^4J_{(C,F)}$ = 3.6 Hz), 130.9 (d, $^3J_{(C,F)}$ = 7.9 Hz), 115.0 (d, $^2J_{(C,F)}$ = 21.8 Hz), 104.4, 83.6, 59.6, 39.6, 32.1, 29.4, and 28.4. IR (neat) ν = 3061 (br), 2977 (m), 2920 (m), 2866 (w), 1968 (w), 1900 (w) 1699 (s), 1483 (m) cm^{-1}. HRMS [ESI, $(C_{24}H_{24}F_2O_2+Na)^+$] Calcd: 405.1642, Found: *m/z* 405.1650.

2,2-bis(4-Methoxyphenyl)-5-cycloheptylienepent-4-enoic acid



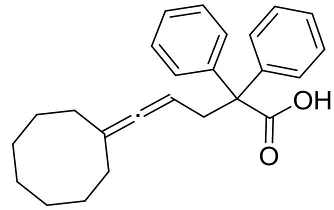
White solid (mp = 118-119 ^{o}C), yield 0.24 g (89%), R_f = 0.47 (3:4, EtOAc/hexanes).[1]H NMR (500 MHz, $CDCl_3$) δ 11.2 (br. s, 1H, COOH), 7.23 (d, J = 8.5 Hz, 4H), 6.82 (d, J = 8.5 Hz, 4H), 4.71-4.67 (m, 1H), 3.79 (s, 6H), 3.01 (d, J = 7.5 Hz, 2H), 2.02-1.98 (m, 4H), and 1.51-1.42 (m, 8H). [13]C NMR (126 MHz, $CDCl_3$) δ 204.0, 179.0, 158.5, 134.4, 130.4, 113.3, 103.9, 84.2, 59.2, 55.4, 39.6, 32.1, 29.4, and 28.5. IR (neat) ν 3058 (br), 2970(m), 2928 (m), 2864 (w), 1962 (w), 1903(w) 1697 (s), 1481 (m) cm^{-1}. HRMS [ESI, $(C_{26}H_{30}O_4+Na)^+$] Calcd: 429.2042, Found: m/z 429.2040.

9-(3-Cycloheptylideneallyl)-9H-xanthene-9-carboxylic acid



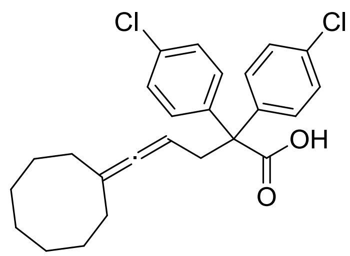
White solid (>90 ^{o}C charring), yield 0.55 g (89%), R_f = 0.53 (1:4, EtOAc/hexanes).[1]H NMR (500 MHz, $CDCl_3$) δ 11.3 (br. s, 1H, COOH), 7.28-7.24 (m, 4H), 7.09-7.05 (m, 4H), 4.43-4.39 (m, 1H), 2.96 (d, J = 7.5 Hz, 2H), 1.75-1.64 (m, 4H), and 1.42-1.34 (m, 8H). [13]C NMR (126 MHz, $CDCl_3$) δ 204.3, 178.8, 150.9, 128.9, 127.5, 123.4, 120.6, 116.9, 104.2, 82.2, 50.2, 40.7, 32.0, 29.5, and 28.3. IR (neat) ν 3075 (w), 2920 (m), 2848 (m), 2627 (w), 1961 (w), 1698 (s), and 1574 (m) cm^{-1}. HRMS [ESI, $(C_{24}H_{24}O_3+Na)^+$] Calcd: 383.1623, Found: m/z 383.1627.

5-Cyclooctylidene-2,2-diphenylpent-4-enoic acid



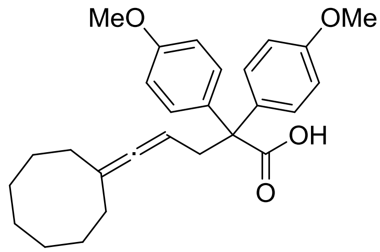
White solid (146-147 ^{o}C), yield 0.34 g (93%), R_f = 0.55 (1:4, EtOAc/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.2 (br. s, 1H, COOH), 7.34-7.24 (m, 10H), 4.78-4.75 (m, 1H), 3.09 (d, J = 7.5 Hz, 2H), 1.92-1.88 (m, 4H), and 1.52-1.43 (m, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 204.1, 142.1, 129.4, 129.3, 128.0, 127.1, 103.9, 84.7, 60.2, 38.9, 31.3, 26.8, and 26.2. IR (neat) ν = 3068 (w), 2920 (m), 2846 (w), 2631 (w), 1692 (s), and 1599 cm^{-1}. HRMS [ESI, $(C_{25}H_{28}O_2+Na)^+$] Calcd: 383.1987, Found: *m/z* 383.1988.

2,2-bis(4-Chlorophenyl)-5-cyclooctylienepent-4-enoic acid



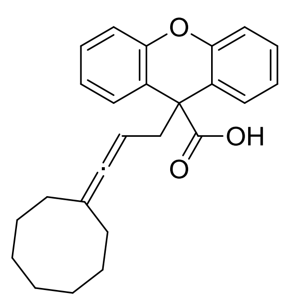
White solid (mp = 141-142.5 °C), yield 0.29 g (95%), R_f = 0.47 (1:4, EtOAc/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.2 (br. s, 1H, COOH), 7.29-7.22 (m, 8H), 4.73-4.70 (m, 1H), 3.01 (d, J = 7.5 Hz, 2H), 1.90-1.88 (m, 4H), and 1.48-1.42 (m, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 204.3, 140.2, 133.4, 130.7, 130.7, 128.3, 128.3, 104.5, 84.0, 59.9, 38.9, 31.3, 26.8, and 26.2. IR (neat) ν 3059 (br), 2972 (m), 2924 (m), 2634 (w), 1960 (w), 1903(w) 1698 (s), 1480 (m) cm^{-1}. HRMS [ESI, $(C_{25}H_{26}Cl_2O_2+Na)^+$] Calcd: 451.1208, Found: *m/z* 451.1209.

2,2-bis(4-Methoxyphenyl)-5-cyclooctylienepent-4-enoic acid



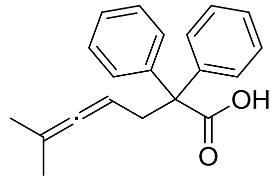
White solid (118-119 °C), yield 0.55 g (92%), R_f = 0.51 (2:3, EtOAc/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.2 (br. s, 1H, COOH), 7.24 (d, *J* = 9.0 Hz, 4H), 6.83 (d, *J* = 9.0 Hz, 4H), 4.76-4.73 (m, 1H), 3.80 (s, 6H), 3.02 (d, *J* = 7.5 Hz, 2H), 1.94-1.91 (m, 4H), and 1.51-1.44 (m, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 203.9, 158.4, 134.2, 130.2, 130.1, 113.2, 103.7, 84.7, 59.1, 55.2, 38.9, 31.2, 26.7, 26.7, and 26.1. IR (neat) ν 3007 (w), 2921 (m), 2846 (m), 2637 (w), 1959 (w), 1690 (s), and 1608 cm^{-1}. HRMS [ESI, $(C_{27}H_{32}O_4+Na)^+$] Calcd: 443.2198, Found: *m/z* 443.2192.

9-(3-Cycloheptylideneallyl)-9H-xanthene-9-carboxylic acid



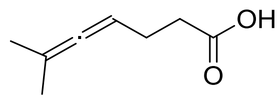
White solid (147-148 °C), yield 0.22 g (91%), R_f = 0.54 (1:4, EtOAc/hexanes).^{1}H NMR (500 MHz, $CDCl_3$) δ 11.3 (br. s, 1H, COOH), 7.28-7.25 (m, 4H), 7.09-7.06 (m, 4H), 4.43-4.40 (m, 1H), 2.95 (d, *J* = 7.5 Hz, 2H), 1.69-1.62 (m, 4H), and 1.43-1.31 (m, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 204.4, 150.9, 129.0, 127.6, 123.4, 120.7, 116.9, 104.1, 82.9, 50.3, 40.8, 31.1, 26.8, 26.7 and 26.1. IR (neat) ν 3078 (w), 2918 (m), 2858 (m), 2631 (w), 1960 (w), 1695 (s), and 1605 cm^{-1}. HRMS [ESI, $(C_{25}H_{26}O_3+Na)^+$] Calcd: 397.1780, Found: *m/z* 397.1788.

6-Methyl-2,2-diphenylhepta-4,5-dienoic acid



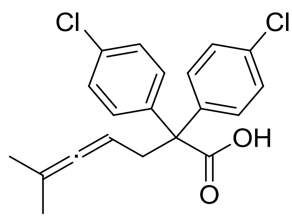
Analytical data is in agreement with literature data. [18]

6-Methylhepta-4,5-dienoic acid



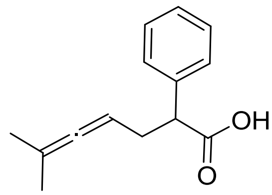
Analytical data is in agreement with literature.[10a]

2,2-bis(4-Chlorophenyl)-6-methylhepta-4,5-dienoic acid



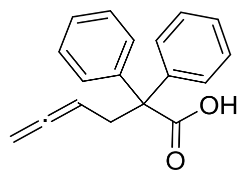
White solid (150-151 ^{o}C), yield 0.15 g (93%), R_f = 0.54 (1:4, EtOAc/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.3 (br. s, 1H, COOH), 7.09-7.01 (m, 8H), 4.59 (m, 1H), 2.79 (d, J = 7.5 Hz, 2H), 1.47 (s, 3H), and 1.46 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 203.8, 181.2, 141.2, 132.6, 130.6, 127.8, 94.7, 84.7, 60.4, 39.1, and 20.0. IR (neat) ν 3054 (br), 2977(m), 2908 (m), 2854 (w), 1961 (w), 1903(w) 1693 (s), 1482 (m) cm^{-1}. HRMS [ESI, $(C_{20}H_{18}Cl_2O_2+Na)^+$] Calcd: 383.0582, Found: *m/z* 383.0588.

6-Methyl-2-phenylhepta-4,5-dienoic acid



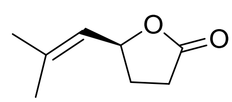
Viscous oil, yield 0.11 g (90%), R_f = 0.56 (1:4, EtOAc/hexanes). ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.3 (br. s, 1H, COOH), 7.31-7.25 (m, 5H), 4.97-4.92 (m, 1H), 3.67 (dd, J = 9.0, 6.5 Hz, 1H), 2.76-2.70 (m, 1H), 2.42-2.36 (m, 1H), 1.57 (d, J = 2.5 Hz, 3H), and 1.53 (d, J = 2.5 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 202.3, 178.8, 138.2, 128.6, 128.0, 127.4, 96.9, 86.0, 50.9, 32.5, and 204. HRMS [ESI, $(C_{14}H_{16}O_2+Na)^+$] Calcd: 239.1048, Found: *m/z* 239.1050.

2,2-Diphenylhexa-4,5-dienoic acid[18]



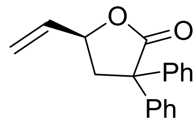
Analytical data are in agreement with literature data.

(*S*)-5-5(2-Methylprop-1-en-1-yl)dihydrofuran-2(3*H*)-one[18]



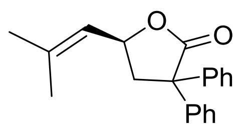
Viscous oil, yield (29.0 mg, 92%), R_f 0.42 (1:1 Et_2O/hexanes); 92% *ee*, t_{R1} = 56.92 min (minor), t_{R2} = 58.73 min (major). Chiral HPLC conditions: Chiralcel OD-H, 0.5 mL/min, hexanes/*i*-PrOH 99:1. $[\alpha]_D^{23}$ = +118.5 (c = 0.3, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.24 (d, J = 8.4 Hz, 1H), 5.21-5.16 (m, 1H), 2.58-2.48 (m, 2H), 2.40-2.32 (m, 1H), 1.98-1.88 (m, 1H), 1.77 (s, 3H), and 1.74 (s, 3H).

(*S*)-3,3-Diphenyl-5-vinyldihydrofuran-2(3*H*)-one[19]



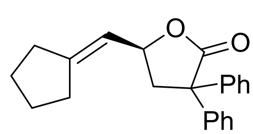
Viscous oil, yield (27.0 mg, 86%), R_f 0.48 (2:3 Et_2O/hexanes); 86% *ee*, t_{R1} = 7.36 min (major), t_{R2} = 8.90 min (minor). Chiral HPLC conditions: Chiralcel OD-H, 1.0 mL/min, hexanes/*i*-PrOH 100:5. $[\alpha]_D^{23.2} = -83.4$ (c = 0.5, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$) δ 7.42-7.19 (m, 10H), 5.92 (ddd, J = 17.2, 10.4, 6.4 Hz, 1H), 5.42 (d, J = 17.0 Hz, 1H), 5.30 (d, J = 10.5 Hz, 1H), 4.79-4.76 (1 H, m), 3.10 (dd, J = 13.0, 5.0 Hz, 1H), and 2.76 (dd, J = 13.0, 10.5 Hz, 1H).

(*S*)-5-(2-Methylprop-1-en-1-yl)-3,3-diphenyldihydrofuran-2(3H)-one[19]



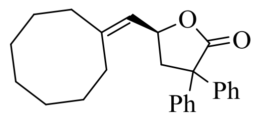
Viscous oil, yield (29.0 mg, 97%), R_f 0.44 (2:3 Et_2O/hexanes); 84% *ee*, t_{R1} = 24.36 min (minor), t_{R2} = 29.16 min (major). Chiral HPLC conditions: Chiralpack AD-H, 0.5 mL/min, hexanes/*i*-PrOH 100:5. $[\alpha]_D^{23.1} = -88.9$ (c = 0.5, THF). ^1H NMR (500 MHz, $CDCl_3$) δ 7.43-7.22 (m, 10H), 5.28-5.26 (m, 1H), 5.04 (ddd, J = 10.6, 8.4, 427 4.8 Hz, 1H), 3.06 (dd, J = 13.0, 5.0 Hz, 1H), 2.69 (dd, J = 13.0, 10.5 Hz, 1H), 1.78 (d, J = 1.5 Hz, 3H), 1.68 (d, J = 1.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 177.3, 142.3, 140.9, 139.9, 129.1, 128.5, 127.9, 127.8, 127.5, 127.3, 122.2, 74.1, 58.4, 44.4, 25.9, and 18.7.

(*S*)-5-(Cyclopentylidenemethyl)-3,3-diphenyldihydrofuran-2(3*H*)-one[18]



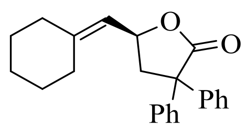
White solid (mp = 56-57 °C, reported[7] 52-55 °C), yield (26.0 mg, 89%), R_f 0.46 (2:3, Et_2O/hexanes); 89% *ee*, t_{R1} = 7.17 min (major), t_{R2} = 12.56 min (minor). Chiral HPLC conditions: Chiralpack AD-H, 1.0 mL/min, hexanes/*i*PrOH 100:5. $[\alpha]_D^{22.3} = -63.3$ (*c* = 0.3, THF). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41-7.22 (m, 10H), 5.39-5.35 (m, 1H), 4.94 (ddd, *J* = 10.5, 8.6, 5.2 Hz, 1H), 3.07 (dd, *J* = 13.0, 5.0 Hz, 1H), 2.69 (dd, *J* = 13.0, 10.5 Hz, 1H), 2.38-2.15 (m, 4H), 1.72-1.54 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.2, 152.5, 142.4, 139.9, 129.0, 128.4, 127.8, 127.8, 127.5, 127.2, 117.4, 75.7, 58.3, 44.2, 34.1, 29.3, 26.3, and 26.0.

(*S*)-5-Cyclohexylidenemethyl)-3,3-diphenyldihydrofuran-2(3*H*)-one



Viscous oil, yield (28.8 mg, 96%), R_f 0.47 (2:3, Et_2O/hexanes); 79% *ee*, t_{R1} = 6.08 min (minor), t_{R2} = 9.15 min (major). Chiral HPLC conditions: Chiralcel OD-H, 1.0 mL/min, hexanes/*i*PrOH 100:5. $[\alpha]_D^{23.8} = -62.2$ (*c* = 0.2, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43-7.25 (m, 10H), 5.33 (d, *J* = 8.5 Hz, 1H), 5.14-5.09 (m, 1H), 3.11 (dd, *J* = 13.5, 5.0 Hz, 1H), 2.71 (dd, *J* = 13.5, 10.5 Hz, 1H), 2.27-2.23 (m, 4H), 1.74-1.67 (m, 3H), and 1.57-1.49 (m, 7H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 177.5, 151.2, 142.9, 140.3, 129.3, 128.6, 128.1, 128.1, 127.7, 127.5, 122.7, 74.3, 58.6, 44.5, 37.8, 29.8, 28.5, 27.6, 26.6, 26.4, and 26.2. IR (neat) ν = 3059 (w), 2922 (m), 2851 (m), 1978 (w), and 1760 (s) cm^{-1}. HRMS [ESI, $(C_{25}H_{28}O_2+Na)^+$] Calcd: 383.1987, Found: *m/z* 383.1989.

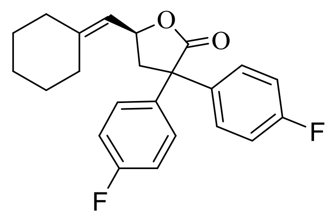
(*S*)-5-(Cyclooctylidenemethyl)-3,3-diphenyldihydrofuran-2(3*H*)-one[18]



Yield (28.0 mg, 92%), R_f 0.47 (2:3, Et_2O/hexanes); 86% *ee*, t_{R1} = 6.18 min (major), t_{R2} = 12.27 min (minor). Chiral HPLC conditions: Chiralcel OD-H, 1.0 mL/min, hexanes/*i*-PrOH 100:5. $[\alpha]_D^{21.8}$ =

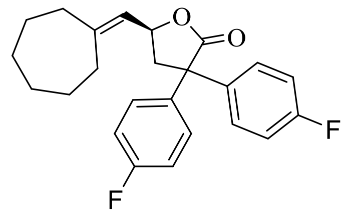
−98.7 (c = 0.3, THF). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.36 (m, 4H), 7.34-7.28 (m, 5H), 5.22 (d, J = 8.4 Hz, 1H), 5.12-5.06 (m, 1H), 3.04 (dd, J = 12.0, 4.8 Hz, 1H), 2.70 (dd, J = 13.2, 10.4 Hz, 1H), 2.20-2.07 (m, 4H), 157.1.53 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.4, 148.7, 142.3, 139.9, 129.1, 128.5, 127.9, 127.8, 127.5, 127.3, 118.9, 73.4, 58.4, 44.7, 37.1, 29.7, 28.3, 27.9, and 26.6.

(*S*)-5-(Cyclohexylidenemethyl)-3,3-bis(4-fluorophenyl)dihydrofuran-2(3H)-one



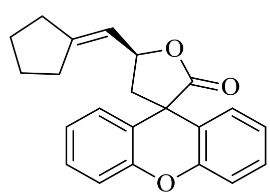
Viscous oil, yield (27 mg, 91%), R_f 0.49 (2:3, Et_2O/hexanes); 81% *ee*, t_{R1} = 12.00 min (major), t_{R2} = 17.99 min (minor). Chiral HPLC conditions: Chiralpack AD-H, 1.0 mL/min, hexanes/*i*-PrOH 100:5. $[\alpha]_D^{20.9}$ = −76.8 (c = 0.2, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37-7.34 (m, 2H), 7.28-7.24 (m, 2H), 7.09-7.05 (m, 2H), 7.01-6.97 (m, 2H), 5.20 (d, J = 8.5 Hz, 1H), 5.10-5.05 (m, 1H), 2.98 (dd, J = 13.0, 5.0 Hz, 1H), 2.64 (dd, J = 13.0, 10.5 Hz, 1H), 2.22-2.06 (m, 4H), and 1.58-1.50 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.1, 162.3 (d, $^1J_{(C,F)}$ = 249 Hz), 162.1 (d, $^1J_{(C,F)}$ = 249 Hz), 149.1, 137.9, 135.6, 129.5 (d, $^3J_{(C,F)}$ = 8.3 Hz), 129.2 (d, $^3J_{(C,F)}$ = 8.3 Hz), 118.6, 116.1 (d, $^2J_{(C,F)}$ = 21.4 Hz), 115.4 (d, $^2J_{(C,F)}$ = 21.4 Hz), 103.9, 57.3, 44.8, 37.1, 29.7, 28.3, 27.9, and 26.5. IR (neat) ν 3078 (w), 3039 (w), 2930 (m), 2854 (m), 1892 (w), 1759 (s), and 1605 (m) cm^{-1}. HRMS [ESI, $(C_{25}H_{20}O_2+Na)^+$] Calcd: 391.1486, Found: m/z 391.1500.

(*S*)-5-(Cycloheptylidenemethyl)-3,3-bis(4-fluorophenyl)dihydrofuran-2(3H)-one



Viscous oil, yield (29 mg, 97%), R_f 0.52 (2:3, Et_2O/hexanes); 82% *ee*, t_{R1} = 11.80 min (minor), t_{R2} = 17.02 min (major). Chiral HPLC conditions: Chiralpack AD-H, 1.0 mL/min, hexanes/*i*PrOH 100:5. $[\alpha]_D^{22.5} = -70.2$ (c = 0.3, $CHCl_3$). ^1H NMR (600 MHz, $CDCl_3$) δ 7.35 (dd, J = 9.0, 5.4 Hz, 2H), 7.26 (dd, J = 9.0, 5.4 Hz, 2H), 7.07 (dd, J = 9.0, 8.4 Hz, 2H), 6.99 (dd, J = 9.0, 8.4 Hz, 2H), 5.26 (d, J = 8.4 Hz, 1H), 5.06-5.02 (m, 1H), 3.01 (dd, J = 13.2, 4.8 Hz, 1H), 2.71 (dd, J = 13.2, 10.2 Hz, 1H), 2.34-2.21 (m, 4H), and 1.63-1.47 (m, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 177.1, 162.3 (d, $^1J_{(C,F)}$ = 248 Hz), 162.0 (d, $^1J_{(C,F)}$ = 248 Hz), 150.8, 138.0 (d, $^4J_{(C,F)}$ = 3.3 Hz), 135.6 (d, $^4J_{(C,F)}$ = 3.3 Hz), 129.5 (d, $^3J_{(C,F)}$ = 8.3 Hz), 129.2 (d, $^3J_{(C,F)}$ = 8.3 Hz), 121.9, 116.1 (d, $^2J_{(C,F)}$ = 21.6 Hz), 115.4 (d, $^2J_{(C,F)}$ = 21.6 Hz), 73.9, 57.3, 44.6, 37.9, 30.6, 29.7, 29.1, 28.7, and 27.3. IR (neat) ν = 3084 (w), 3052 (w), 2929 (m), 2851 (m), 1882 (w), 1749 (s), and 1605 (m) cm^{-1}. HRMS [ESI, $(C_{24}H_{24}F_2O_2)^+$] Calcd: 382.1744, Found: *m/z* 382.1752.

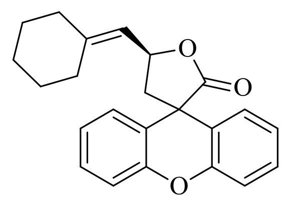
(*S*)-5-(Cyclopentylidenemethyl)-4,5-dihydro-2*H*-spiro[furan-3,9'-xanthen]-2'-one



White solid (mp = 150-151 °C), yield 28 mg (97%), R_f = 0.42 (2:3, Et_2O/hexanes)); 96% *ee*, t_{R1} = 11.29 min (major), t_{R2} = 15.30 min (minor). Chiral HPLC conditions: Chiralcel OD-H, 1.0 mL/min, hexanes/*i*-PrOH 100:3. $[\alpha]_D^{23.4} = -117.8$ (c = 0.2, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$) δ 7.35-7.26 (m, 3H), 7.23 (dd, J = 3.2, 1.2 Hz, 1H), 7.21-7.20 (m, 1H), 7.18-7.12 (m, 3H), 5.44-5.40 (m, 1H), 5.32-5.26 (m, 1H), 2.74 (dd, J = 13.6, 6.0 Hz, 1H), 2.48-2.19 (m, 4H), 2.26 (dd, J = 13.6, 10.0 Hz, 1H), and 1.78-

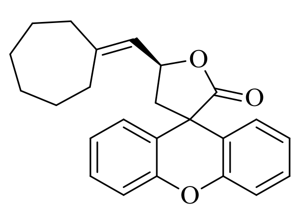
1.59 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.3, 152.9, 151.7, 151.0, 129.3, 129.0, 127.4, 125.9, 124.3, 124.1, 123.7, 122.9, 117.6, 117.6, 116.7, 76.2, 50.2, 34.2, 29.4, 26.3, and 26.0. IR (neat) ν 3055 (w), 2969 (m), 2922 (w), 1913 (w), 1765 (s), 1599 (m) cm^{-1}. HRMS [ESI, $(C_{22}H_{20}O_3+Na)^+$] Calcd: 355.1310, Found: *m/z* 355.1310.

(*S*)-5-(Cyclohexylidenemethyl)-4,5-dihydro-2*H*-spiro[furan-3,9'-xanthen]-2'-one



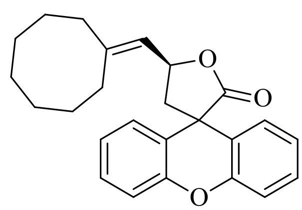
Viscous oil, yield 28 mg (92%), R_f = 0.43 (2:3, Et_2O/hexanes), 84% *ee*, t_{R1} = 9.00 min (major), t_{R2} = 11.23 min (minor). Chiral HPLC conditions: Chiralcel OD-H, 1.0 mL/min, hexanes/*i*-PrOH 100:5. $[\alpha]_D^{23.7}$ = −67.9 (*c* = 0.2, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$) δ 7.35-7.12 (m, 8H), 5.44 (ddd, *J* = 10.0, 8.4, 6.0 Hz, 1H), 5.25 (d, *J* = 8.4 Hz, 1H), 2.74 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.31-2.12 (m, 4H), 2.26 (dd, *J* = 13.6, 10.0 Hz, 1H), and 1.64-1.48 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.3, 151.7, 151.0, 148.8, 129.3, 129.0, 127.5, 125.9, 124.3, 124.1, 123.7, 122.9, 119.0, 117.6, 116.7, 73.8, 50.8, 50.3, 37.1, 29.8, 28.4, 27.9, and 26.6. IR (neat): ν 2955 (w), 2769 (w), 1909 (w), 1751 (s), 1685 (w), 1616 (m) cm^{-1}. HRMS [ESI, $(C_{23}H_{22}O_3+Na)^+$] Calcd: 369.1467, Found: *m/z* 369.1477.

(*S*)-5-(Cycloheptylidenemethyl)-4,5-dihydro-2*H*-spiro[furan-3,9'-xanthen]-2'-one



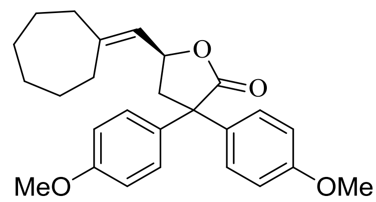
Viscous oil, yield 29 mg (93%), R_f = 0.44 (2:3, Et_2O/hexanes), 87% *ee*, t_{R1} = 8.90 min (major), t_{R2} = 11.32 min (minor). Chiral HPLC conditions: Chiralcel OD-H, 1.0 mL/min, hexanes/*i*-PrOH 100:5. $[\alpha]_D^{23.7}$ = −96.9 (*c* = 0.1, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$) δ 7.36-7.13 (m, 8H), 5.41 (ddd, *J* = 10.0, 9.0, 6.0 Hz, 1H), 5.33 (d, *J* = 9.0 Hz, 1H), 2.75 (dd, *J* = 13.5, 6.0 Hz, 1H), 2.45-2.26 (m, 4H), 2.26 (dd, *J* = 13.5, 10.0 Hz, 1H), and 1.70-1.47 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.3, 151.7, 151.0, 150.6, 129.3, 129.0, 127.5, 125.9, 124.3, 124.1, 123.7, 122.9, 122.4, 117.6, 116.7, 74.3, 50.6, 50.2, 37.9, 30.7, 29.7, 29.1, 28.7, and 27.3. IR (neat): ν = 3039 (w), 2923 (w), 2850 (w), 1882 (w), 1758 (s), and 1607 (m) cm^{-1}. HRMS [ESI, $(C_{24}H_{24}O_3+Na)^+$] Calcd: 383.1623, Found: *m/z* 383.1603.

(*S*)-5-(Cyclooctylidenemethyl)-4,5-dihydro-2*H*-spiro[furan-3,9'-xanthen]-2'-one



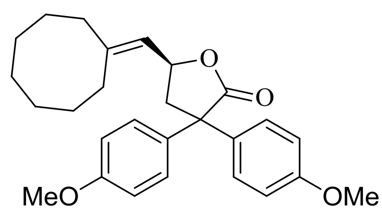
Viscous oil, yield 27.5 mg (92%), R_f = 0.45 (2:3, Et_2O/hexanes), 90% *ee*, t_{R1} = 8.20 min (major), t_{R2} = 9.65 min (minor). Chiral HPLC conditions: Chiralcel OD-H, 1.0 mL/min, hexanes/*i*-PrOH 100:5. $[\alpha]_D^{23.7}$ = −158.8 (*c* = 0.5, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$) δ 7.36-7.14 (m, 8H), 5.48-5.43 (m, 1H), 5.35 (d, *J* = 9.0 Hz, 1H), 2.75 (dd, *J* = 13.5, 6.5 Hz, 1H), 2.32-2.24 (m, 5H), and 1.79-1.43 (m, 10H) ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.4, 151.7, 151.2, 150.9, 129.3, 129.0, 127.5, 125.8, 124.3, 124.1, 123.7, 122.9, 122.4, 117.6, 116.7, 74.4, 50.5, 50.2,l 37.6, 29.7, 28.2, 27.3, 26.3, 26.1, and 25.8. IR (neat): ν 3039 (w), 2923 (w), 2854 (w), 1909 (w), 1776 (s), 1657 (w), 1600 (m) cm^{-1}. HRMS [ESI, $(C_{25}H_{26}O_3+Na)^+$] Calcd: 397.1780, Found: *m/z* 397.1765.

(*S*)-5-(Cycloheptylidenemethyl)-3,3-bis(4-methoxyphenyl)dihydrofuran-2(3*H*)-one



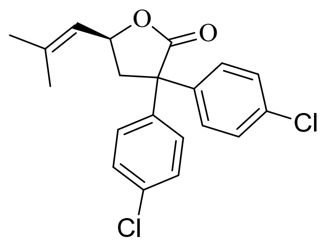
Viscous oil, yield 29.0 mg (97%), R_f = 0.42 (1:1, Et_2O/hexanes), 81% *ee*, t_{R1} = 13.90 min (major), t_{R2} = 17.87 min (minor). Chiral HPLC conditions: Chiralcel OD-H, 1.0 mL/min, hexanes/*i*PrOH 100:5. $[\alpha]_D^{23.8}$ = −78.9 (*c* = 0.35, THF). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.31 (d, *J* = 9.0 Hz, 2H), 7.19 (d, *J* = 9.0 Hz, 2H), 6.90 (d, *J* = 9.0 Hz, 2H), 6.82 (d, *J* = 9.0 Hz, 2H), 5.27 (d, *J* = 8.5 Hz, H), 5.06-5.01 (m, 1H), 3.81 (s, 3H), 3.77 (s, 3H), 2.99 (dd, *J* = 13.0, 5.0 Hz, 1H), 2.61 (dd, *J* = 13.0, 10.5 Hz, 1H), 2.34-2.20 (m, 4H), and 1.64-1.43 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.0, 159.0, 158.6, 150.2, 134.9, 131.9, 128.9, 128.6, 122.4, 114.4, 113.8, 105.1, 73.8, 57.2, 55.4, 44.7, 37.9, 30.5, 29.7, 29.1, 28.7, and 27.3. IR (neat) ν 3078 (w), 3039 (w), 2930 (m), 2854 (m), 1892 (w), 1759 (s), and 1605 (m) cm^{-1}. HRMS [ESI, $(C_{26}H_{30}O_4+Na)^+$] Calcd: 429.2042, Found: *m/z* 429.2036.

(*S*)-5-(Cyclooctylidenemethyl)-3,3-bis(4-methoxyphenyl)dihydrofuran-2(3*H*)-one



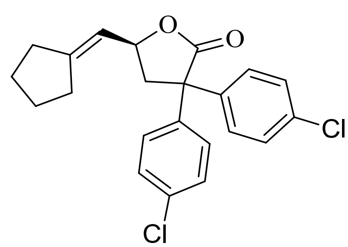
Viscous oil, yield 29.0 mg (97%), R_f = 0.42 (1:1, Et_2O/hexanes), 72% *ee*, t_{R1} = 6.36 min (major), t_{R2} = 12.38 min (minor). Chiral HPLC conditions: Chiralcel OD, 1.0 mL/min, hexanes/*i*-PrOH 100:5. $[\alpha]_D^{22.2}$ = −57.9 (*c* = 0.3, THF). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.32 (d, *J* = 9.0 Hz, 2H), 7.19 (d, *J* = 9.0 Hz, 2H), 6.90 (d, *J* = 9.0 Hz, 2H), 6.82 (d, *J* = 9.0 Hz, 2H), 5.29 (d, *J* = 9.0 Hz, H), 5.09-5.05 (m, 1H), 3.82 (s, 3H), 3.77 (s, 3H), 3.00 (dd, *J* = 13.2, 4.8 Hz, 1H), 2.61 (dd, *J* = 13.2, 10.8 Hz, 1H), 2.36-2.20 (m, 4H), and 1.67-1.45 (m, 10H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 178.0, 159.1, 158.6, 150.7, 135.0, 131.9, 128.9, 128.6, 122.5, 114.4, 113.8, 73.9, 57.1, 55.4, 44.8, 37.6, 29.6, 28.3, 27.3, 26.3, 26.0 and 25.8. IR (neat): ν = 3000 (w), 2923 (m), 2850 (m), 2121 (w), and 1759 (s) cm^{-1}. HRMS [ESI, $(C_{27}H_{32}O_4+Na)^+$] Calcd: 443.2198, Found: *m/z* 443.2184.

(*S*)-3,3-bis(4-Chlorophenyl)-5-(2-methylprop-1-en-1-yl)dihydrofuran-2(3*H*)-one



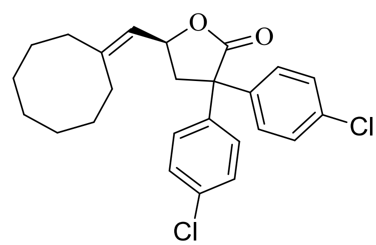
Viscous oil, yield 28.0 mg (95%), R_f = 0.45 (3:7, Et_2O/hexanes), 85% *ee*, t_{R1} = 12.76 min (minor), t_{R2} = 15.88 min (major). Chiral HPLC conditions: Chiralpack AD-H, 1.0 mL/min, hexanes/*i*-PrOH 100:5. $[\alpha]_D^{23.8}$ = −135.8 (*c* = 0.2, $CHCl_3$). ^1H NMR (600 MHz, $CDCl_3$) δ 7.36-7.21 (m, 8H), 5.24-5.23 (m, 1H), 5.02-4.97 (m, 1H), 2.99-2.95 (m, 1H), 2.64-2.60 (m, 1H), 1.77 (d, *J* = 2.4 Hz, 3H), and 1.68 (d, *J* = 2.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ = 176.5, 141.6, 140.3, 138.1, 134.2, 133.6, 129.4, 129.2, 128.8, 128.8, 121.7, 74.0, 57.5, 44.1, 26.0, and 18.7. IR (neat): ν 2979 (w), 2930 (w), 1911 (w), 1758 (s), 1649 (w) cm^{-1}. HRMS [ESI, $(C_{20}H_{18}Cl_2O_2)^+$] Calcd: 360.0684, Found: *m/z* 360.0673.

(*S*)-3,3-bis(4-Chlorophenyl)-5-(cyclopentylidenemethyl)dihydrofuran-2(3*H*)-one



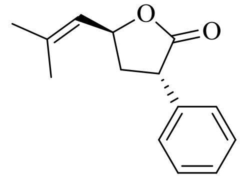
Solid (mp = 103-104 °C), yield 28.0 mg (93%), R_f = 0.46 (3:7, Et_2O/hexanes), 85% *ee*, t_{R1} = 12.76 min (minor), t_{R2} = 15.88 min (major). Chiral HPLC conditions: Chiralpack AD-H, 1.0 mL/min, hexanes/*i*-PrOH 100:5. $[\alpha]_D^{22.1}$ = −81.7 (*c* = 0.3, THF). ^1H NMR (500 MHz, $CDCl_3$) δ 7.37-7.22 (m, 8H), 5.37-5.34 (m, 1H), 4.94-4.89 (m, 1H), 3.00 (dd, J = 13.0, 5.2 Hz, 1H), 2.68 (dd, J = 13.2, 10.4 Hz, 1H), 2.39-2.26 (m, 3H), 2.24- 2.15 (m, 1H), and 1.72-1.54 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 176.6, 153.2, 140.4, 138.2, 134.2, 133.6, 129.4, 129.2, 128.8, 128.8, 117.0, 75.8, 57.5, 43.9, 34.2, 29.4, 26.3, and 26.0. IR (neat) ν = 2977 (w), 2922 (w), 1909 (w), 1752 (s), 1647 (w) cm^{-1}. HRMS [ESI, $(C_{22}H_{20}Cl_2O_2+Na)^+$] Calcd: 409.0738, Found: *m/z* 409.0735.

(*S*)-3,3-bis(4-Chlorophenyl)-5-(cyclooctylidenemethyl)dihydrofuran-2(3*H*)-one



Viscous oil, yield 29.0 mg (97%), R_f = 0.47 (3:7, Et_2O/hexanes), 87% *ee*, t_{R1} = 21.03 min (minor), t_{R2} = 22.74 min (major). Chiral HPLC conditions: Chiralcel OD-H, 0.5 mL/min, hexanes/*i*-PrOH 100:5. $[\alpha]_D^{23.2}$ = −72.3 (c = 0.3, THF). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37-7.22 (m, 8H), 5.27 (d, J = 9.0 Hz, 1H), 5.09-5.05 (m, 1H), 3.00 (dd, J = 13.0, 5.0 Hz, 1H), 2.63 (dd, J = 13.0, 10.5 Hz, 1H), 2.26-2.20 (m, 4H), and 1.67-1.37 (m, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.7, 151.6, 140.5, 138.1, 134.2, 133.6, 129.4, 129.2, 128.8, 128.8, 121.8, 74.0, 57.4, 44.2, 37.6, 29.6, 28.3, 27.3, 26.3, 26.0, and 25.8. IR (neat) ν 3065 (w), 2922 (m), 2851 (m), 1897 (w), and 1760 (s) cm^{-1}. HRMS [ESI, $(C_{25}H_{26}Cl_2O_2+Na)^+$] Calcd: 451.1208, Found: *m/z* 451.1210.

(*3S,5S*)-5-(2-Methylprop-1-en-1-yl)-3-phenyldihydrofuran-2(3*H*)-one



Viscous oil, yield 14.0 mg (48%), R_f = 0.38 (3:7, Et_2O/hexanes), 90% *ee*, t_{R1} = 17.76 min (major), t_{R2} = 19.60 min (minor). Chiral HPLC conditions: Chiralpack AD-H, 1.0 mL/min, hexanes/*i*-PrOH 100:5. $[\alpha]_D^{22.5}$ = 76.4 (*c* = 0.15, THF). ^1H NMR (500 MHz, $CDCl_3$) δ 7.38-7.35 (m, 2H), 7.31-7.28 (m, 3H), 5.30-5.28 (m, 1H), 5.23-5.18 (m, 1H), 3.89 (dd, *J* = 13.0, 8.5 Hz, 1H), 2.79-2.74 (m, 1H), 2.18-2.11 (m, 1H), 1.81 (d, *J* = 1.2 Hz, 3H), and 1.78 (d, *J* = 1.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.9, 140.8, 136.6, 129.0, 128.3, 127.7, 122.6, 75.4, 47.6, 39.0, 25.6, and 18.7. IR (neat) ν 3057 (w), 2983 (w), 2929 (m), 2854 (m), 1972 (w), and 1707 (s) cm^{-1}. HRMS [ESI, $(C_{14}H_{16}O_2+Na)^+$] Calcd: 239.1048, Found: *m/z* 239.1061.

References

[1] B. H. Lipshutz, S. Ghorai, A. R. Abela, R. Moser, T. Nishikata, C. Duplais, A. Krasovskiy, R. D. Gaston, R. C. Gadwood, *J. Org. Chem.* **2011**, *76*, 4379-4391.

[2] M. P. Muñoz, J. Adrio, J. C. Carretero, A. M. Echavarren, *Organometallics* **2005**, *24*, 1293-1300.

[3] A. D. Melhado, M. Luparia, F. D. Toste, *J. Am. Chem. Soc.* **2007**, *129*, 12638-12639.

[4] I. Alonso, B. Trillo, F. López, S. Montserrat, G. Ujaque, L. Castedo, A. Lledós, J. L. Mascareñas, *J. Am. Chem. Soc.* **2009**, *131*, 13020-13030.

[5] S. Handa, L. M. Slaughter, *Angew. Chem., Int. Ed.,* **2012**, *124*, 2966-2969.

[6] C.-M. Chao, E. Genin, P. Y. Toullec, J.-P. Genet, V. Michelet, *J. Organomet. Chem.* **2009**, *694*, 538-545.

[7] A. S. K. Hashmi, M. Hamzić, F. Rominger, J. W. Bats, *Chem. – Eur. J.* **2009**, *15*, 13318-13322.

[8] F. Kleinbeck, F. D. Toste, *J. Am. Chem. Soc.* **2009**, *131*, 9178-9179.

[9] S. G. Sethofer, T. Mayer, F. D. Toste, *J. Am. Chem. Soc.* **2010**, *132*, 8276-8277.

[10] a) G. L. Hamilton, E. J. Kang, M. Mba, F. D. Toste, *Science* **2007**, *317*, 496-499; b) T. Akiyama, H. Morita, P. Bachu, K. Mori, M. Yamanaka, T. Hirata, *Tetrahedron* **2009**, *65*, 4950-4956; c) I. Coric, B. List, *Nature* **2012**, *483*, 315-319; d) J. Guin, G. Varseev, B. List, *J. Am. Chem. Soc.* **2013**, *135*, 2100-2103.

[11] a) S. Handa, "Design and synthesis of novel ligands for tuning of selectivity and reaction pathway in gold catalysis", Ph.D Dissertation, Oklahoma State University, Stillwater, OK **2013**. b) Y.-M. Zhao, Y. Tam, Y.-J. Wang, Z. Li, J. Sun, *Org. Lett.* **2012**, *14*, 1398-1401.

[12] B. M. Trost, J. R. Corte, M. S. Gudiksen, *Angew. Chem., Int. Ed.* **1999**, *38*, 3662-3664.

[13] S. H. Sim, H.-J. Park, S. I. Lee, Y. K. Chung, *Org. Lett.* **2008**, *10*, 433-436.

[14] J. L. Arbour, H. S. Rzepa, A. J. P. White, K. K. Hii, *Chem. Commun.* **2009**, 7125-7127.

[15] B. Trillo, F. Lopez, M. Gulias, L. Castedo, J. L. Mascarenas, *Angew. Chem., Int. Ed.* **2008**, *47*, 951-954.

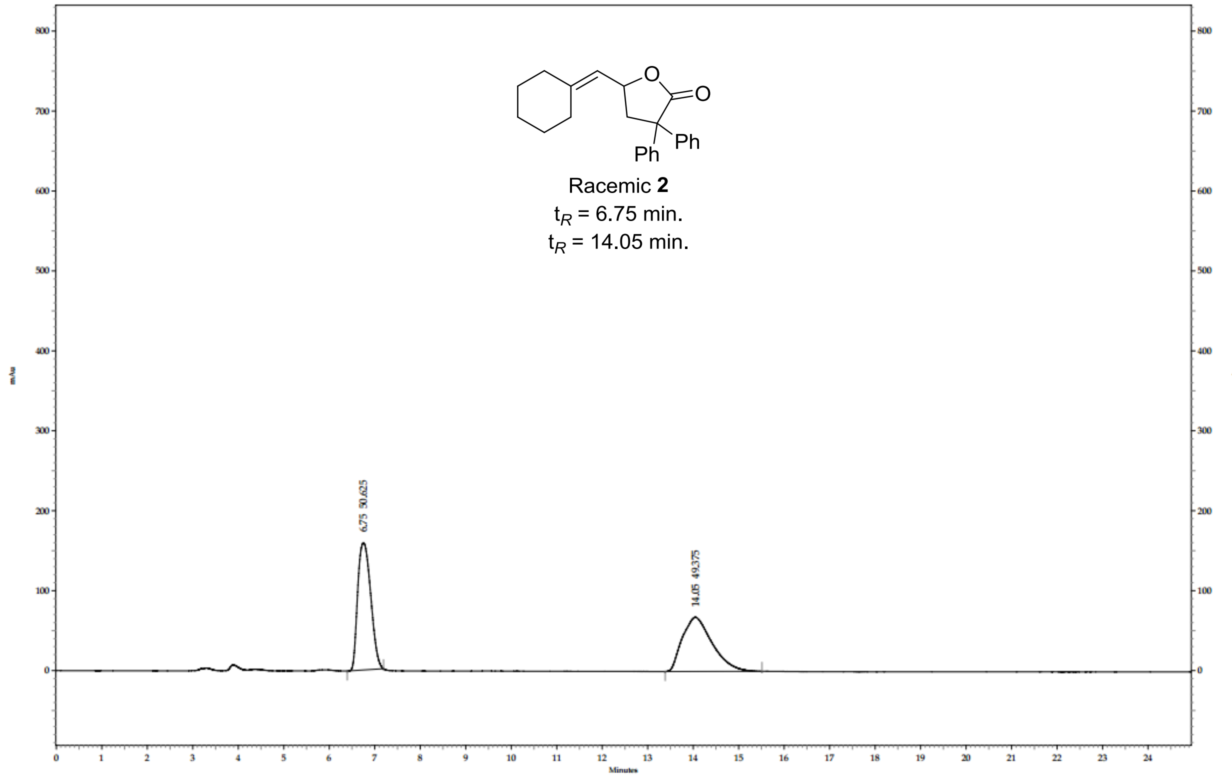
[16] J. Loefstedt, J. Franzen, J.-E. Backvall, *J. Org. Chem.* **2001**, *66*, 8015-8025.

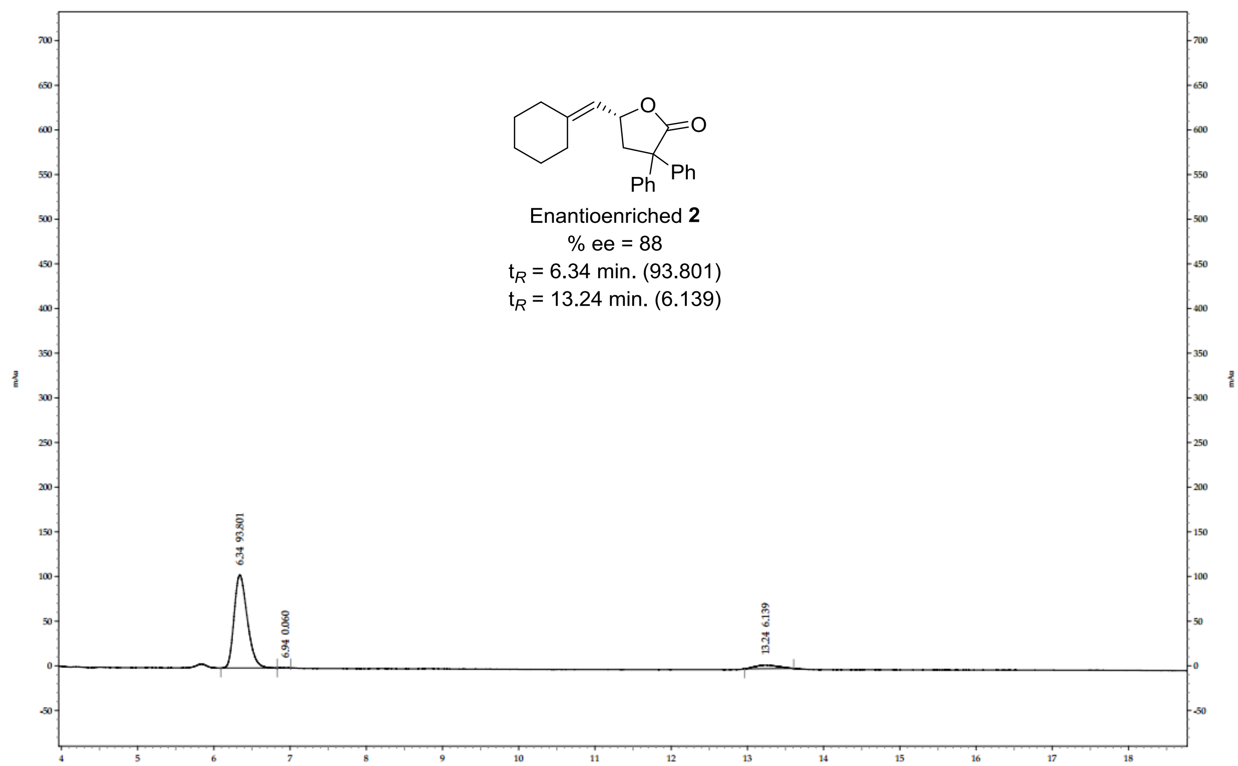
[17] M.-H. Lin, W.-S. Tsai, L.-Z. Lin, S.-F. Hung, T.-H. Chuang, Y.-J. Su, *J. Org. Chem.* **2011**, *76*, 8518-8523.

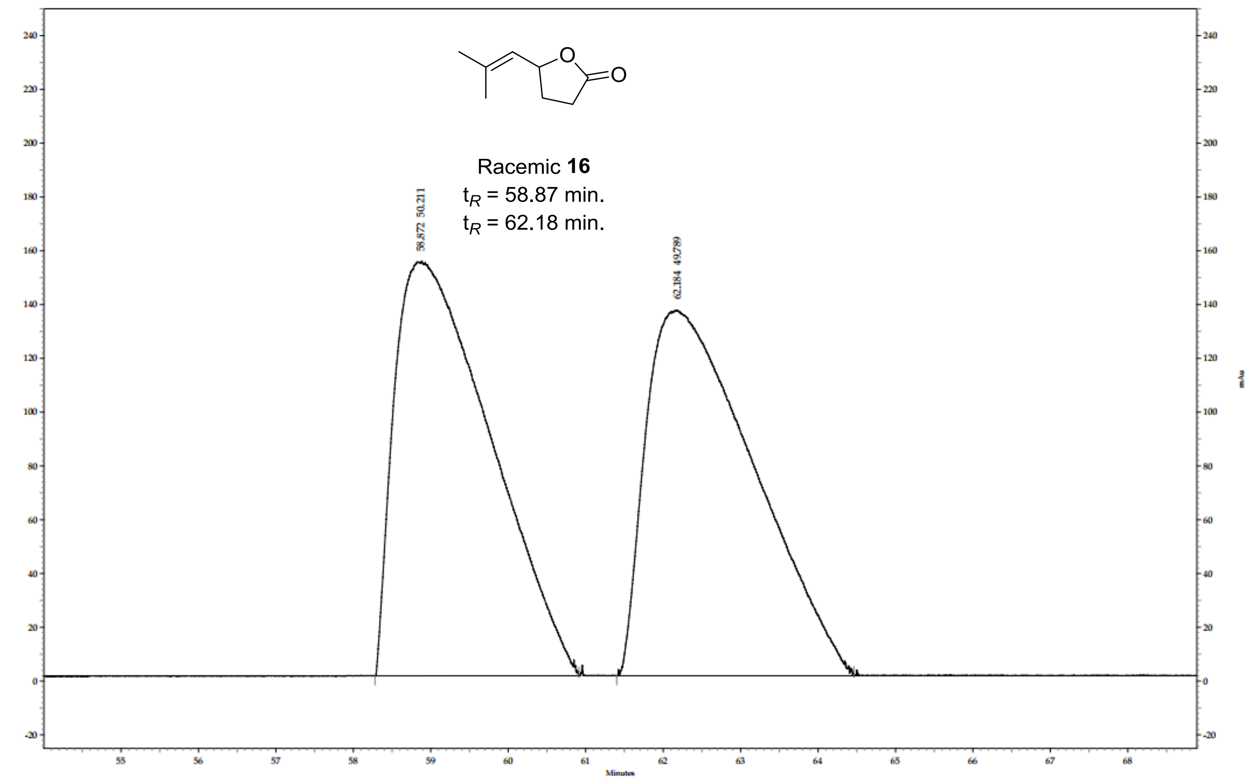
[18] J. L. Arbour, H. S. Rzepa, J. Contreras-García, L. A. Adrio, E. M. Barreiro, K. K. Hii, *Chem. – Eur. J.* **2012**, *18*, 11317-11324.

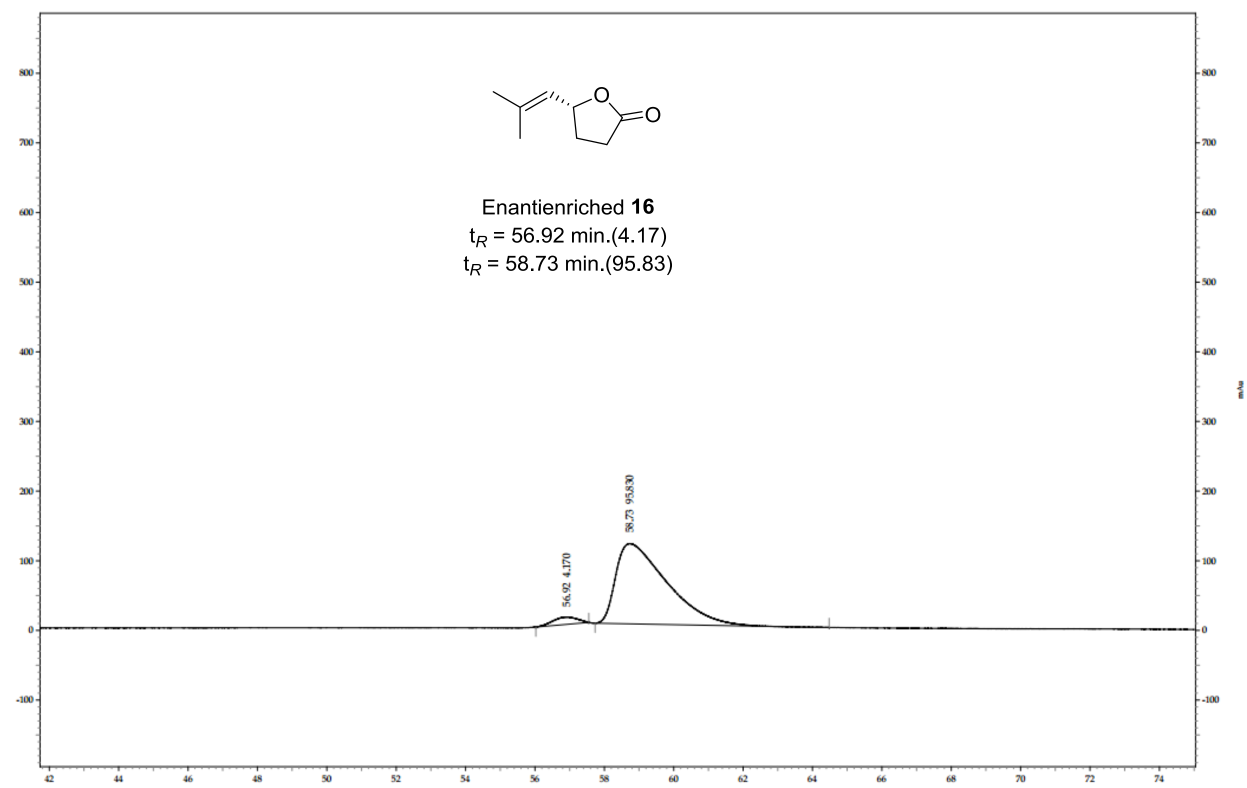
[19] K. Takenaka, M. Akita, Y. Tanigaki, S. Takizawa, H. Sasai, *Org. Lett.* **2011**, *13*, 3506-3509.

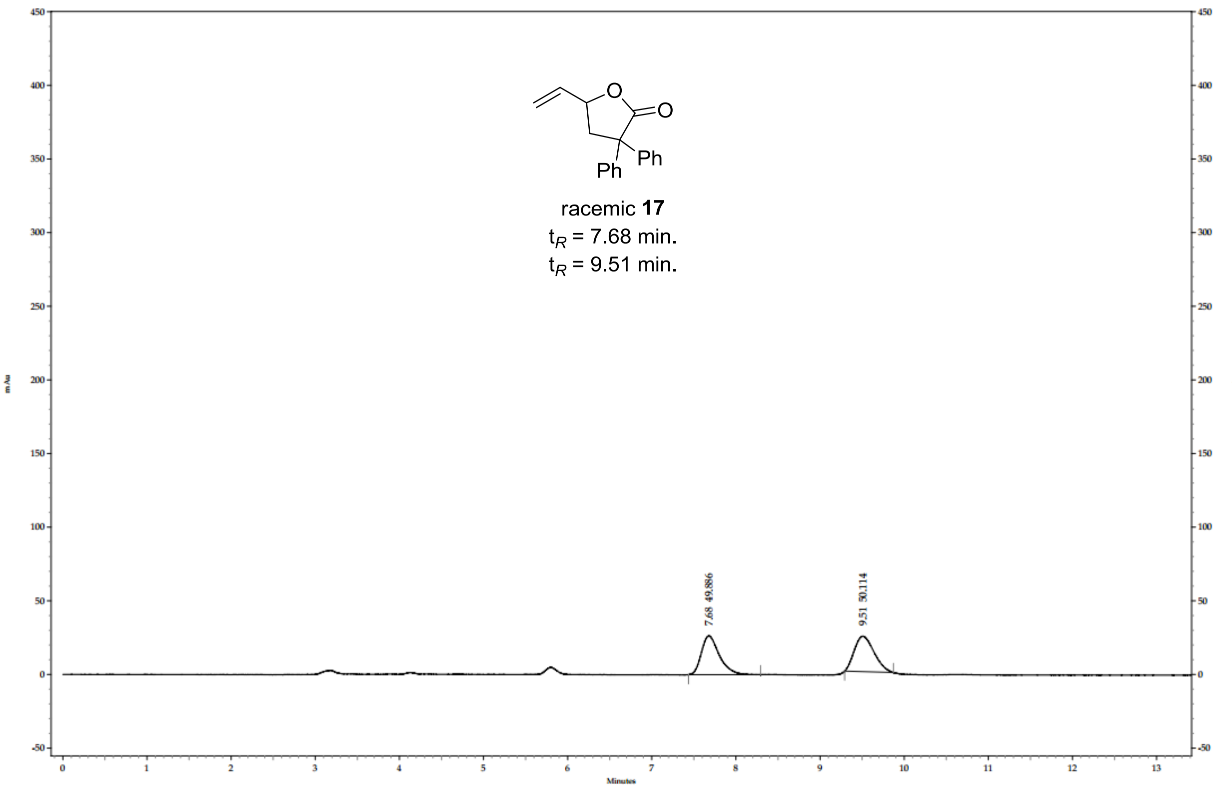
PART 17: HPLC CHROMATOGRAMS



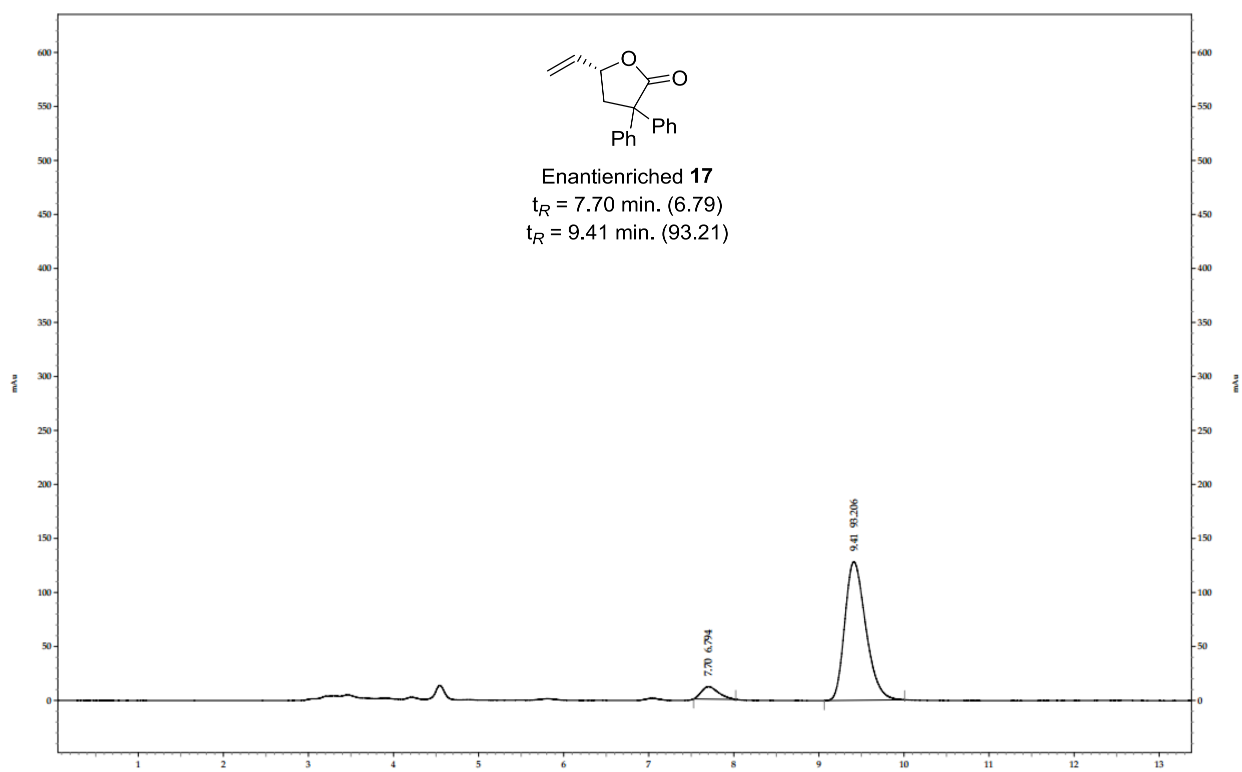



Racemic 16
t_R = 58.87 min.
t_R = 62.18 min.
58.872 50.211
62.184 49.789
Minutes
mAu

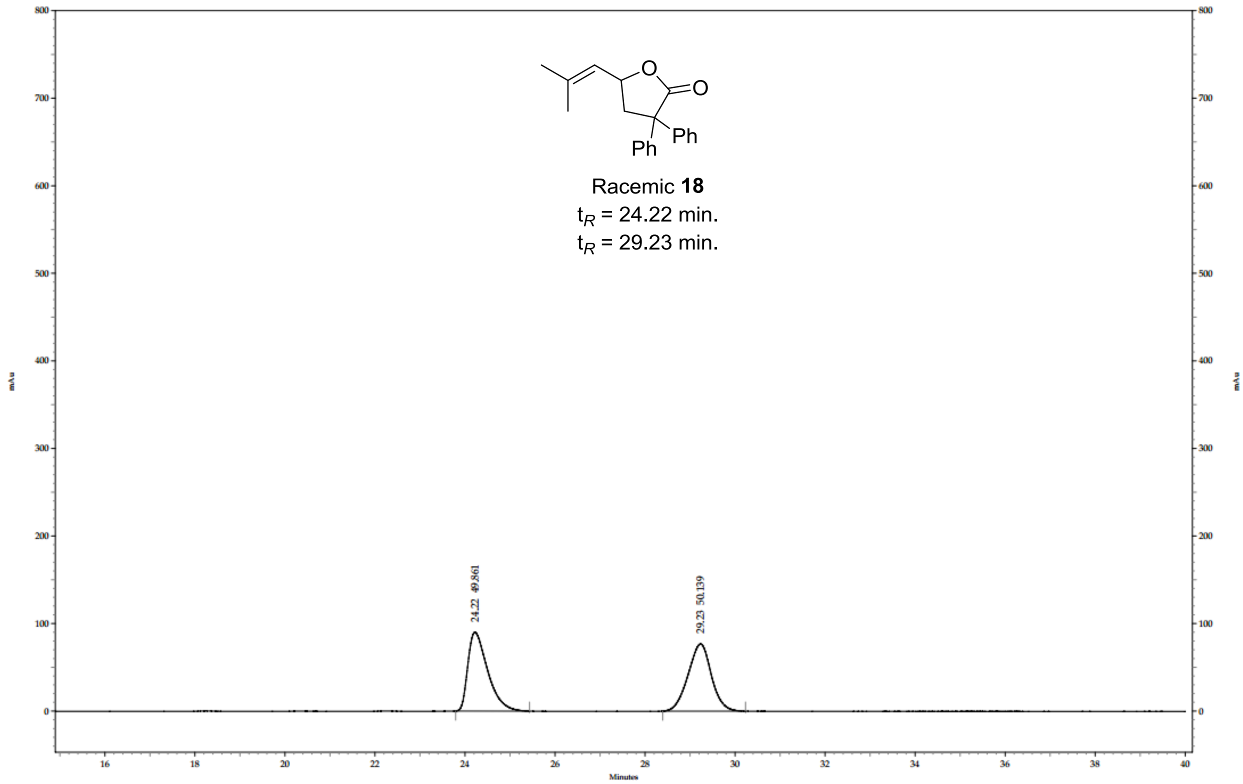

Enantienriched 16
t_R = 56.92 min.(4.17)
t_R = 58.73 min.(95.83)
56.92 4.170
58.73 95.830
Minutes
mAu

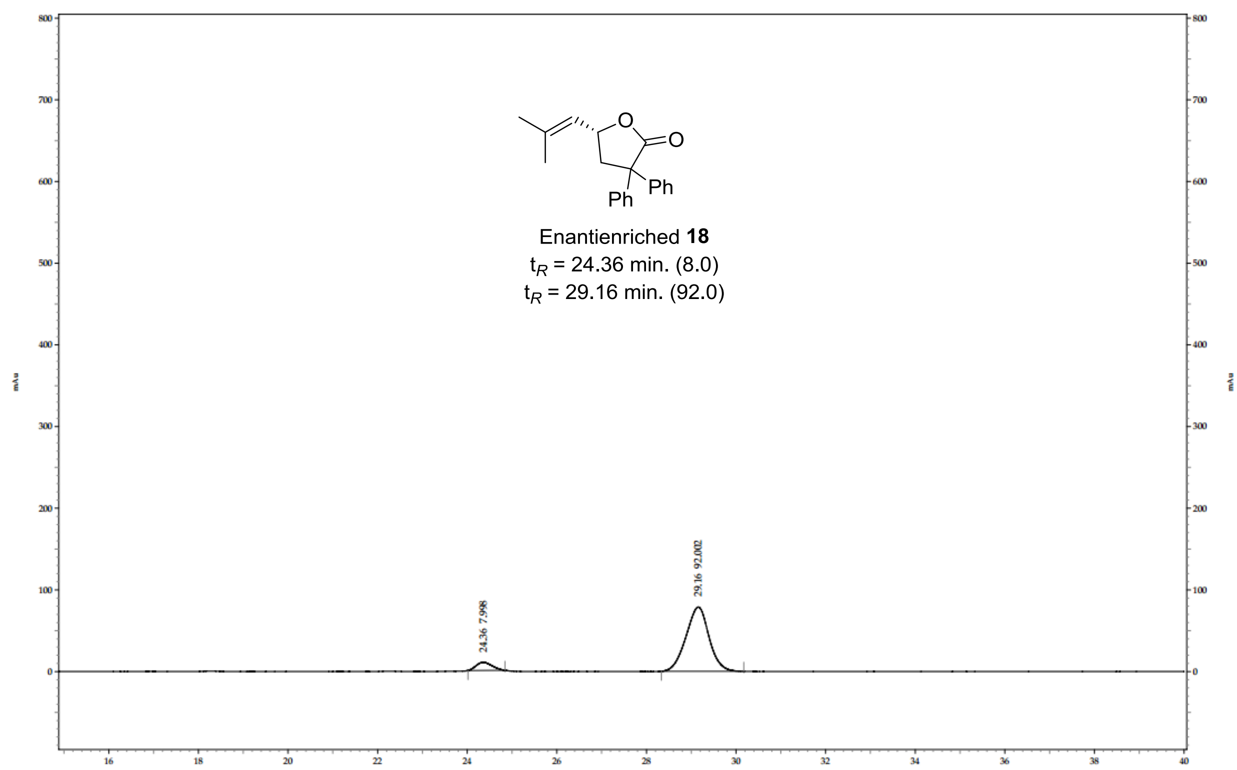


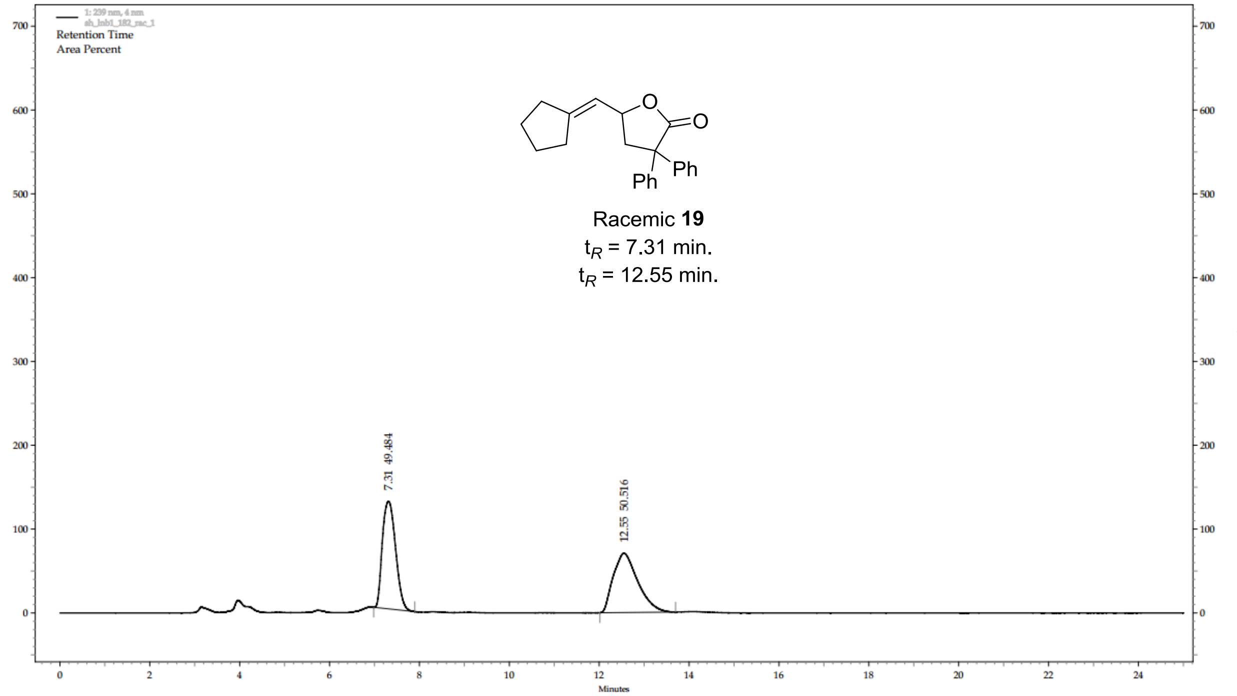
Ph
Ph
racemic **17**
t_R = 7.68 min.
t_R = 9.51 min.
7.68 49.886
9.51 50.114
mAu
Minutes

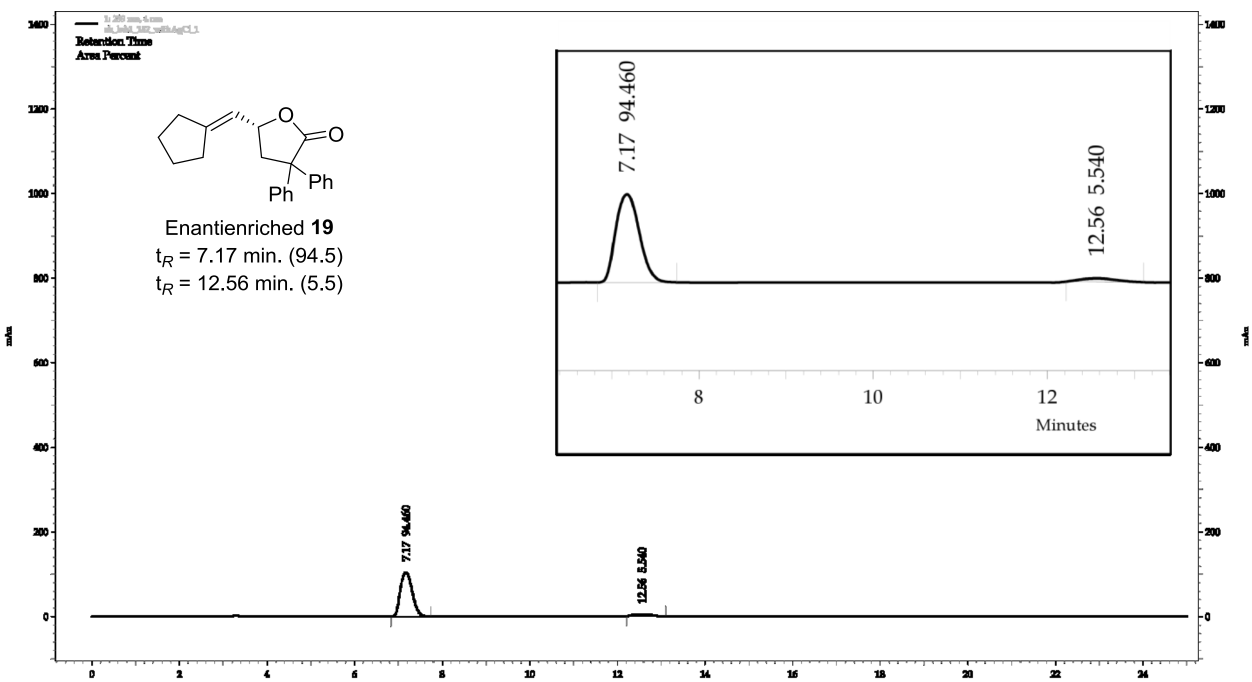


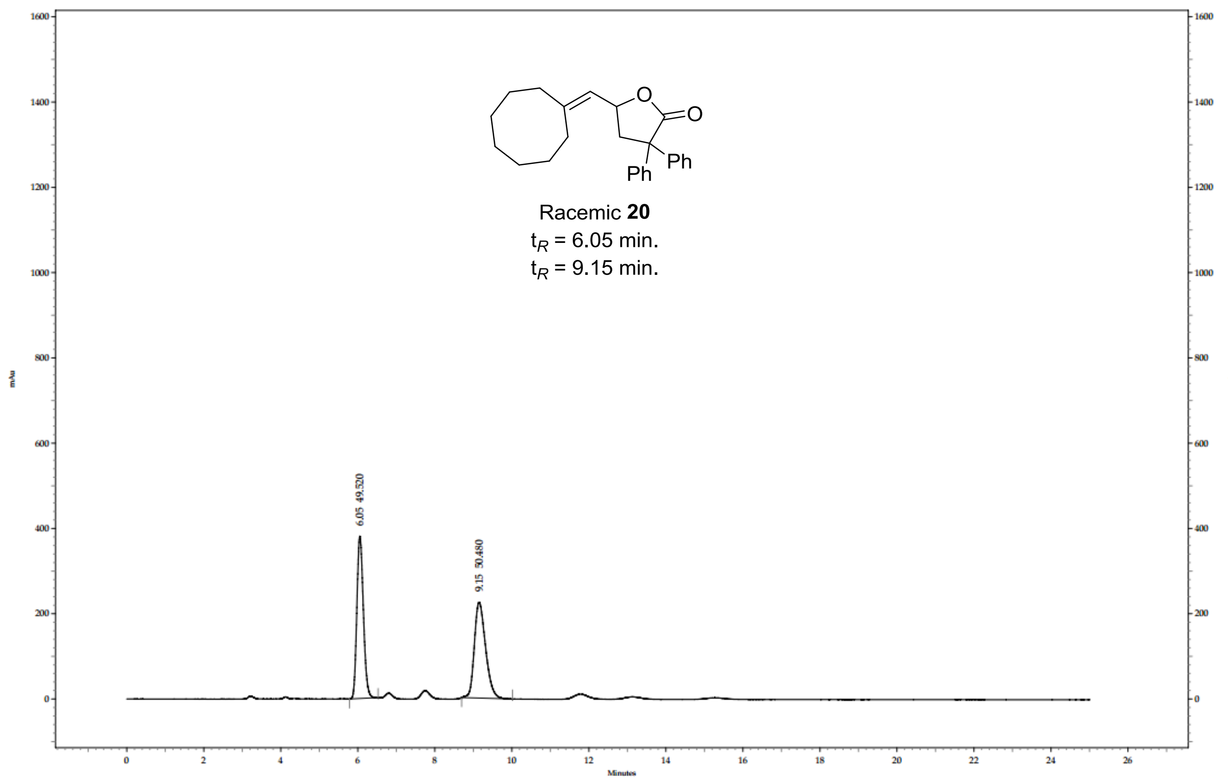
Ph
Ph
Enantienriched **17**
t_R = 7.70 min. (6.79)
t_R = 9.41 min. (93.21)
7.70 6.794
9.41 93.206
mAu
Minutes

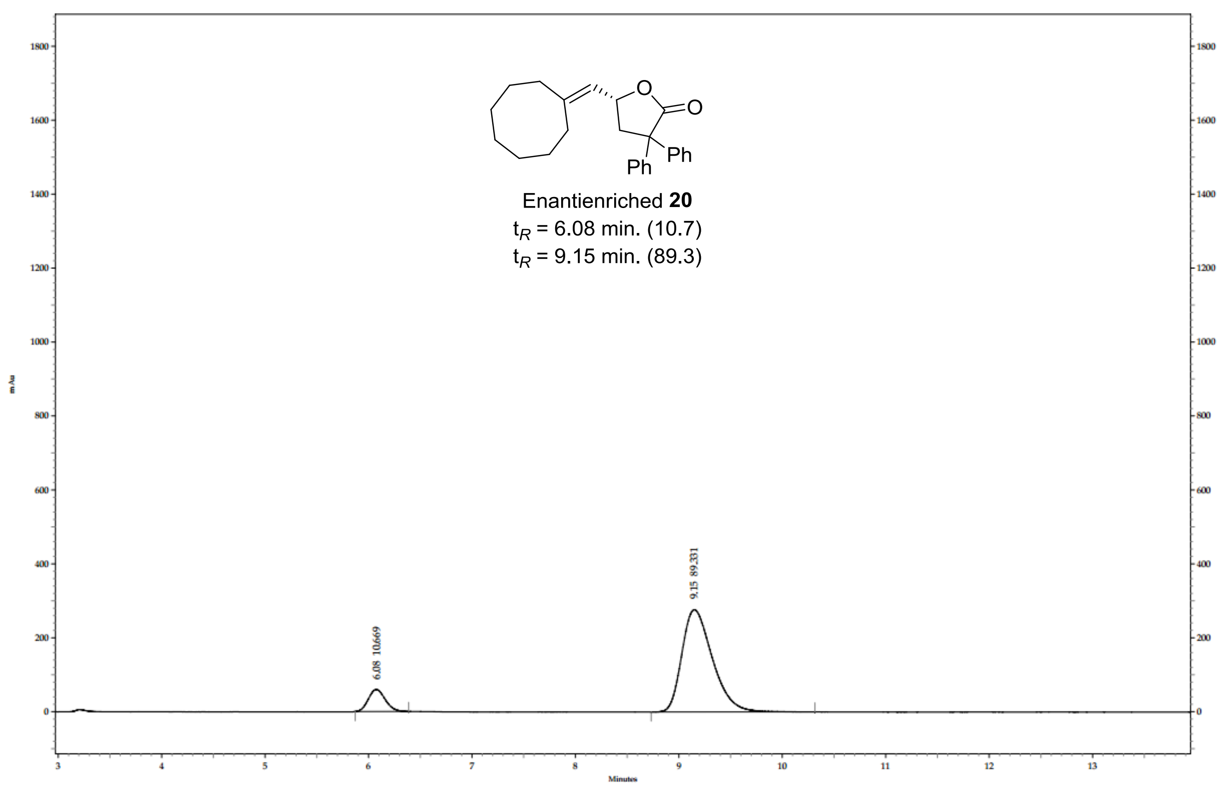

O
O
Ph
Ph
Racemic **18**
t_R = 24.22 min.
t_R = 29.23 min.
24.22 49.861
29.23 50.139
mAu
Minutes

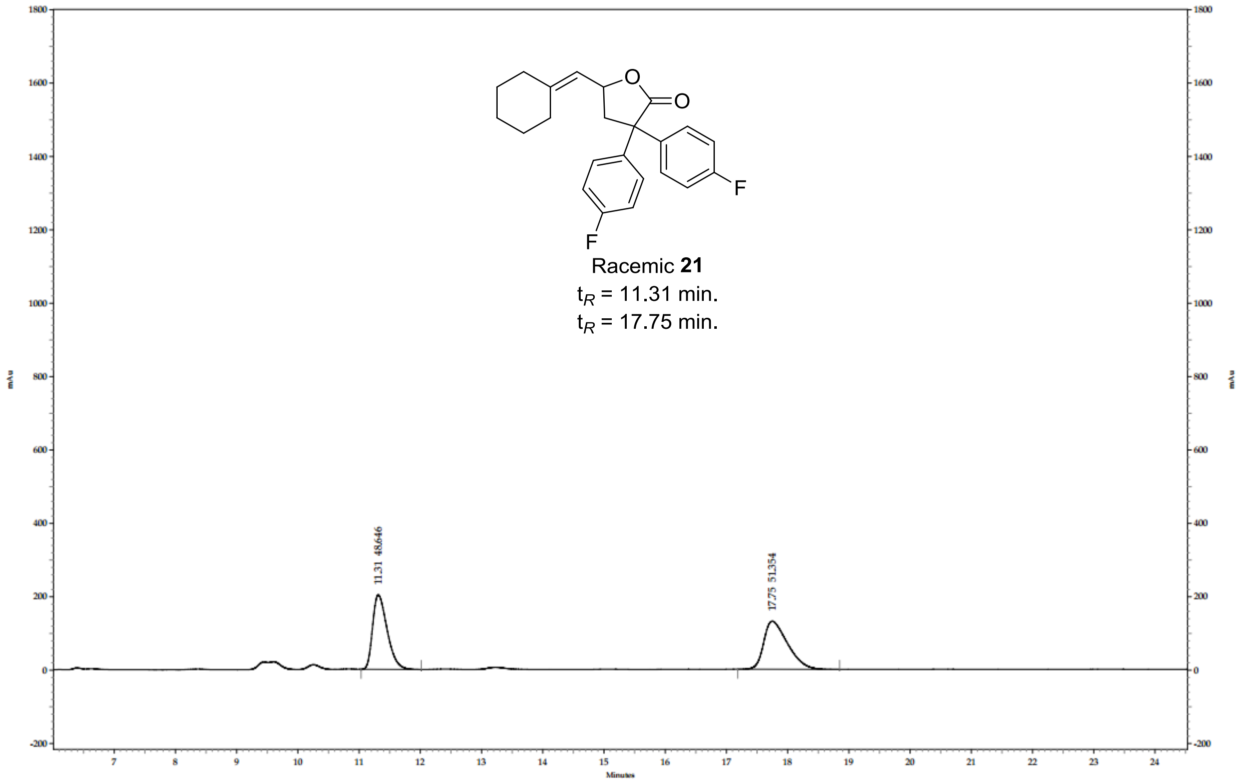

O
O
Ph
Ph
Enantienriched **18**
t_R = 24.36 min. (8.0)
t_R = 29.16 min. (92.0)
24.36 7.998
29.16 92.002
mAu
Minutes


Retention Time
Area Percent
Ph
Ph
Racemic **19**
t_R = 7.31 min.
t_R = 12.55 min.
7.31 49.484
12.55 50.516
Minutes
mAu

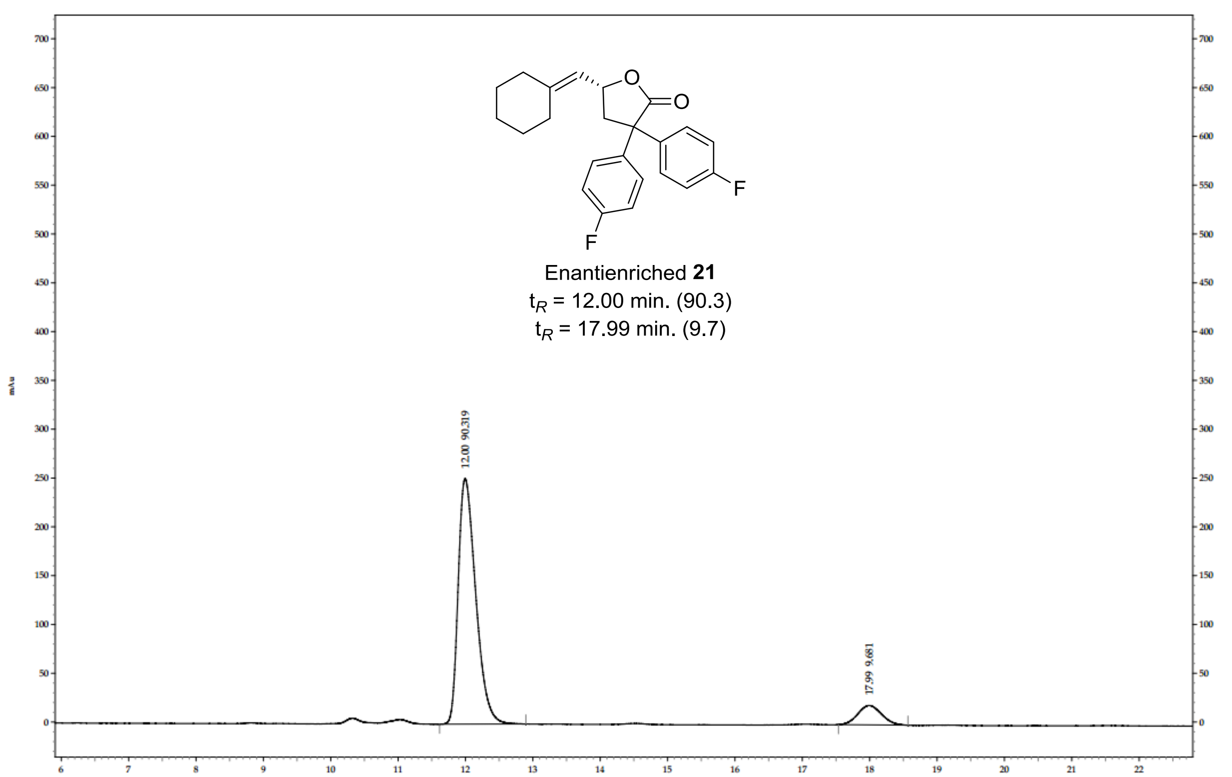

Retention Time
Area Percent
Ph
Ph
Enantienriched **19**
t_R = 7.17 min. (94.5)
t_R = 12.56 min. (5.5)
7.17 94.460
12.56 5.540
Minutes
mAu


Racemic **20**
t_R = 6.05 min.
t_R = 9.15 min.
6.05 49.520
9.15 50.480
Minutes
mAu

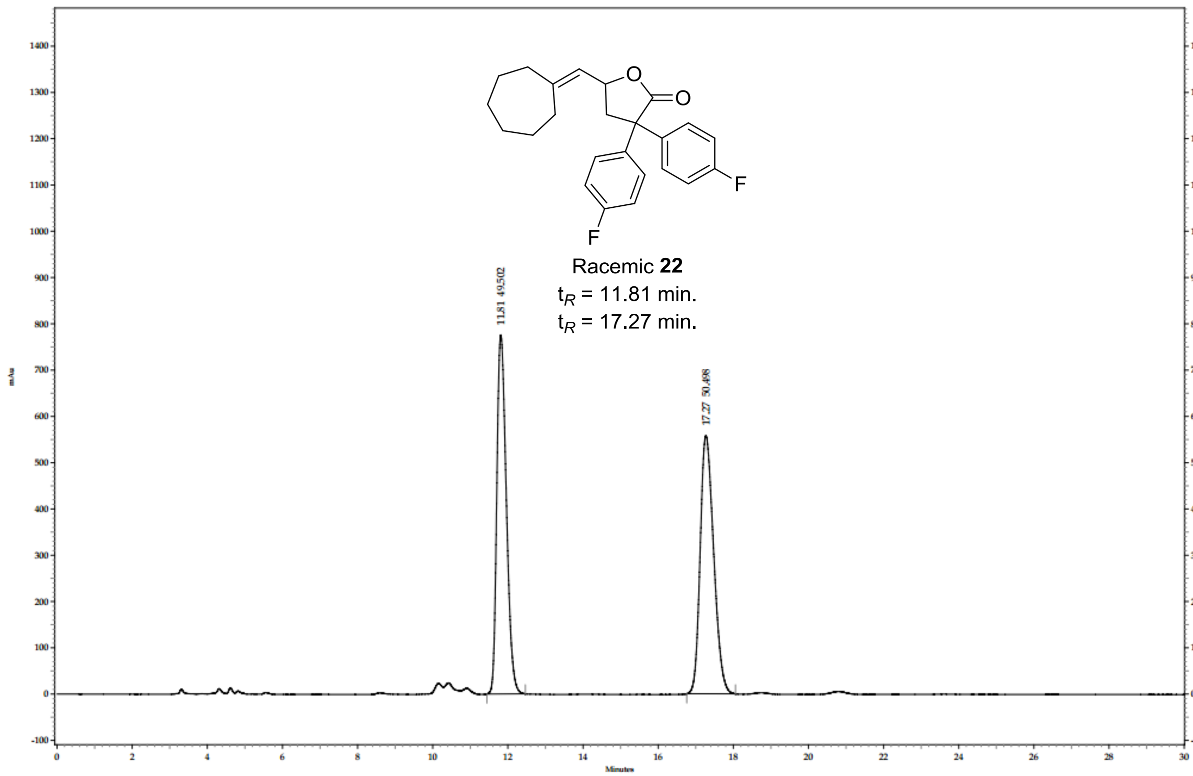

Enantienriched **20**
t_R = 6.08 min. (10.7)
t_R = 9.15 min. (89.3)
6.08 10.669
9.15 89.331
Minutes
mAu

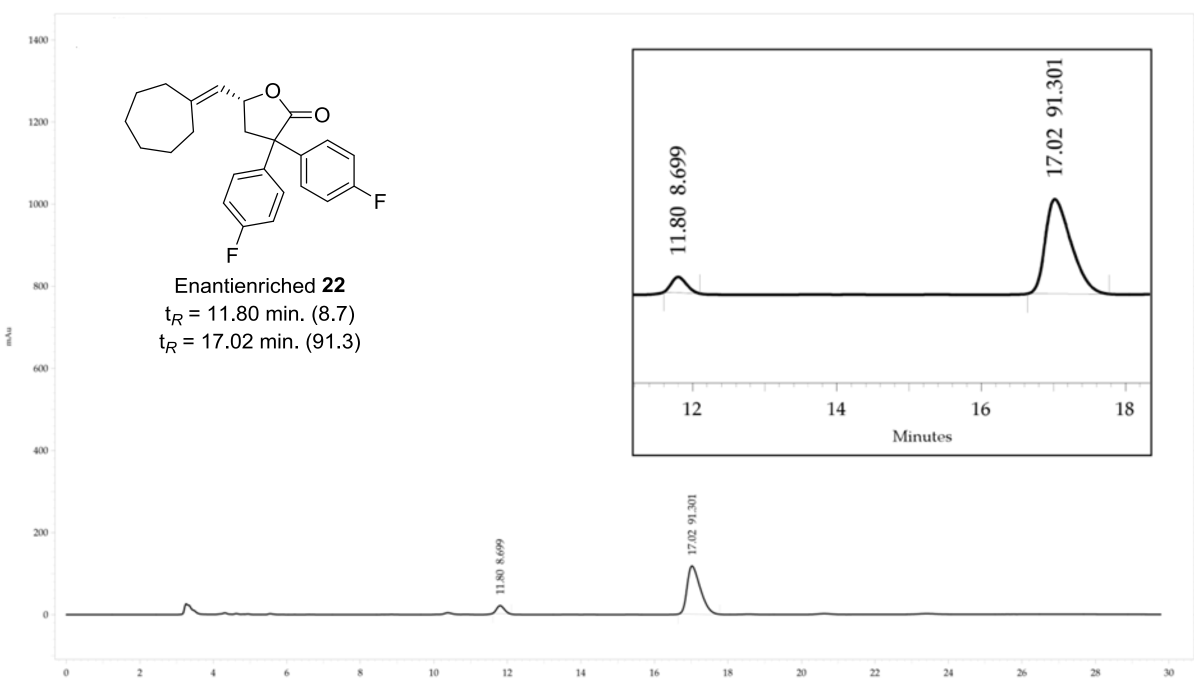


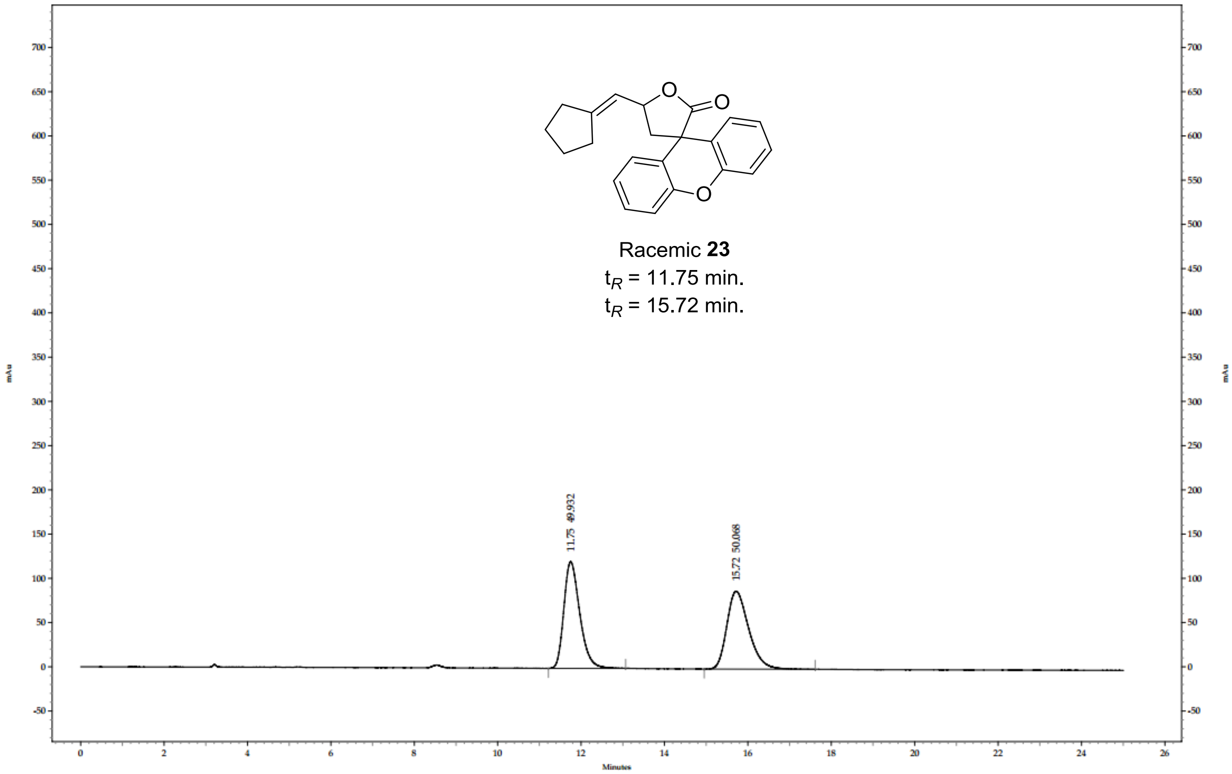
Racemic **21**
t_R = 11.31 min.
t_R = 17.75 min.
11.31 48.646
17.75 51.354
mAu
Minutes

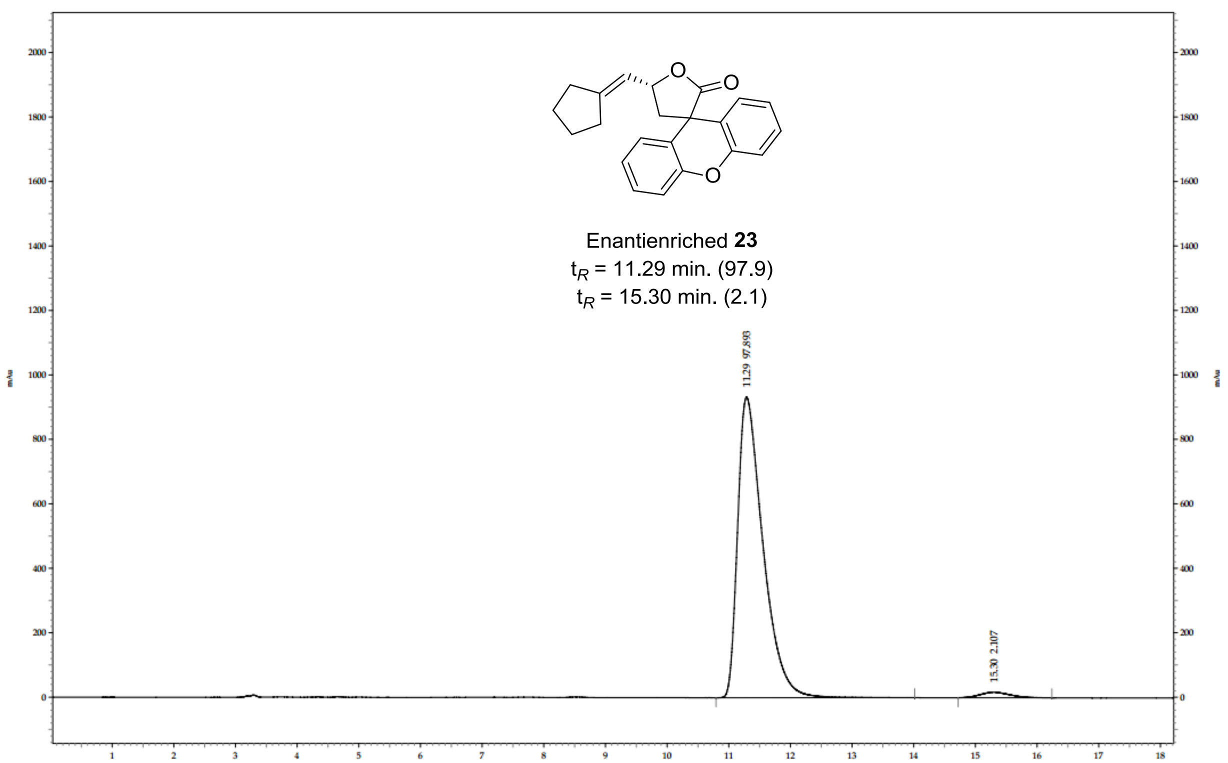


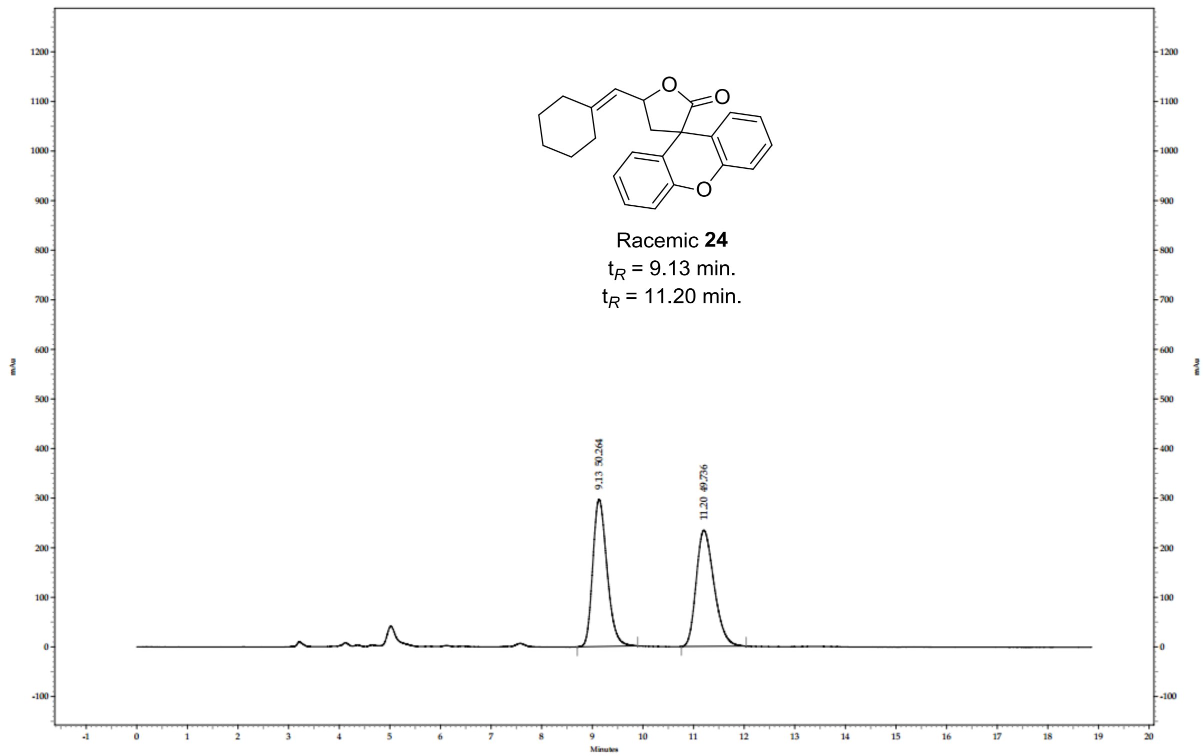
Enantienriched **21**
t_R = 12.00 min. (90.3)
t_R = 17.99 min. (9.7)
12.00 90.319
17.99 9.681
mAu
Minutes

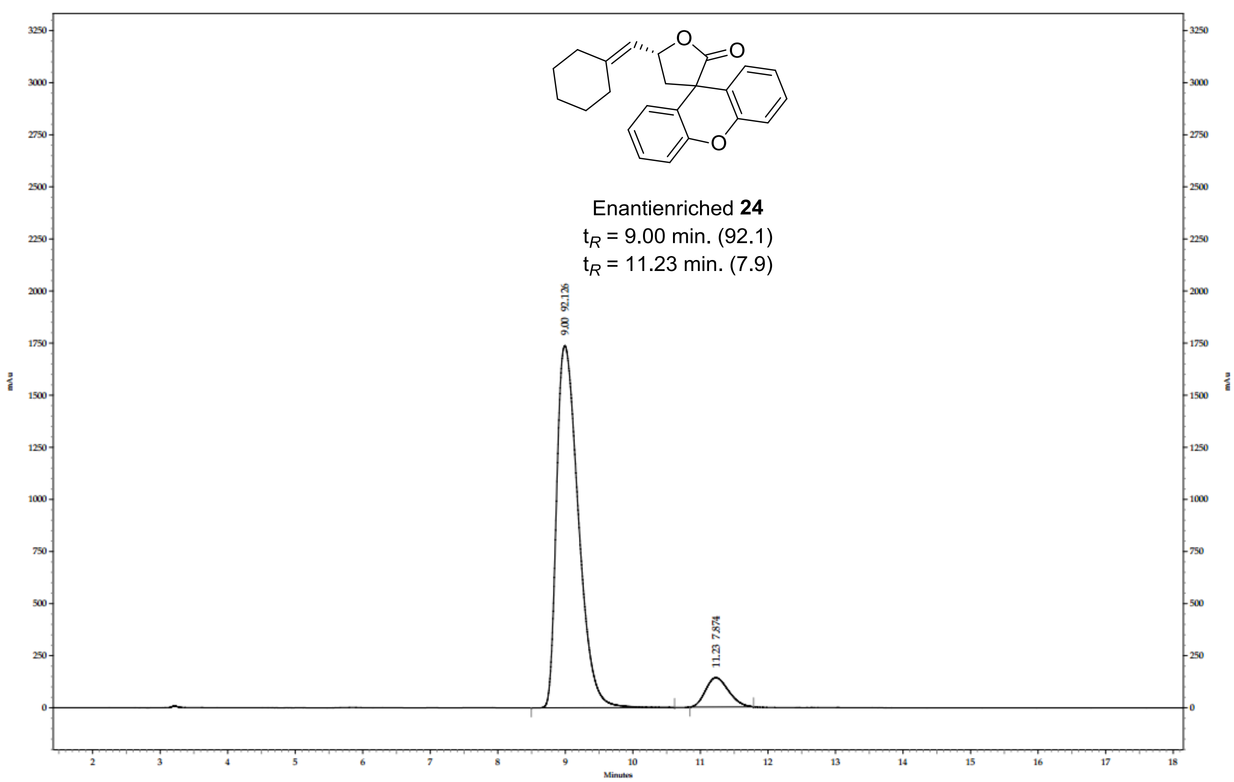

Racemic **22**
t_R = 11.81 min.
t_R = 17.27 min.
11.81 49.502
17.27 50.498
mAu
Minutes

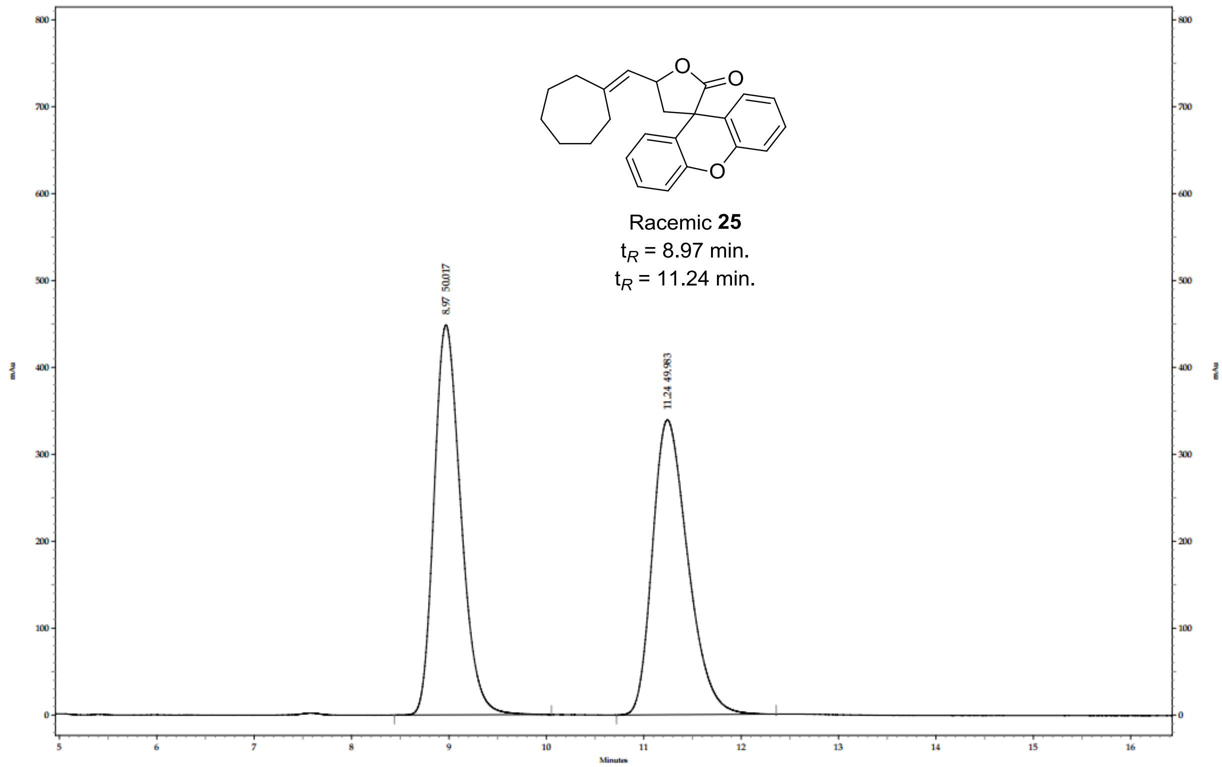

Enantienriched **22**
t_R = 11.80 min. (8.7)
t_R = 17.02 min. (91.3)
11.80 8.699
17.02 91.301
Minutes
mAu

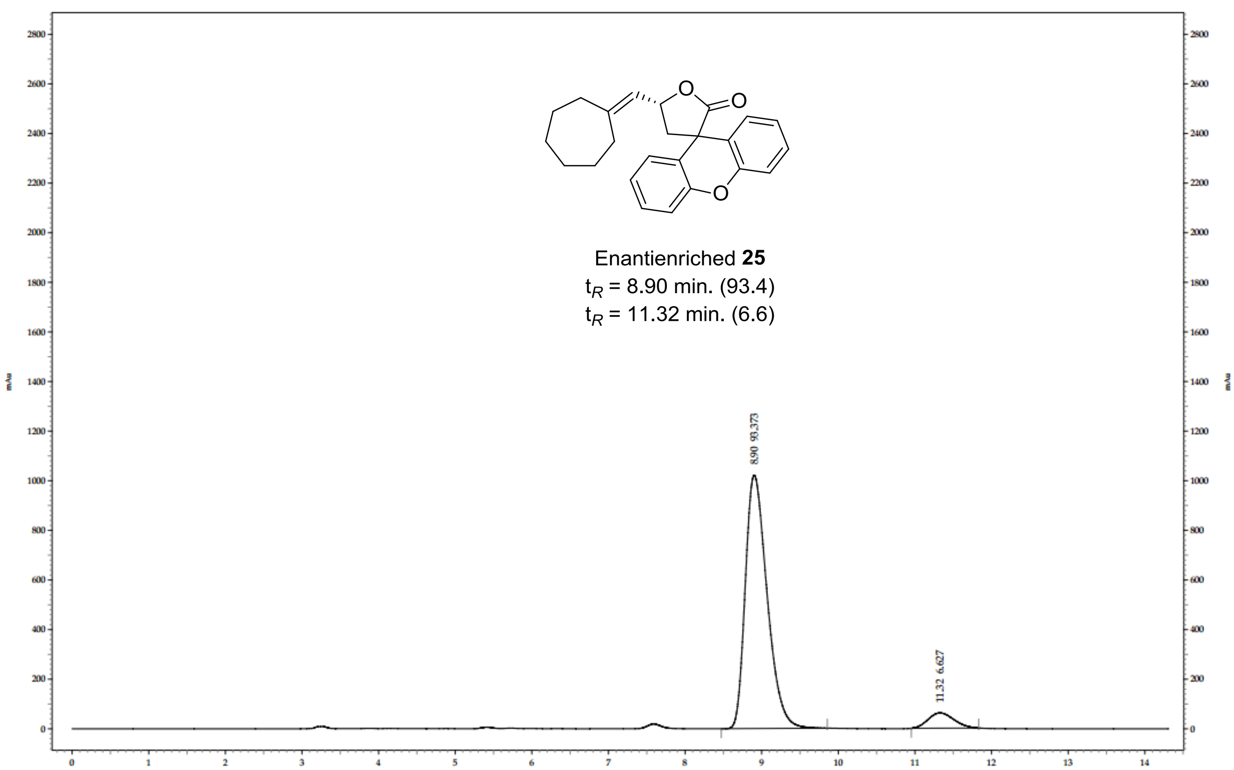

Racemic **23**
t_R = 11.75 min.
t_R = 15.72 min.
11.75 49.932
15.72 50.068
mAu
Minutes

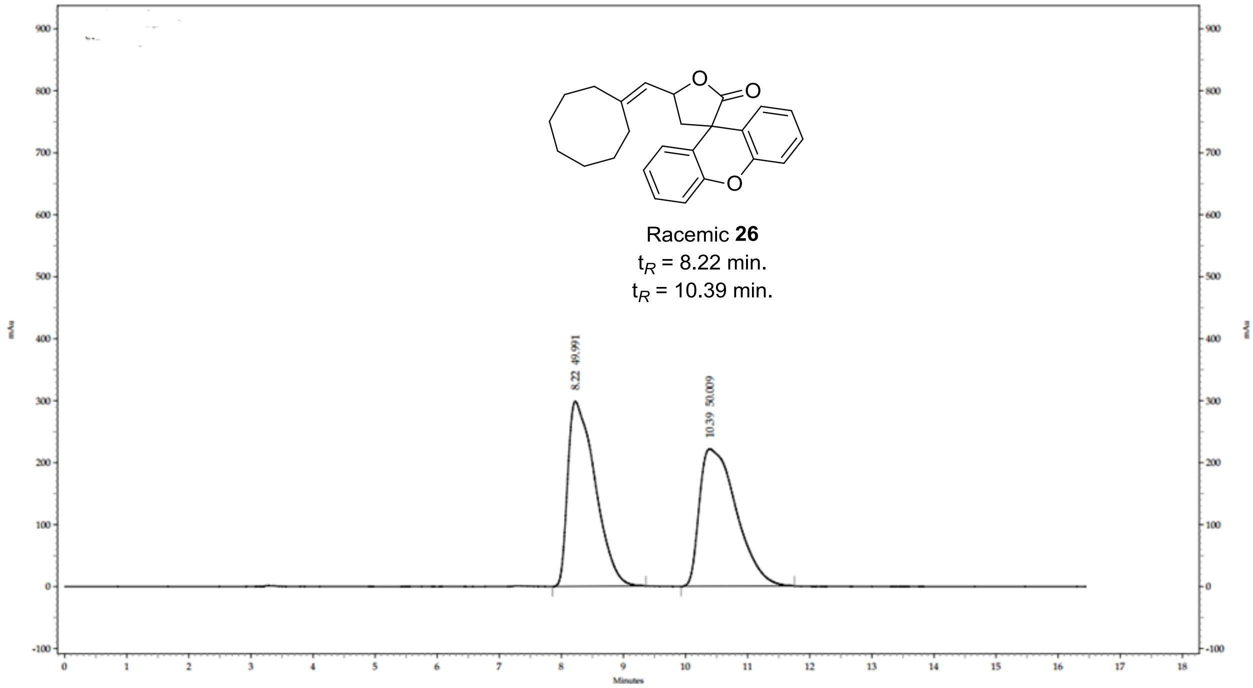

Enantienriched **23**
t_R = 11.29 min. (97.9)
t_R = 15.30 min. (2.1)
11.29 97.893
15.30 2.107
mAu
Minutes

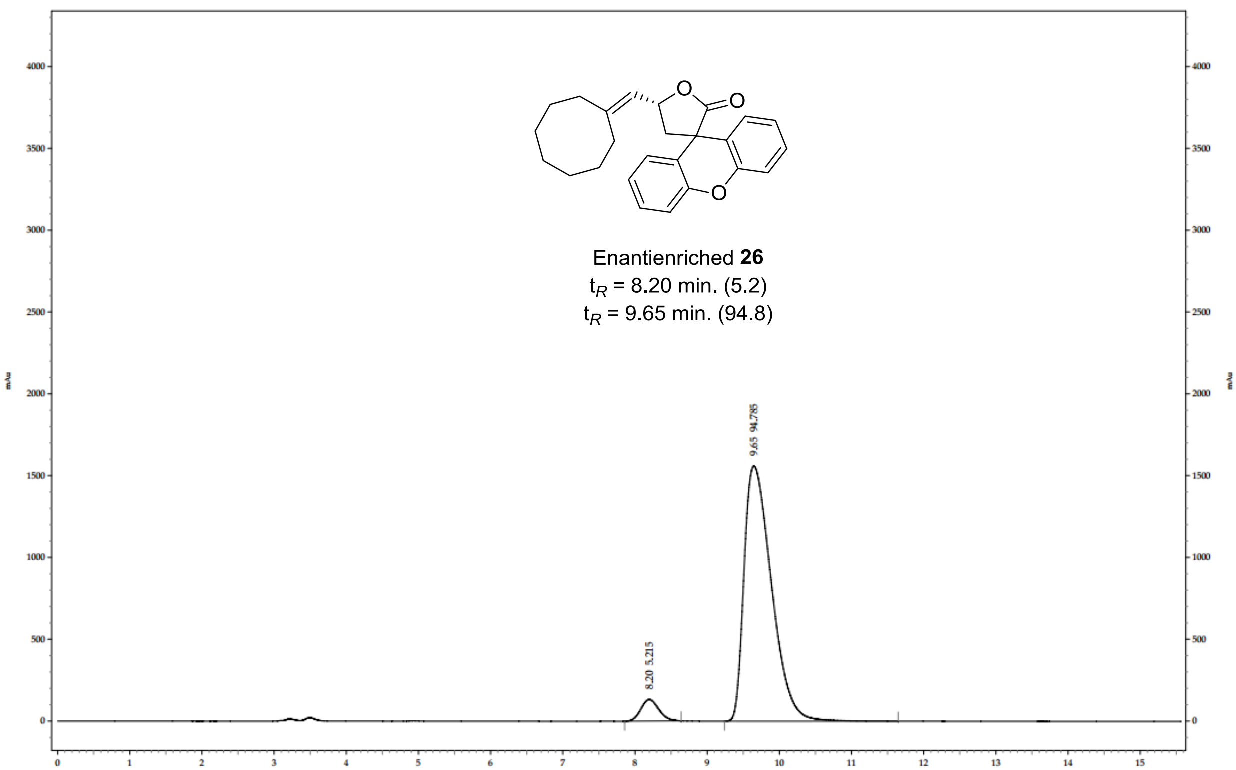

Racemic **24**
t_R = 9.13 min.
t_R = 11.20 min.
9.13 50.264
11.20 49.736
mAu
Minutes

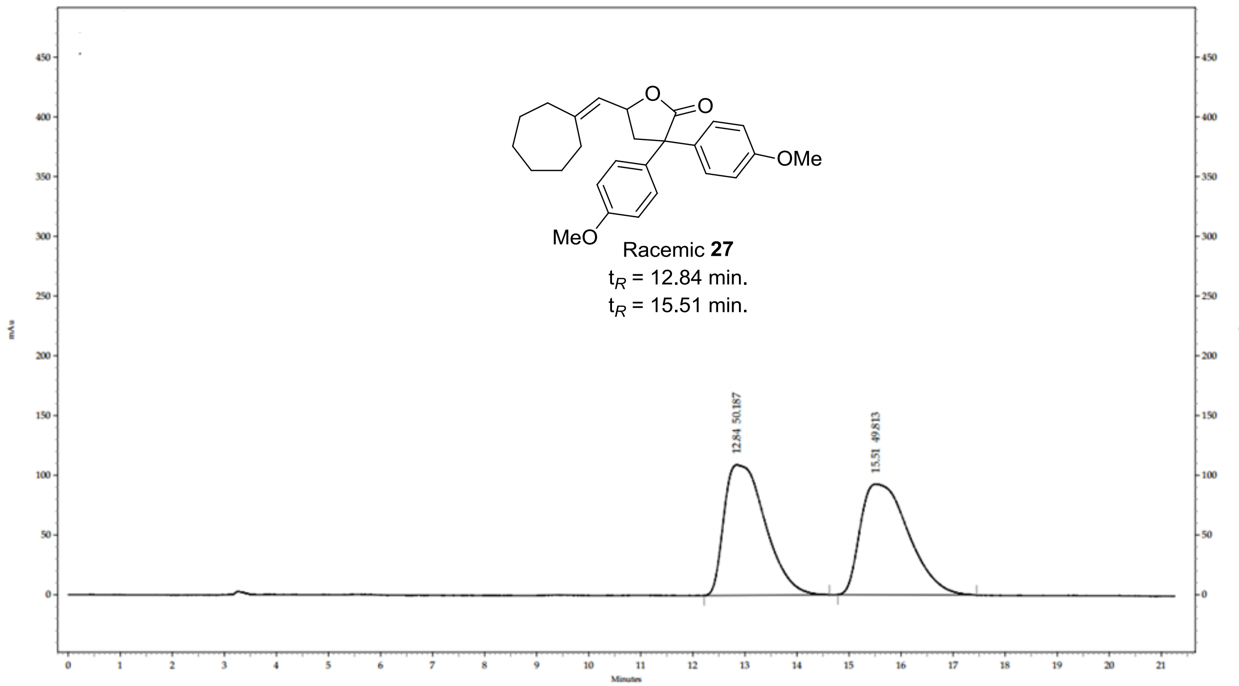

Enantienriched **24**
t_R = 9.00 min. (92.1)
t_R = 11.23 min. (7.9)
9.00 92.126
11.23 7.874
mAu
Minutes

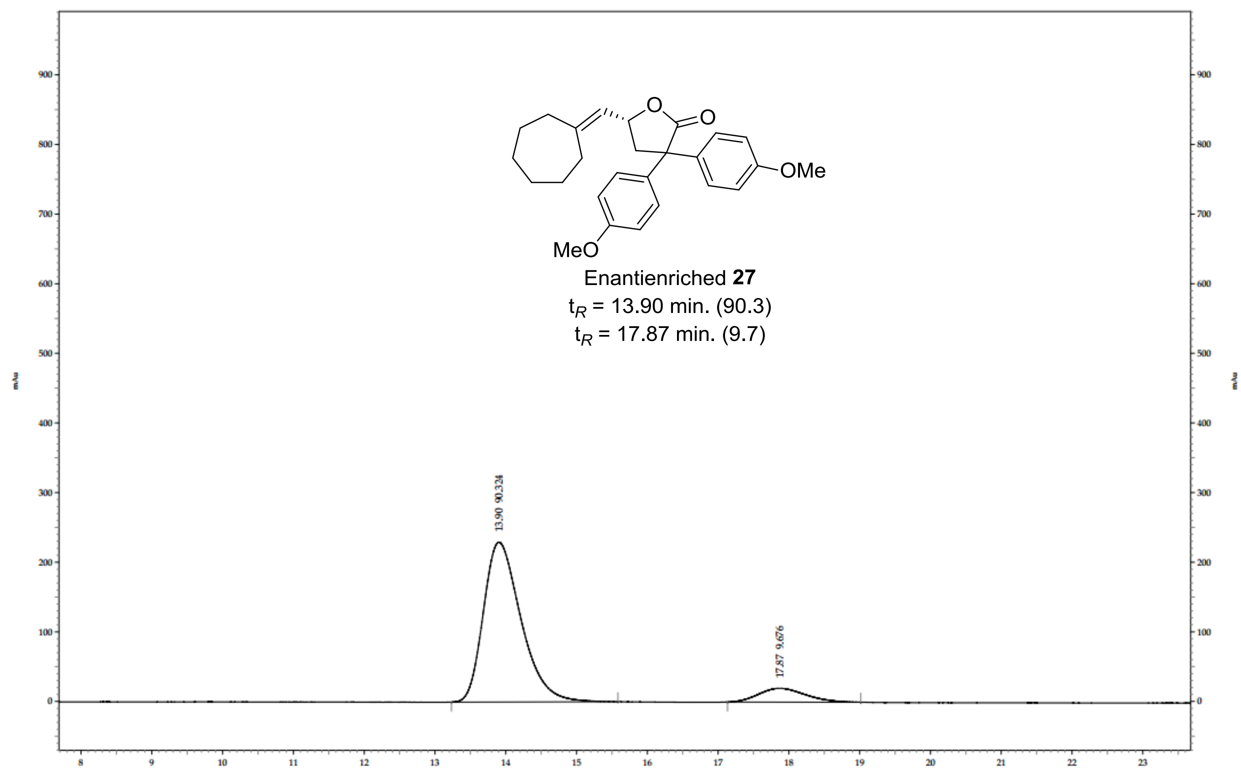

Racemic **25**
t_R = 8.97 min.
t_R = 11.24 min.
8.97 50.017
11.24 49.983
Minutes
mAu

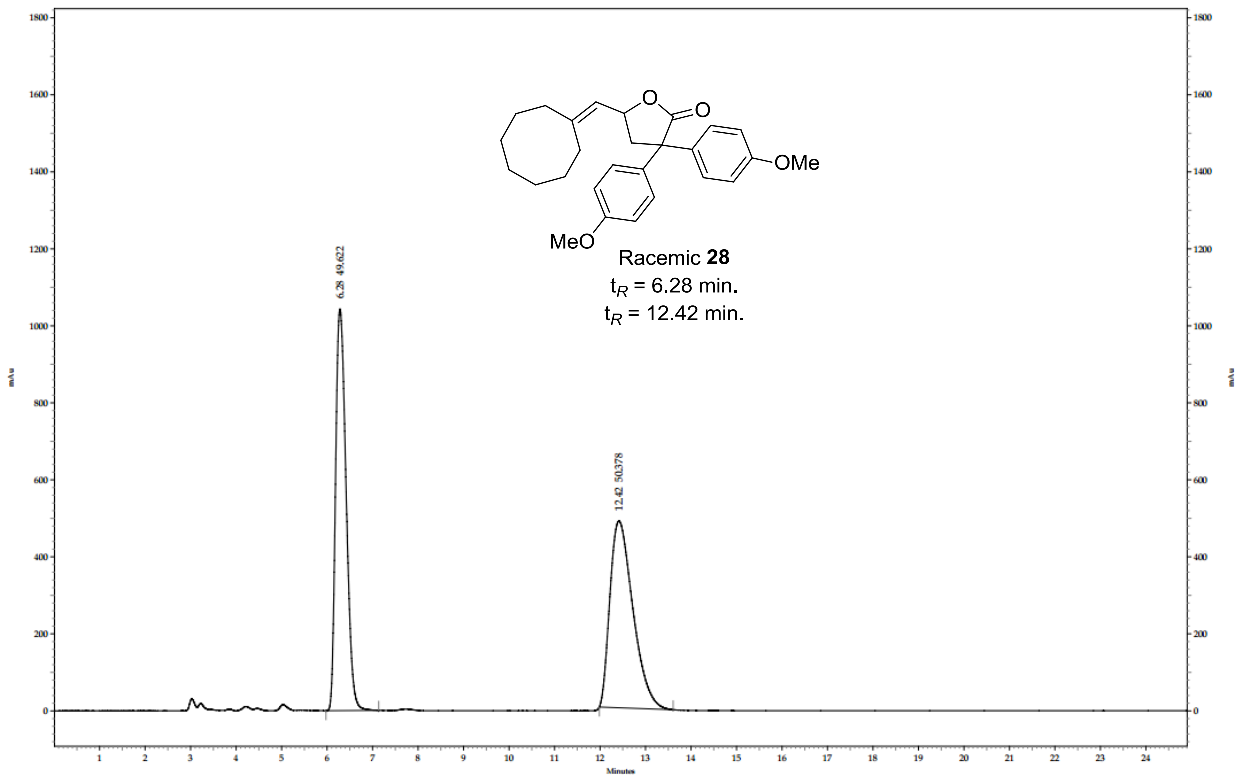

Enantienriched **25**
t_R = 8.90 min. (93.4)
t_R = 11.32 min. (6.6)
8.90 93.373
11.32 6.627
Minutes
mAu

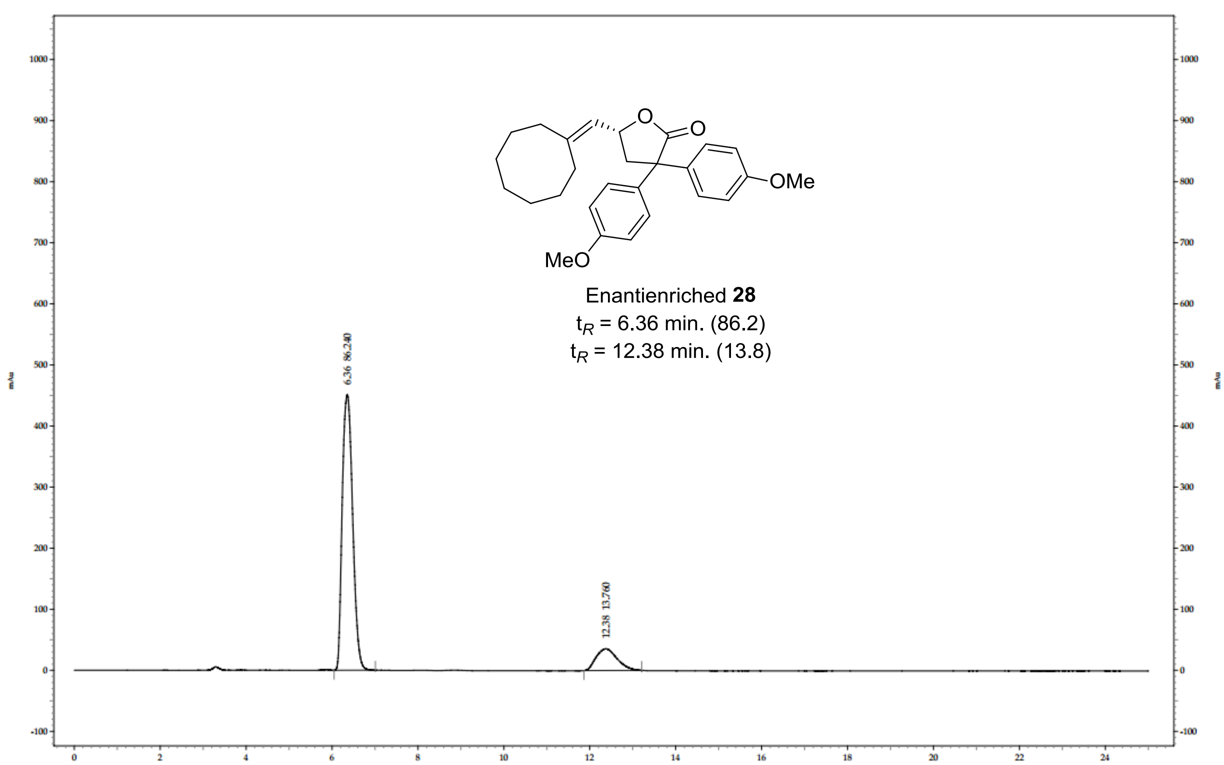

O
O
O
Racemic 26
tR = 8.22 min.
tR = 10.39 min.
8.22 49.991
10.39 50.009
Minutes
mAu

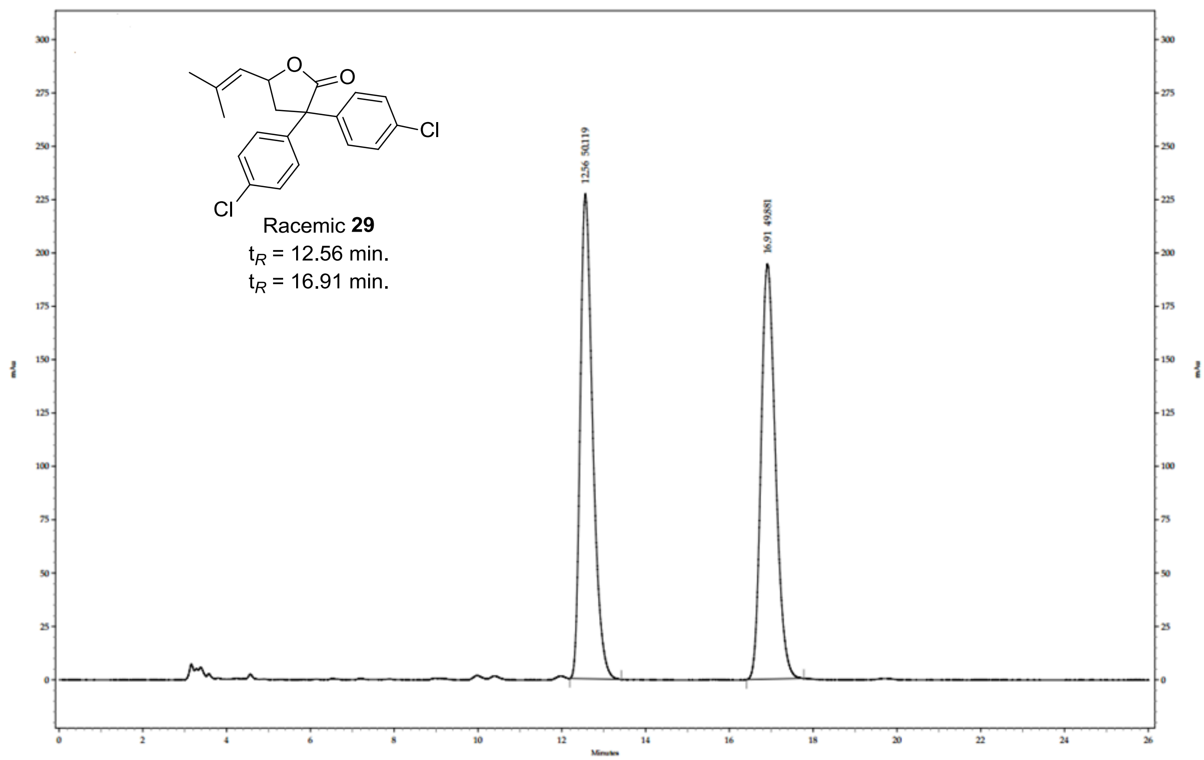

O
O
O
Enantienriched 26
tR = 8.20 min. (5.2)
tR = 9.65 min. (94.8)
8.20 5.215
9.65 94.785
Minutes
mAu

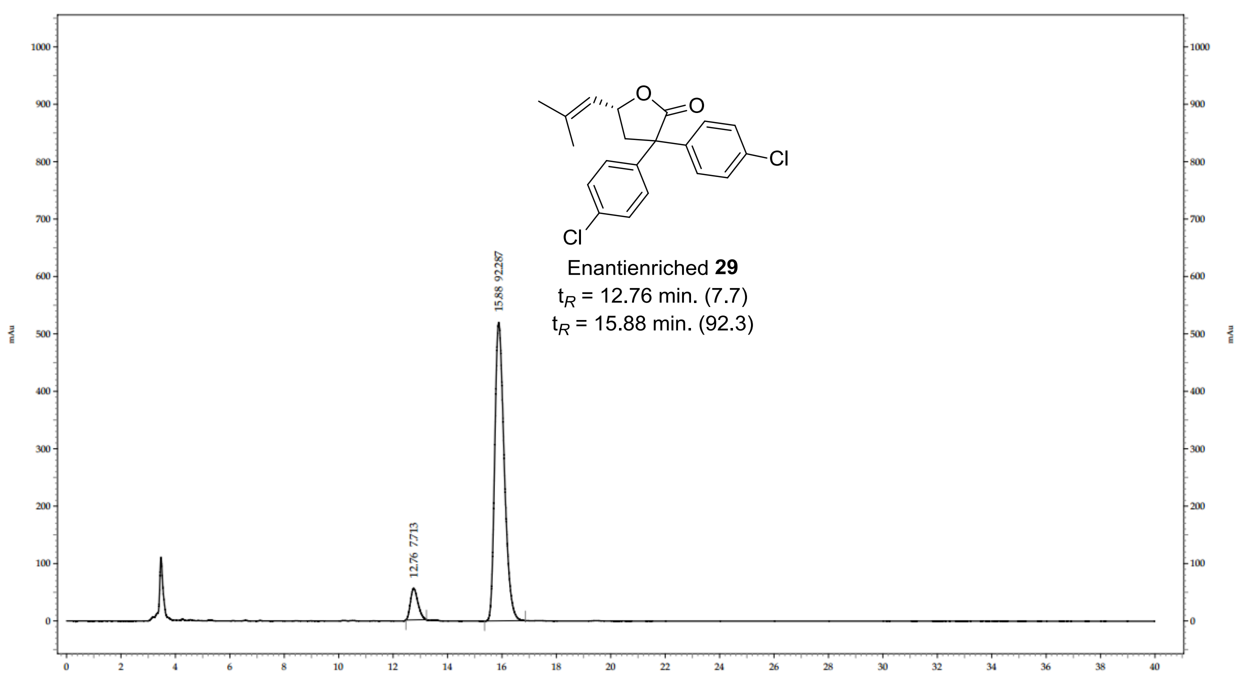

OMe
MeO
Racemic 27
t_R = 12.84 min.
t_R = 15.51 min.
12.84 50.187
15.51 49.813
Minutes
mAu

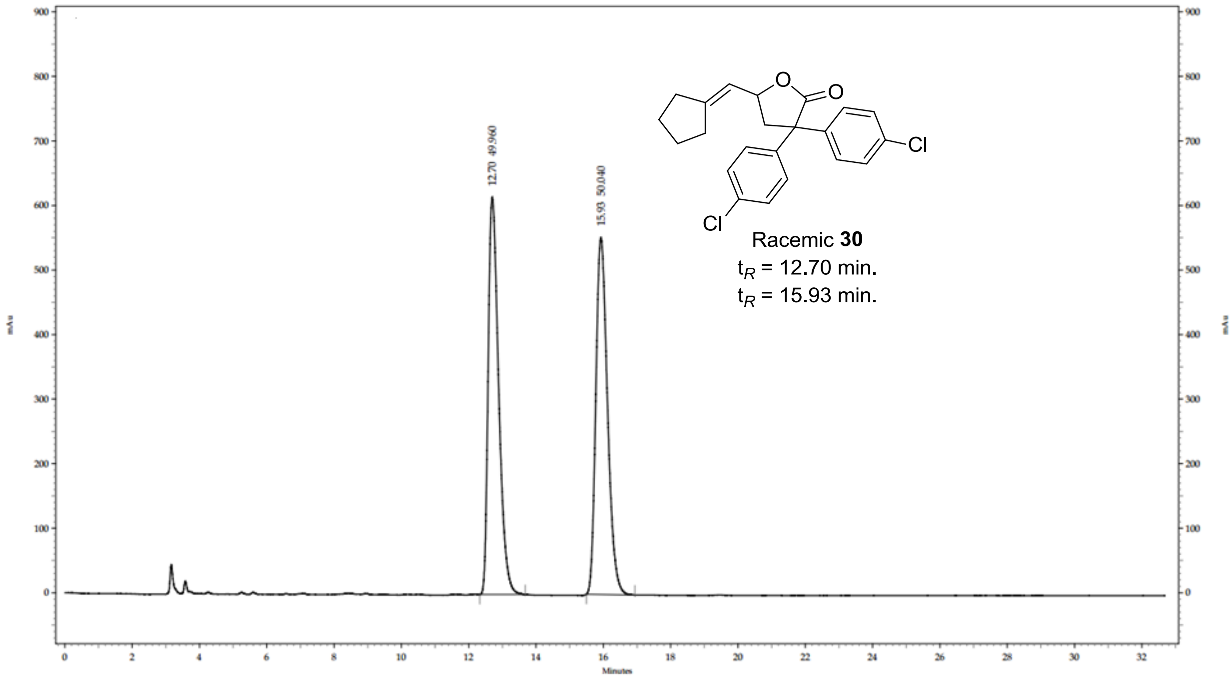

OMe
MeO
Enantienriched 27
t_R = 13.90 min. (90.3)
t_R = 17.87 min. (9.7)
13.90 90.324
17.87 9.676
Minutes
mAu

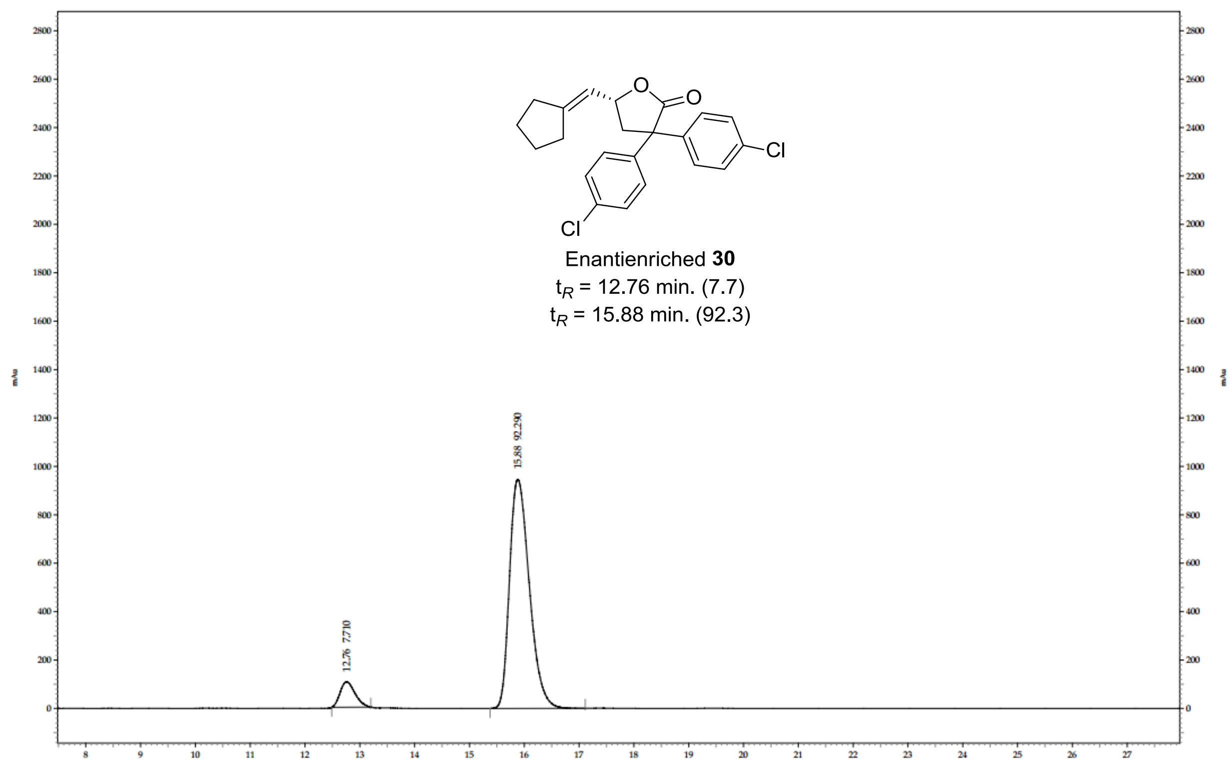

O
O
OMe
MeO
Racemic **28**
t_R = 6.28 min.
t_R = 12.42 min.
6.28 49.622
12.42 50.378
mAu
Minutes

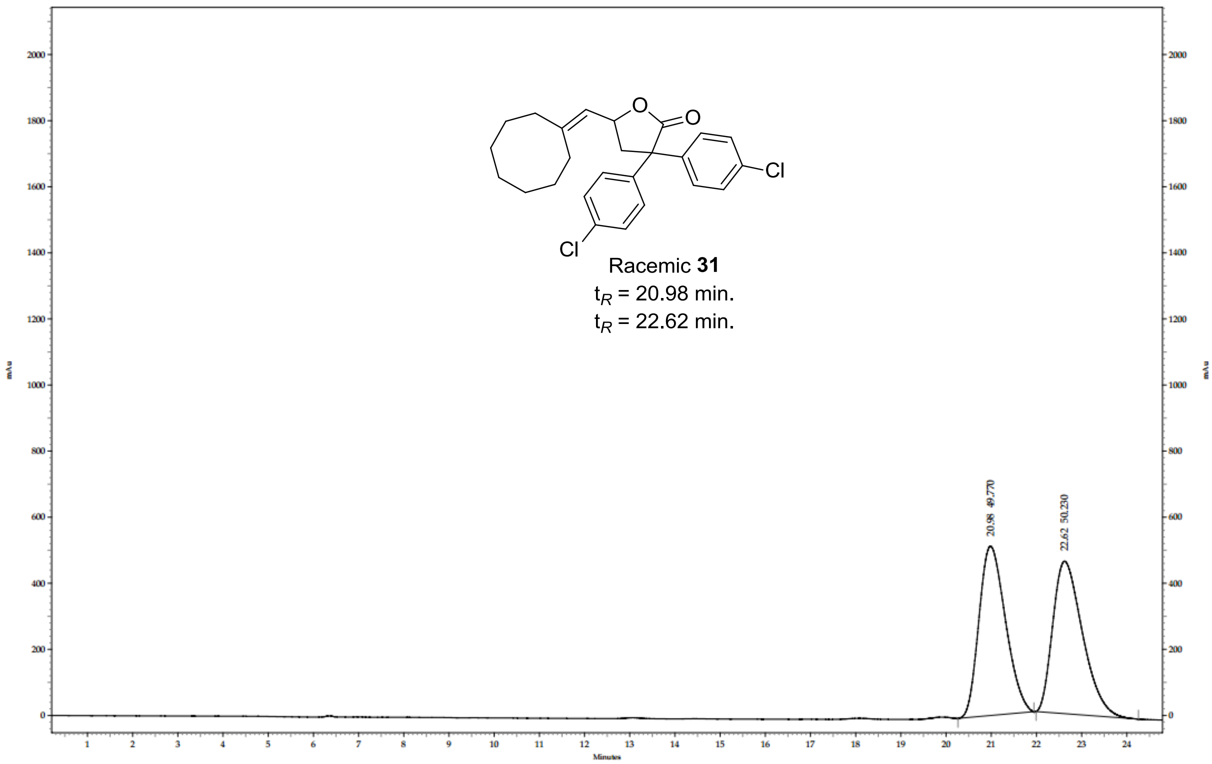

O
O
OMe
MeO
Enantienriched **28**
t_R = 6.36 min. (86.2)
t_R = 12.38 min. (13.8)
6.36 86.240
12.38 13.760
mAu
Minutes

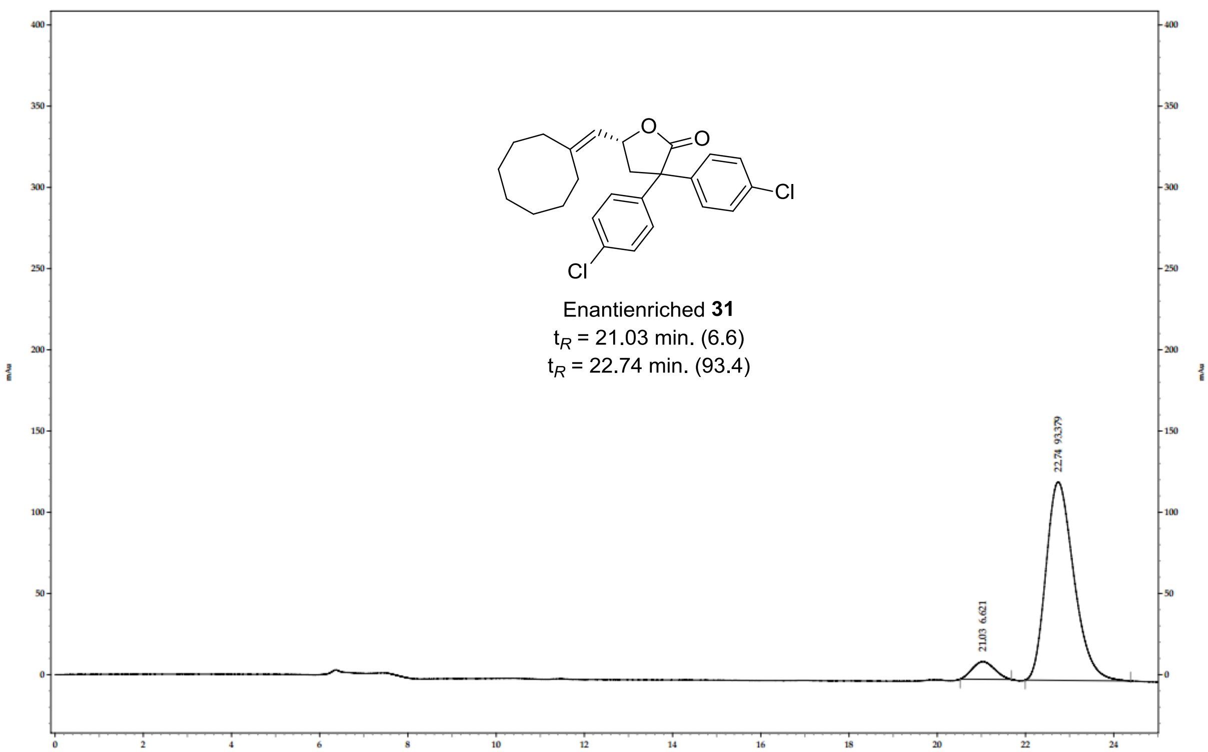

Cl
Cl
Racemic 29
t_R = 12.56 min.
t_R = 16.91 min.
Minutes
mAu

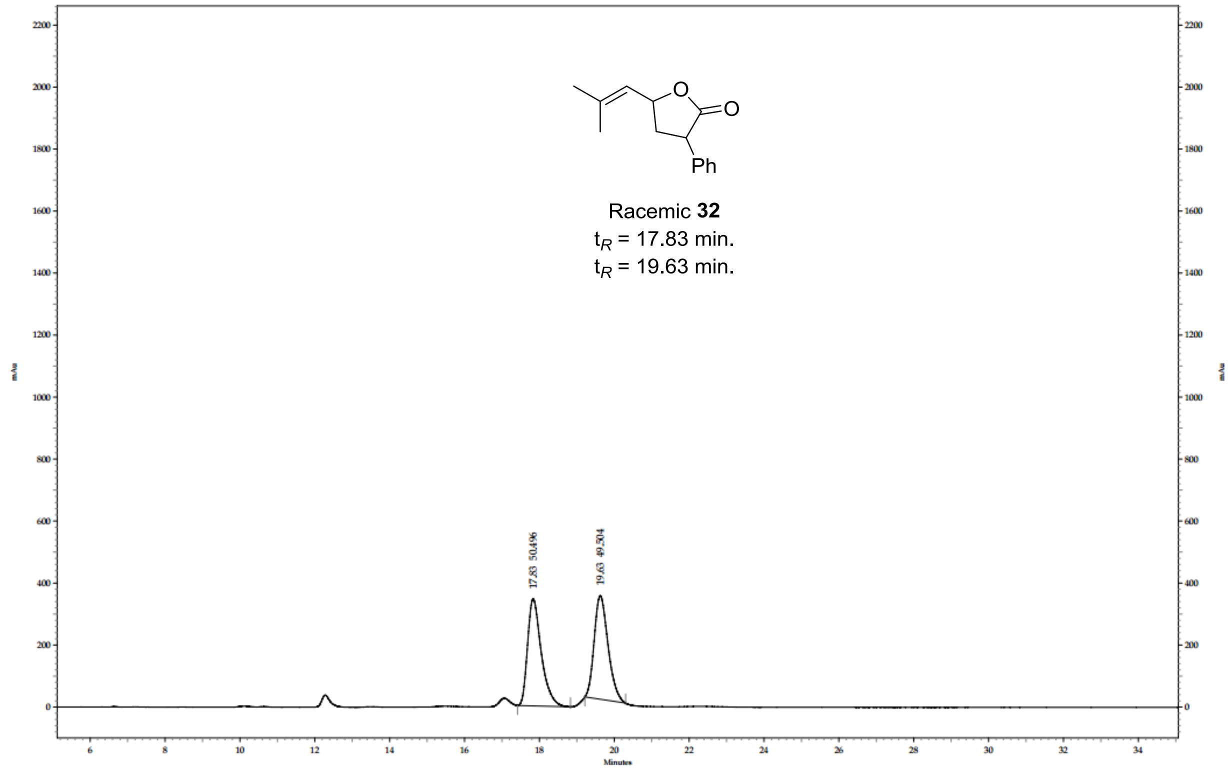

Cl
Cl
Enantienriched 29
t_R = 12.76 min. (7.7)
t_R = 15.88 min. (92.3)
Minutes
mAu

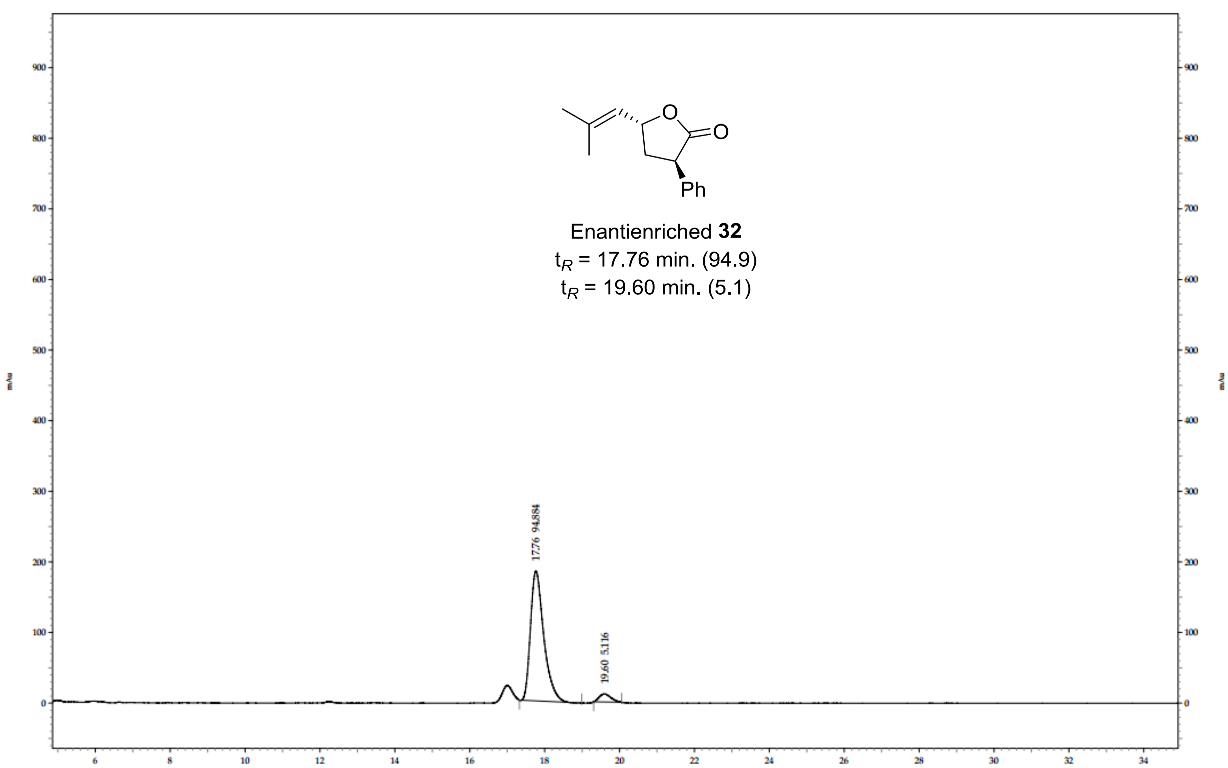

O
O
Cl
Cl
Racemic 30
t_R = 12.70 min.
t_R = 15.93 min.
12.70 49.960
15.93 50.040
mAu
Minutes


O
O
Cl
Cl
Enantienriched 30
t_R = 12.76 min. (7.7)
t_R = 15.88 min. (92.3)
12.76 7.710
15.88 92.290
mAu
Minutes

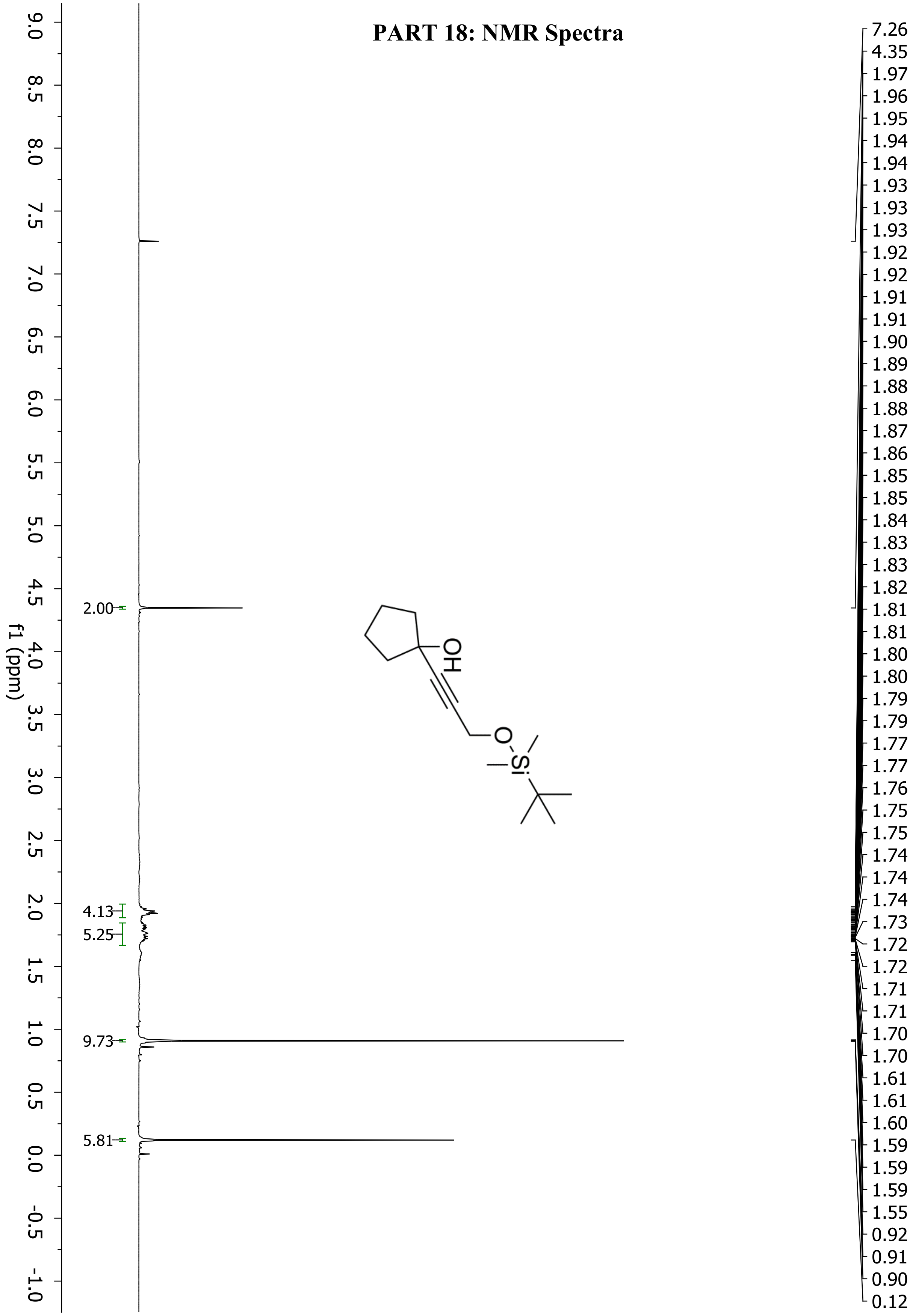

Cl
Cl
Racemic **31**
t_R = 20.98 min.
t_R = 22.62 min.
20.98 49.770
22.62 50.230
mAu
Minutes

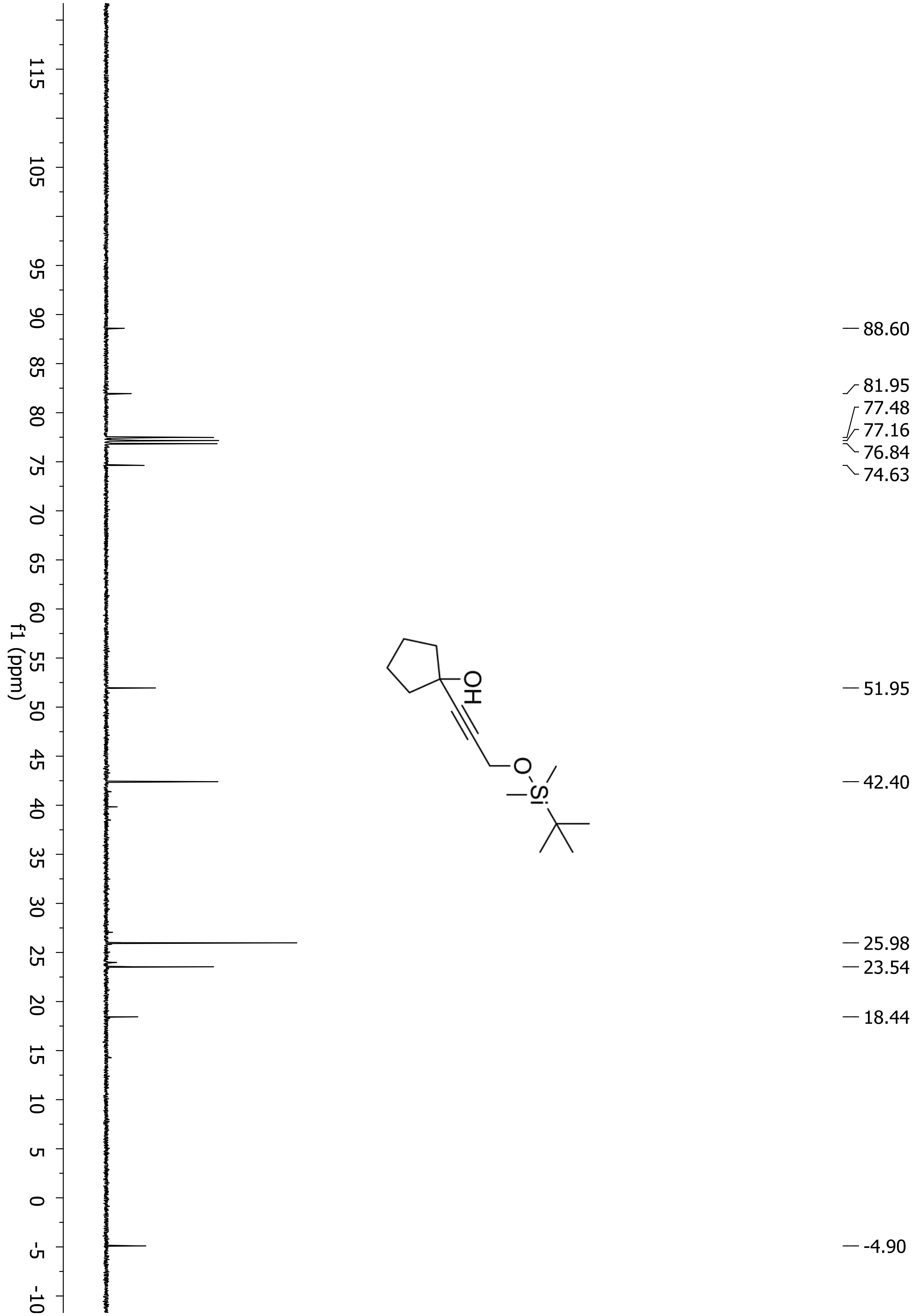

Cl
Cl
Enantienriched **31**
t_R = 21.03 min. (6.6)
t_R = 22.74 min. (93.4)
21.03 6.621
22.74 93.379
mAu
Minutes

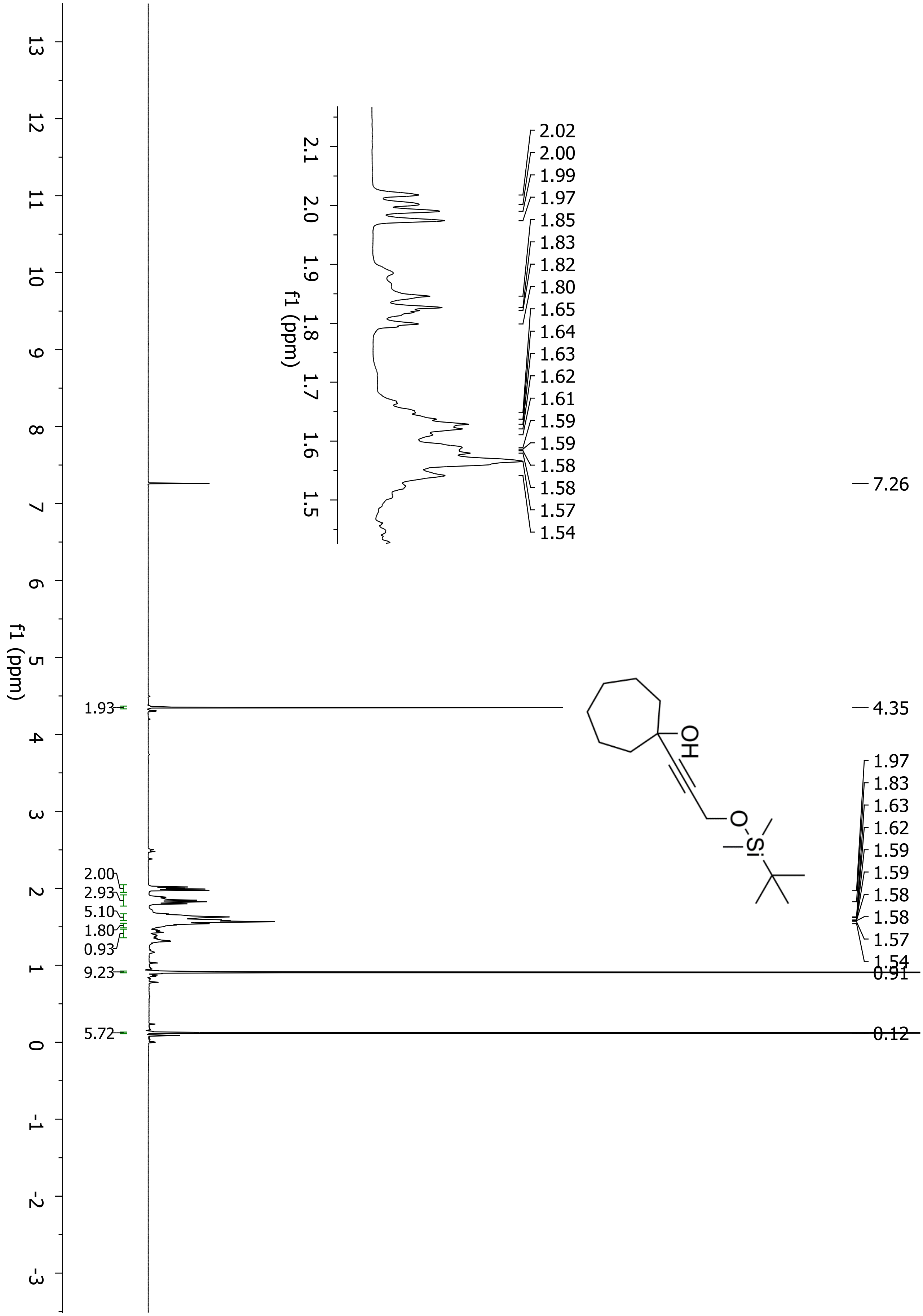

O
O
Ph
Racemic **32**
t_R = 17.83 min.
t_R = 19.63 min.
17.83 50.496
19.63 49.504
mAu
Minutes


O
O
Ph
Enantienriched **32**
t_R = 17.76 min. (94.9)
t_R = 19.60 min. (5.1)
17.76 94.884
19.60 5.116
mAu
Minutes

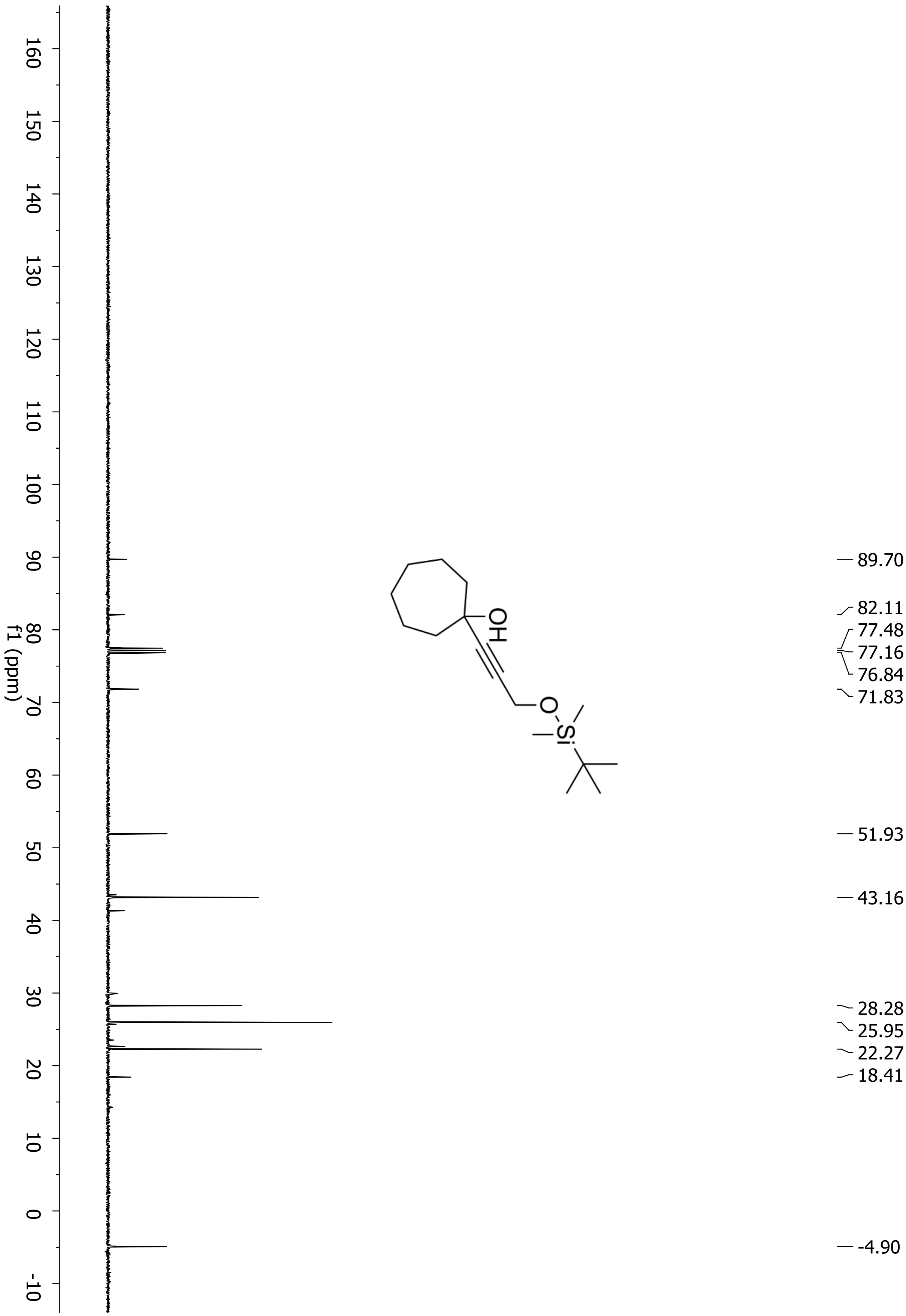
PART 18: NMR Spectra

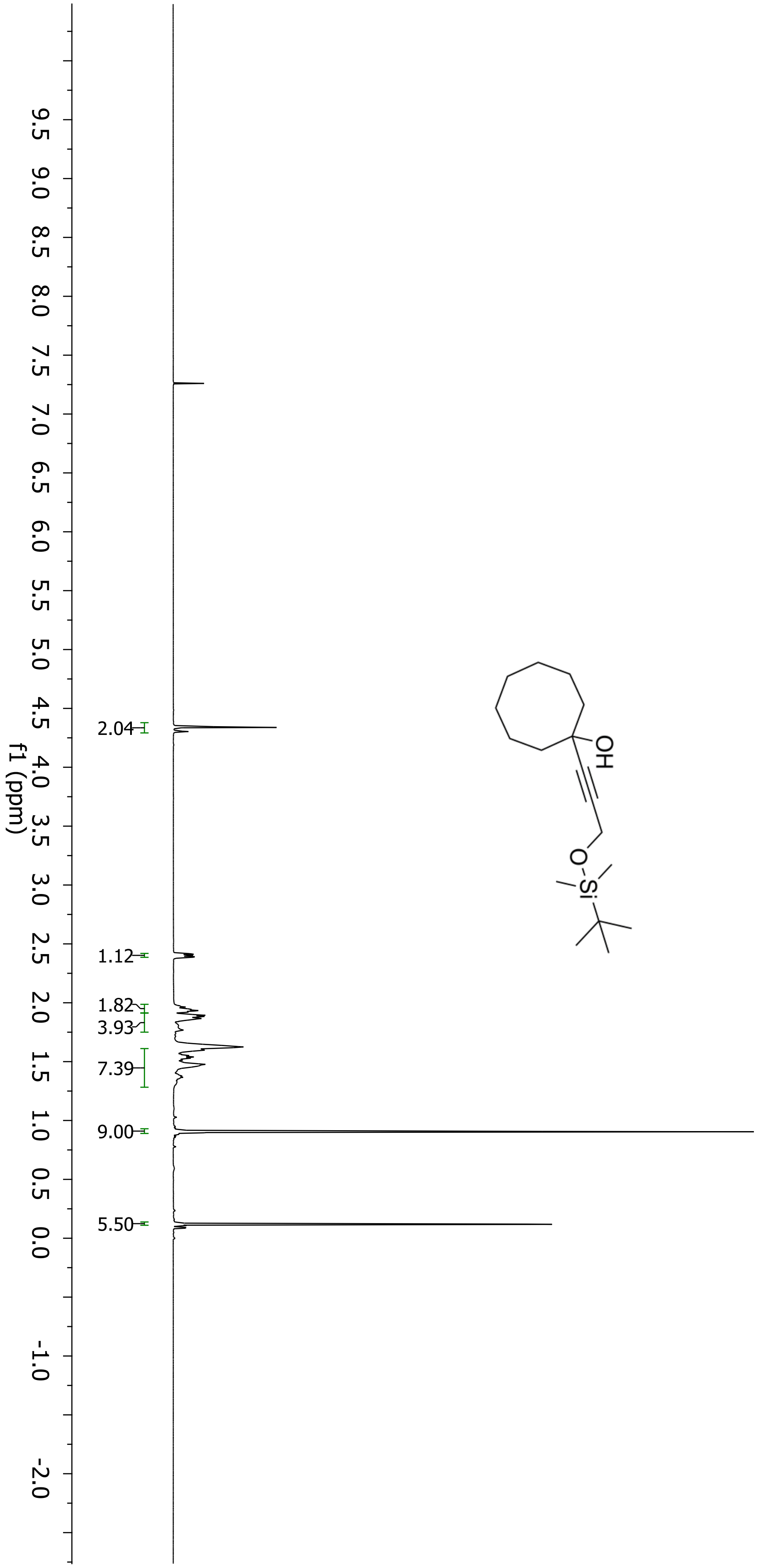



88.60
81.95
77.48
77.16
76.84
74.63
51.95
42.40
25.98
23.54
18.44
-4.90
OH
O
Si
f1 (ppm)
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10

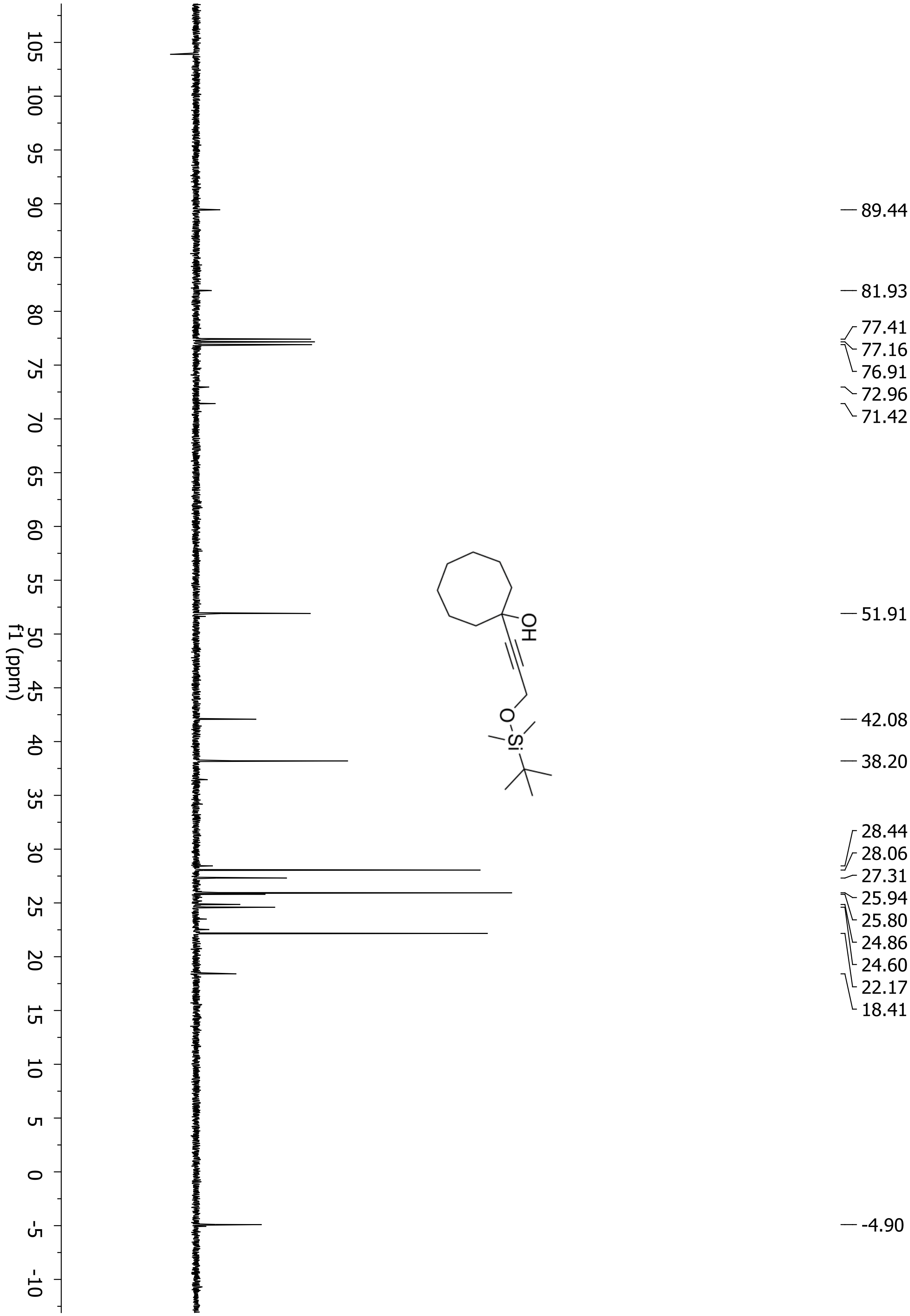


2.02
2.00
1.99
1.97
1.85
1.83
1.82
1.80
1.65
1.64
1.63
1.62
1.61
1.59
1.59
1.58
1.58
1.57
1.54
f1 (ppm)
7.26
4.35
1.97
1.83
1.63
1.62
1.59
1.59
1.58
1.58
1.57
1.54
0.91
0.12
1.93
2.00
2.93
5.10
1.80
0.93
9.23
5.72
OH
O
Si
f1 (ppm)

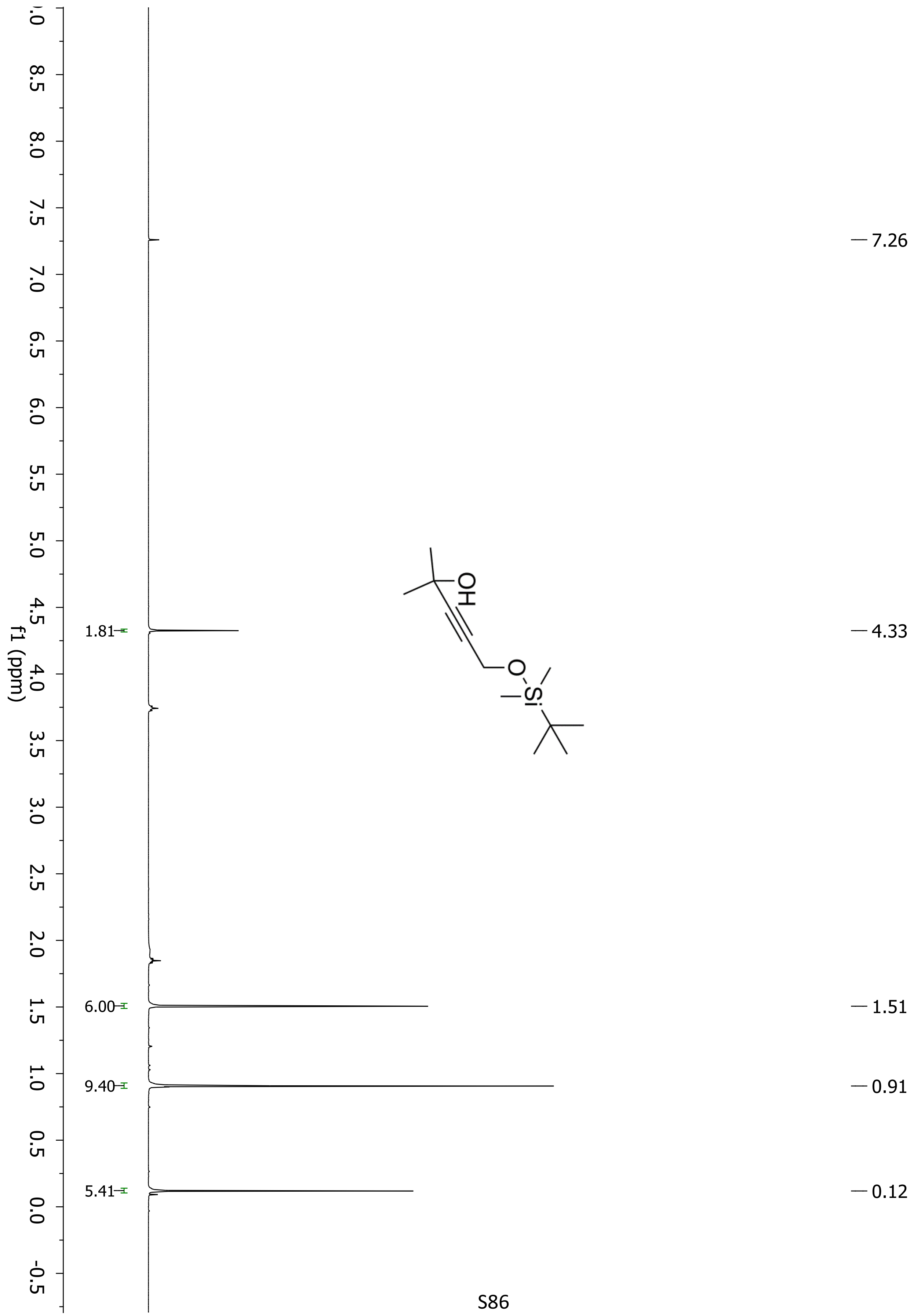

89.70
82.11
77.48
77.16
76.84
71.83
51.93
43.16
28.28
25.95
22.27
18.41
-4.90
f1 (ppm)
OH
O
Si



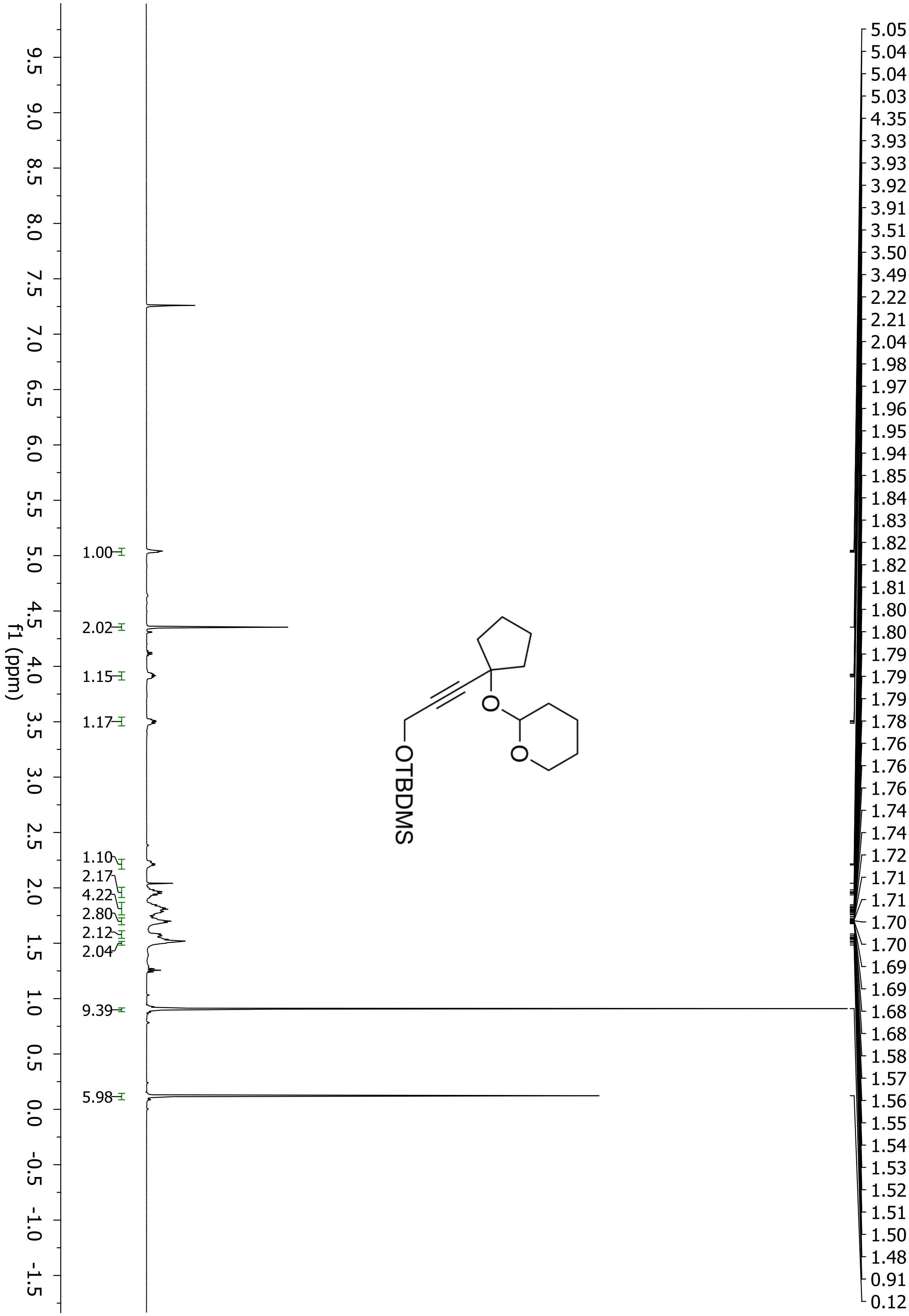
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-1.0
-2.0
f1 (ppm)
2.04
1.12
1.82
3.93
7.39
9.00
5.50
OH
O
Si

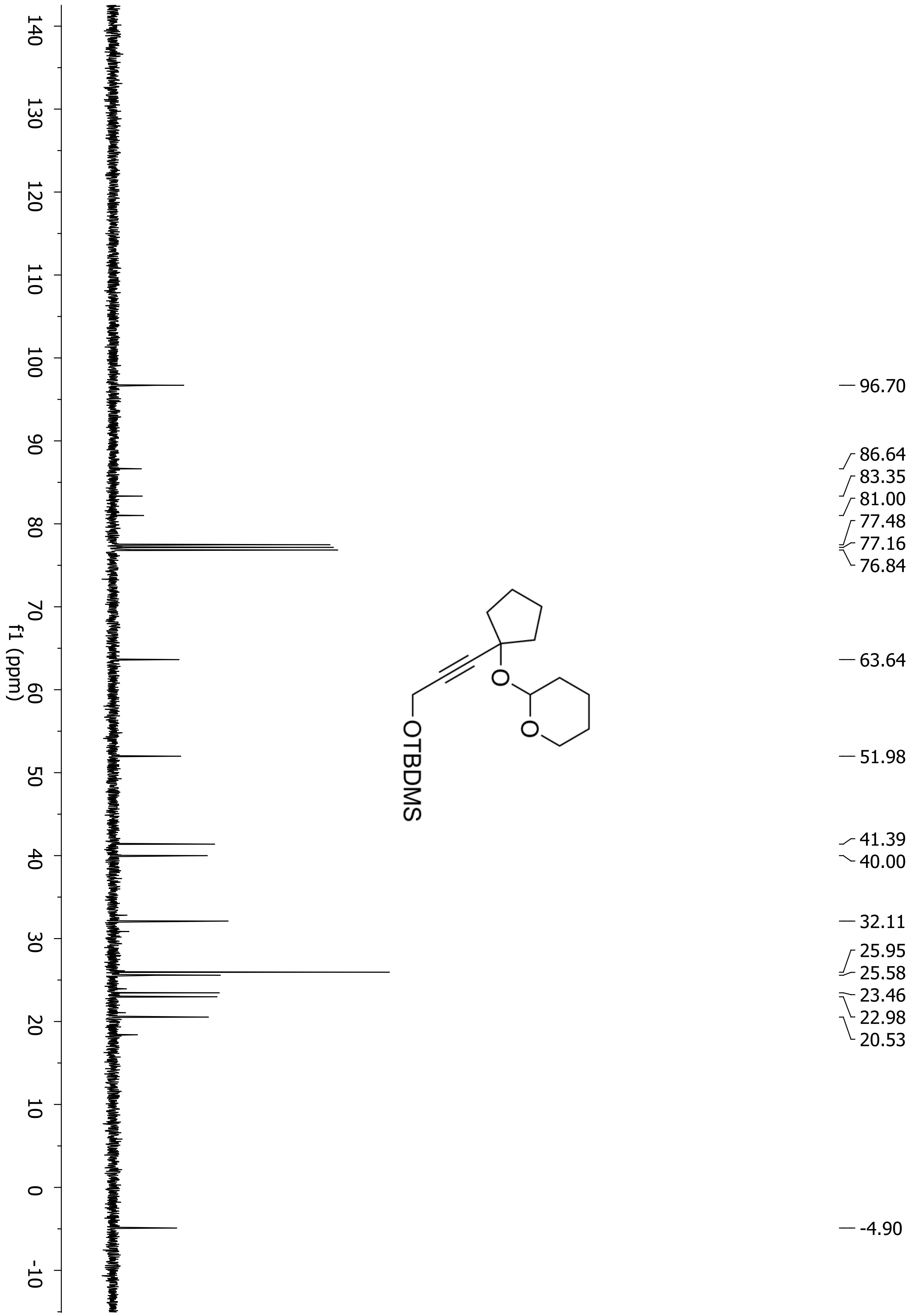


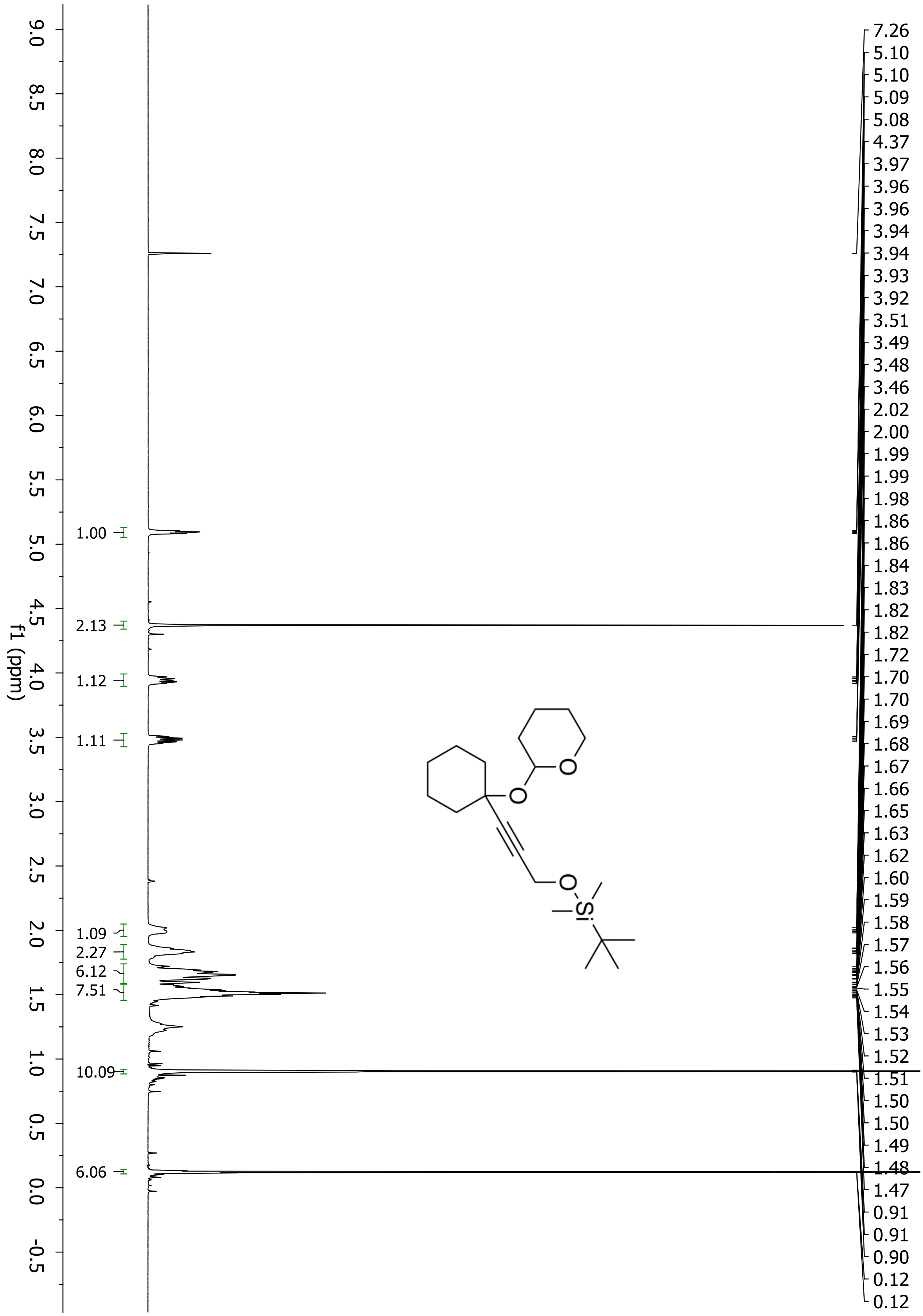
89.44
81.93
77.41
77.16
76.91
72.96
71.42
51.91
42.08
38.20
28.44
28.06
27.31
25.94
25.80
24.86
24.60
22.17
18.41
-4.90
OH
O
Si
f1 (ppm)



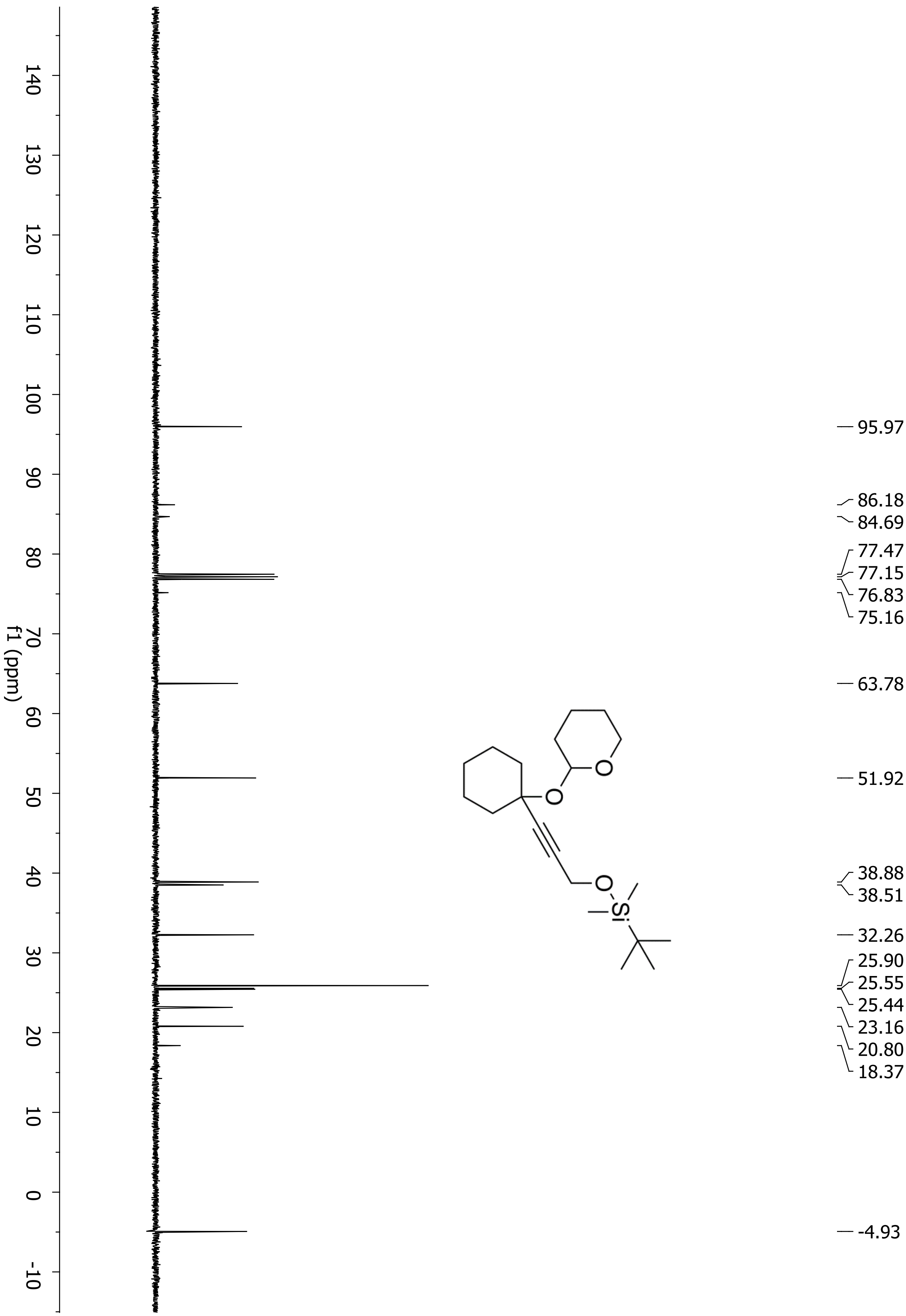
7.26
4.33
1.51
0.91
0.12
1.81
6.00
9.40
5.41
f1 (ppm)
OH
O
Si

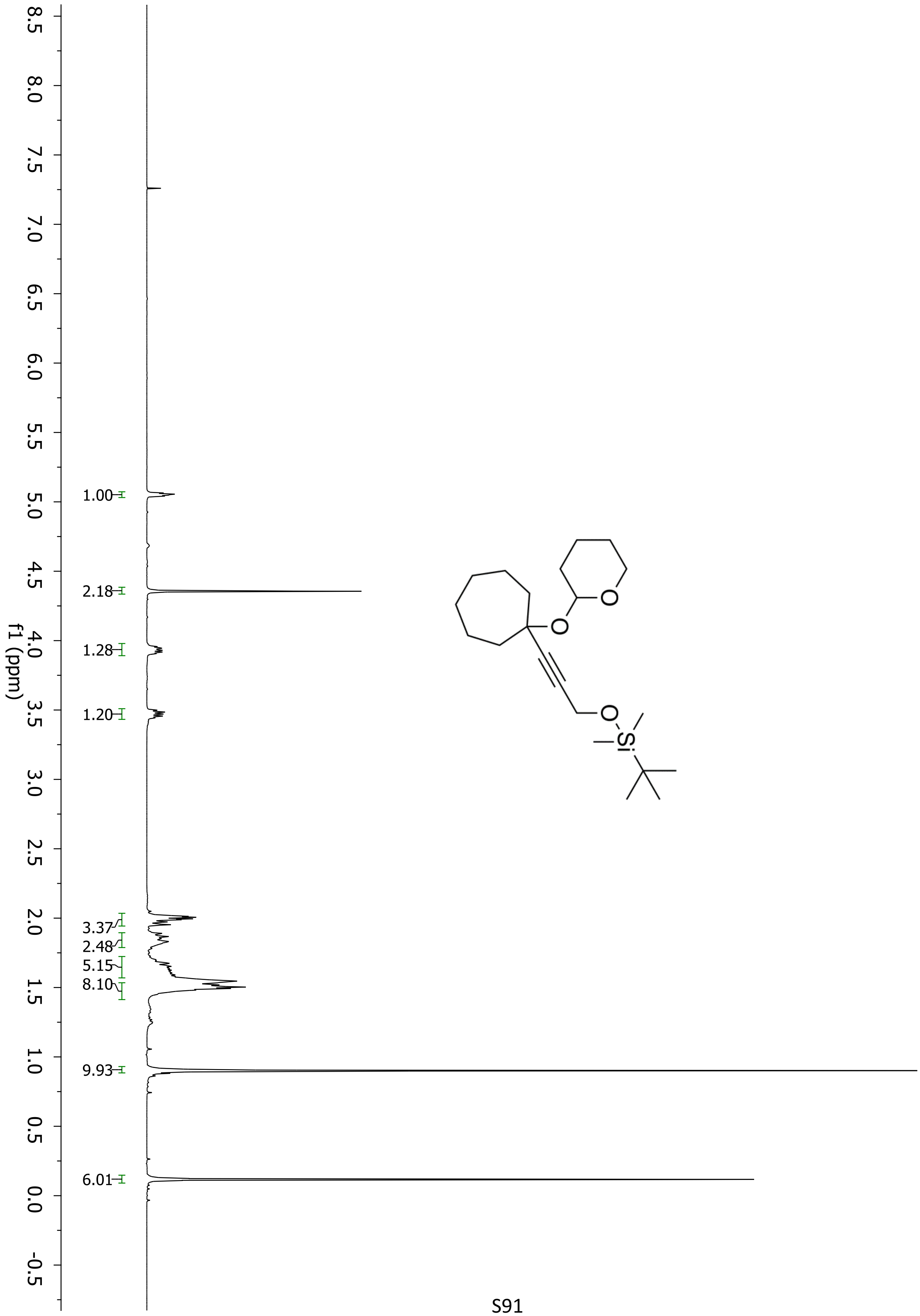

5.05
5.04
5.04
5.03
4.35
3.93
3.93
3.92
3.91
3.51
3.50
3.49
2.22
2.21
2.04
1.98
1.97
1.96
1.95
1.94
1.85
1.84
1.83
1.82
1.82
1.81
1.80
1.80
1.79
1.79
1.79
1.78
1.76
1.76
1.76
1.74
1.74
1.72
1.71
1.71
1.70
1.70
1.69
1.69
1.68
1.68
1.58
1.57
1.56
1.55
1.54
1.53
1.52
1.51
1.50
1.48
0.91
0.12
1.00
2.02
1.15
1.17
1.10
2.17
4.22
2.80
2.12
2.04
9.39
5.98
f1 (ppm)
OTBDMS


96.70
86.64
83.35
81.00
77.48
77.16
76.84
63.64
51.98
41.39
40.00
32.11
25.95
25.58
23.46
22.98
20.53
-4.90
f1 (ppm)
OTBDMS
O
O

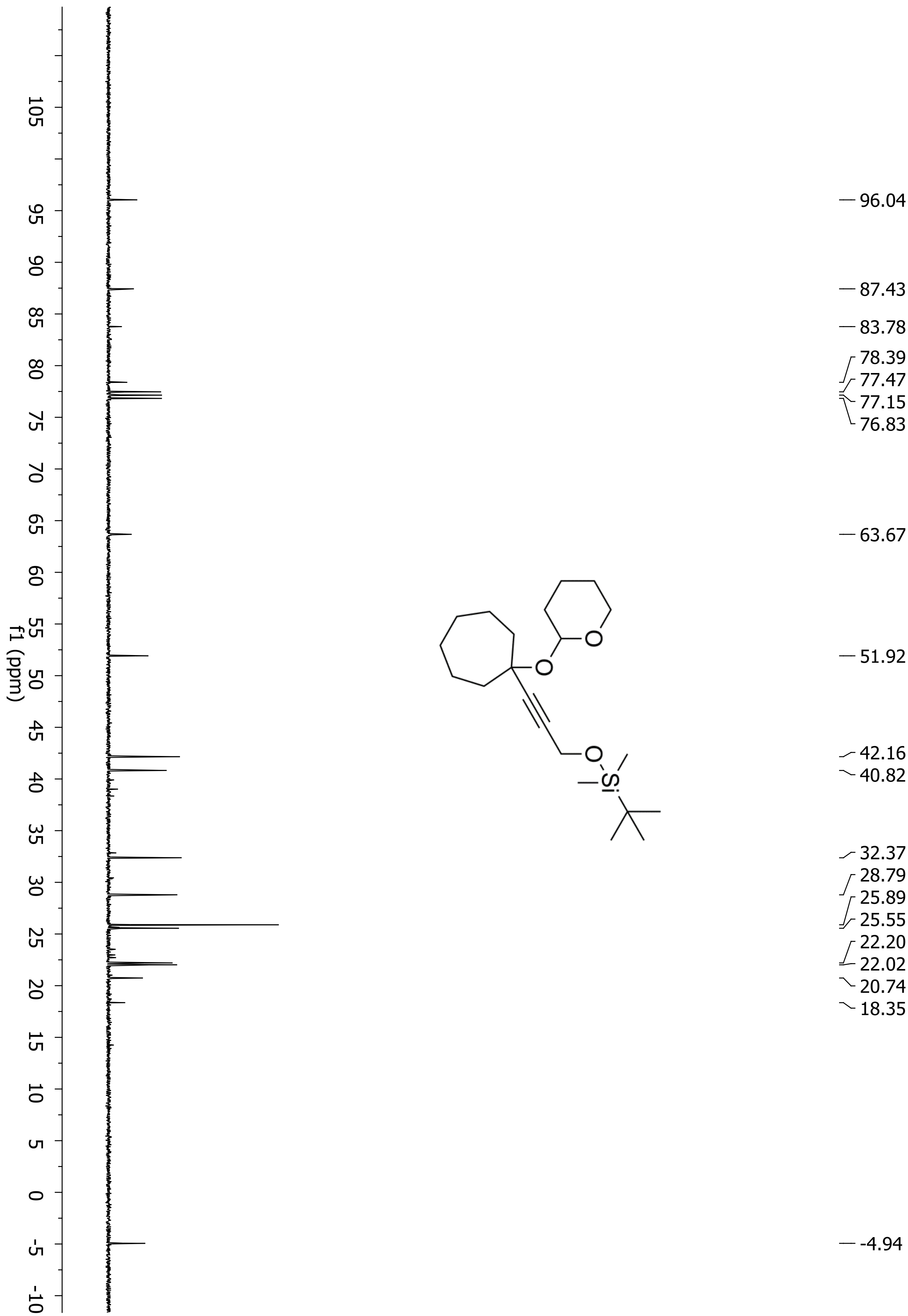


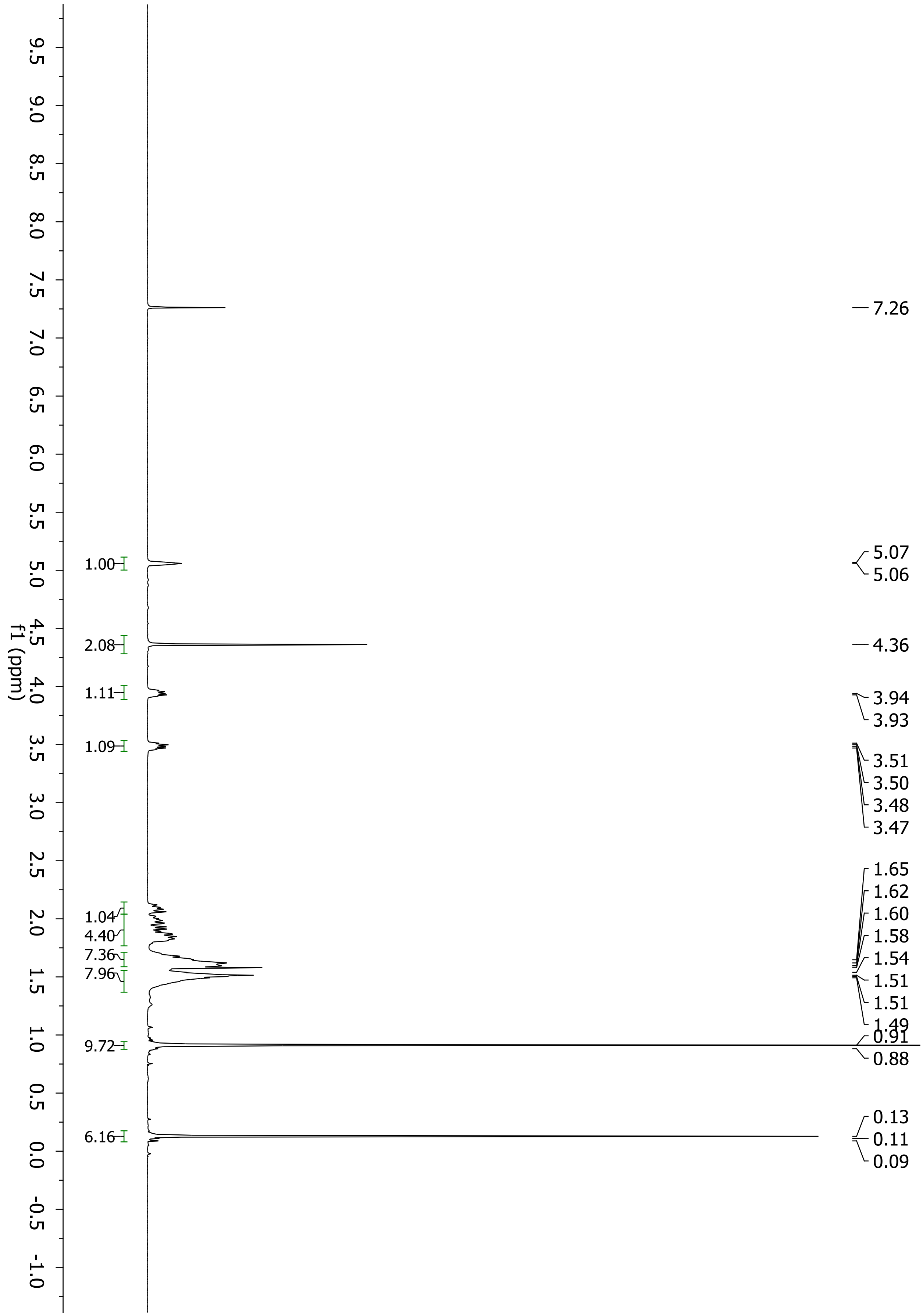
7.26
5.10
5.10
5.09
5.08
4.37
3.97
3.96
3.96
3.94
3.94
3.93
3.92
3.51
3.49
3.48
3.46
2.02
2.00
1.99
1.99
1.98
1.86
1.86
1.84
1.83
1.82
1.82
1.72
1.70
1.70
1.69
1.68
1.67
1.66
1.65
1.63
1.62
1.60
1.59
1.58
1.57
1.56
1.55
1.54
1.53
1.52
1.51
1.50
1.50
1.49
1.48
1.47
0.91
0.91
0.90
0.12
0.12
1.00
2.13
1.12
1.11
1.09
2.27
6.12
7.51
10.09
6.06
f1 (ppm)
O
O
O
Si

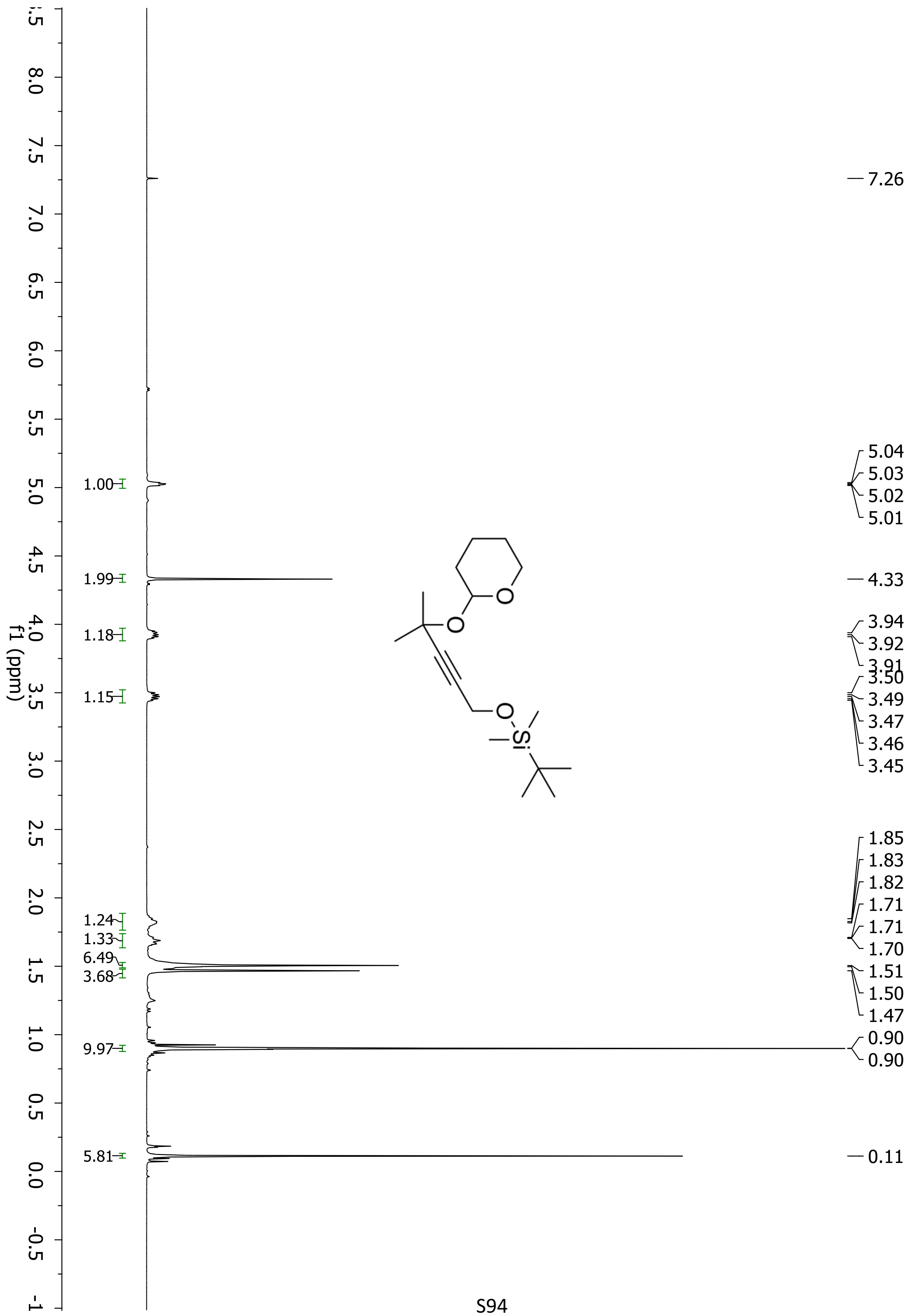

95.97
86.18
84.69
77.47
77.15
76.83
75.16
63.78
51.92
38.88
38.51
32.26
25.90
25.55
25.44
23.16
20.80
18.37
-4.93
f1 (ppm)
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
O
O
O
Si

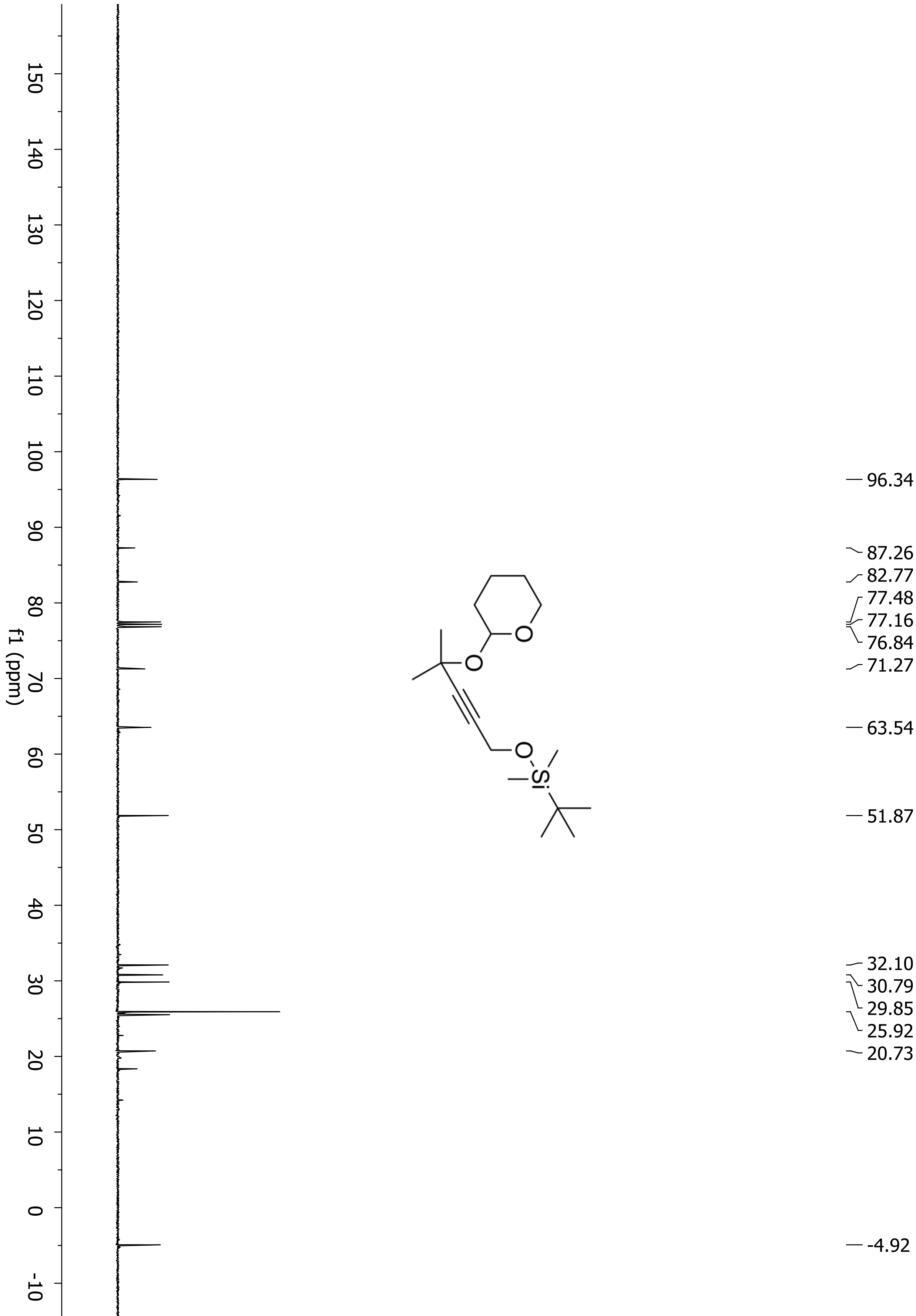


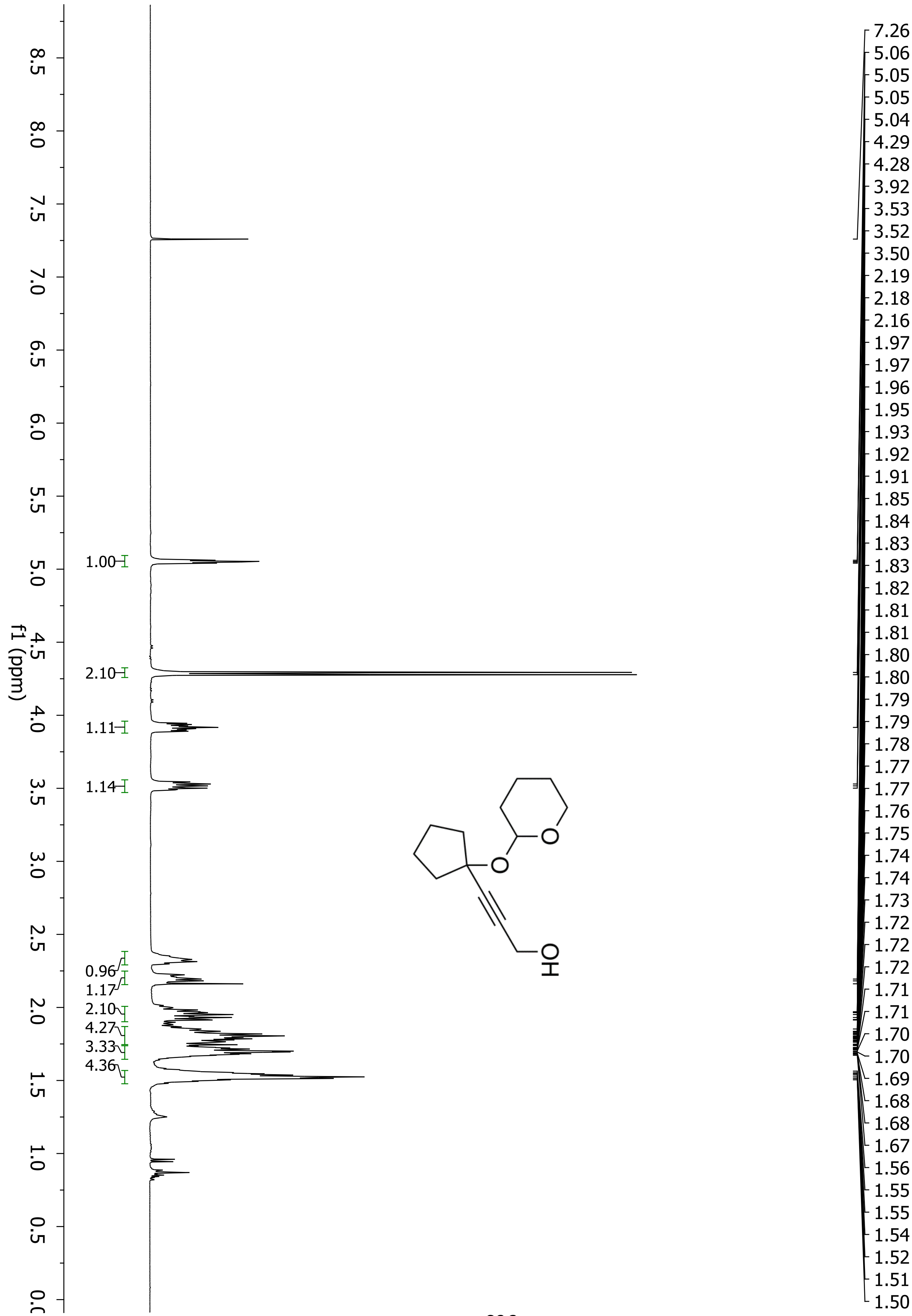
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
1.00
2.18
1.28
1.20
3.37
2.48
5.15
8.10
9.93
6.01
O
O
O
Si

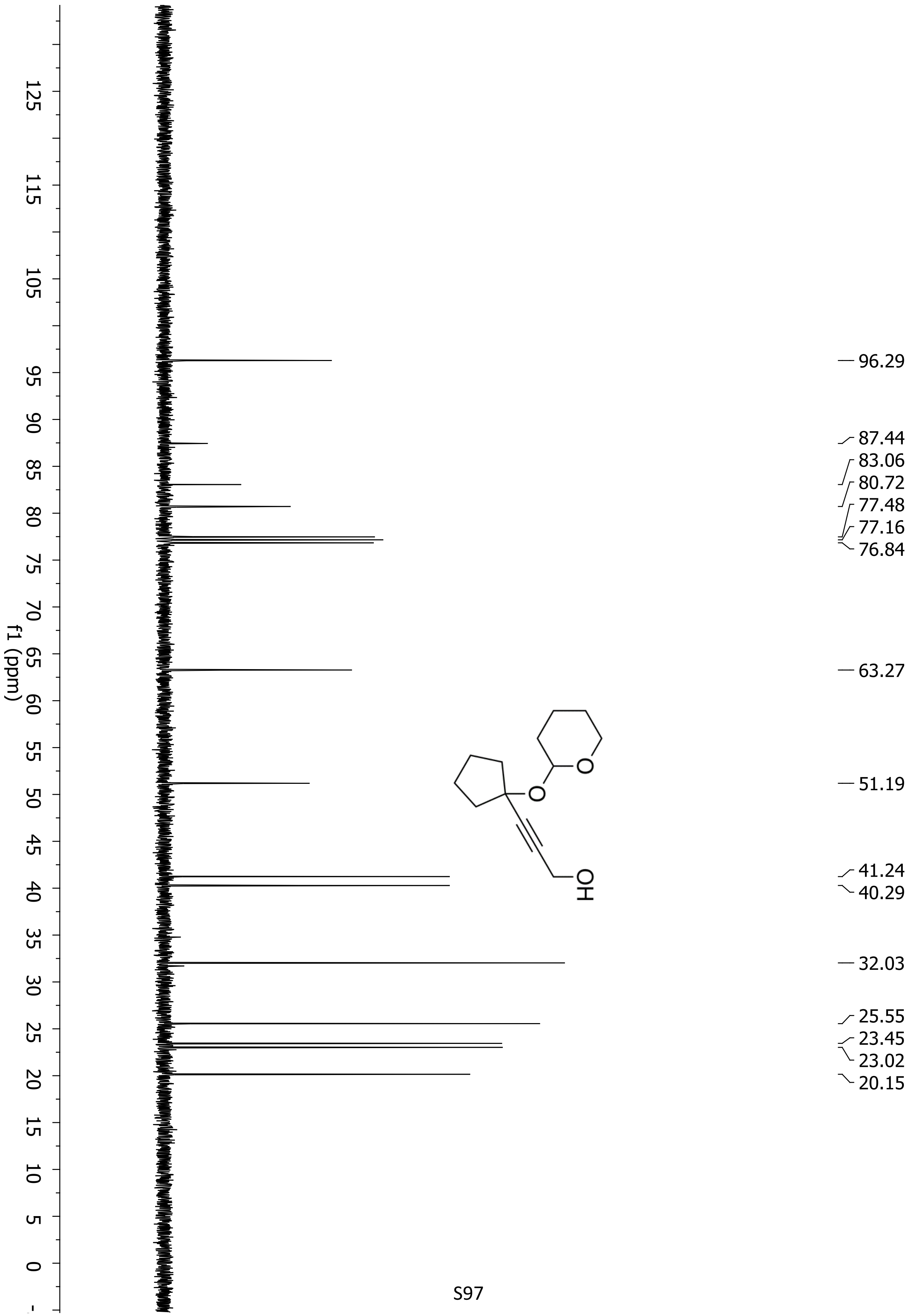

96.04
87.43
83.78
78.39
77.47
77.15
76.83
63.67
51.92
42.16
40.82
32.37
28.79
25.89
25.55
22.20
22.02
20.74
18.35
-4.94
f1 (ppm)
O
O
O
Si

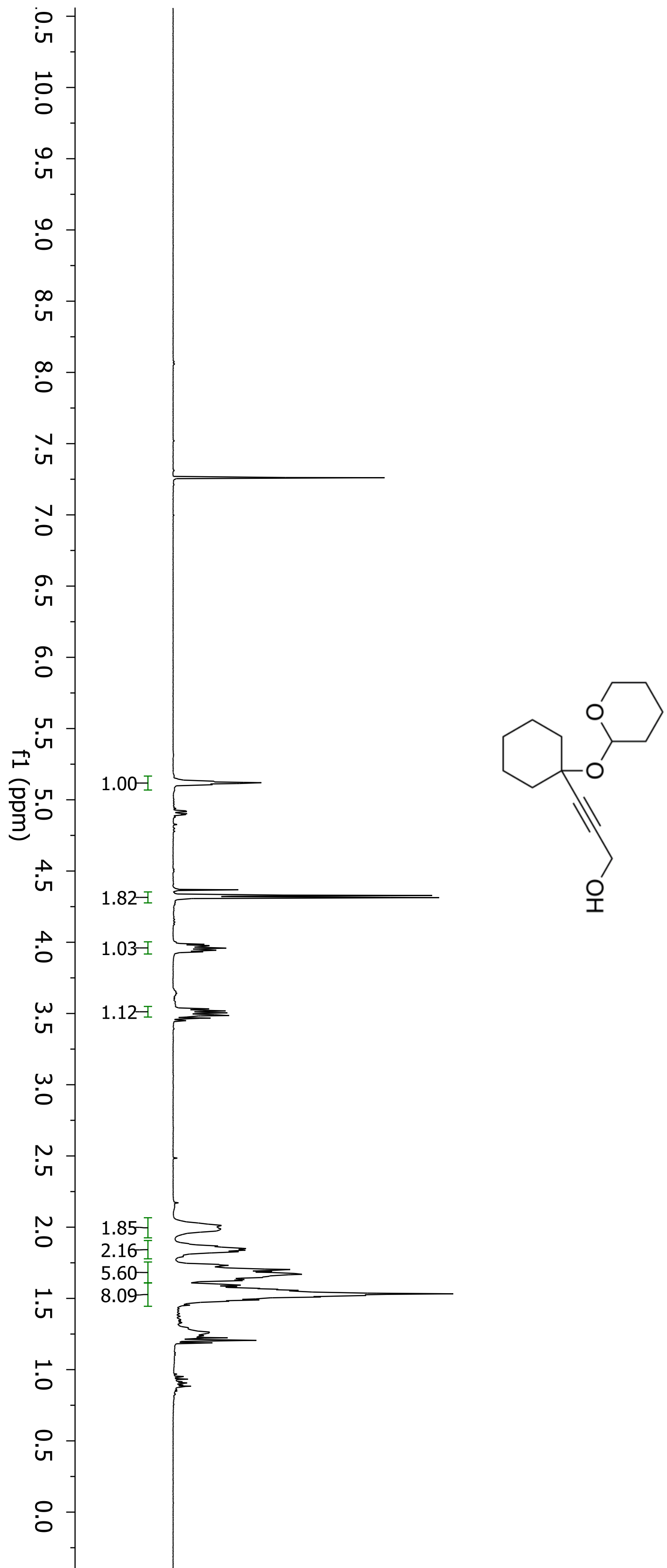

7.26
5.07
5.06
4.36
3.94
3.93
3.51
3.50
3.48
3.47
1.65
1.62
1.60
1.58
1.54
1.51
1.51
1.49
0.91
0.88
0.13
0.11
0.09
1.00
2.08
1.11
1.09
1.04
4.40
7.36
7.96
9.72
6.16
f1 (ppm)


7.26
5.04
5.03
5.02
5.01
4.33
3.94
3.92
3.91
3.50
3.49
3.47
3.46
3.45
1.85
1.83
1.82
1.71
1.71
1.70
1.51
1.50
1.47
0.90
0.90
0.11
1.00
1.99
1.18
1.15
1.24
1.33
6.49
3.68
9.97
5.81
f1 (ppm)
O
O
O
Si

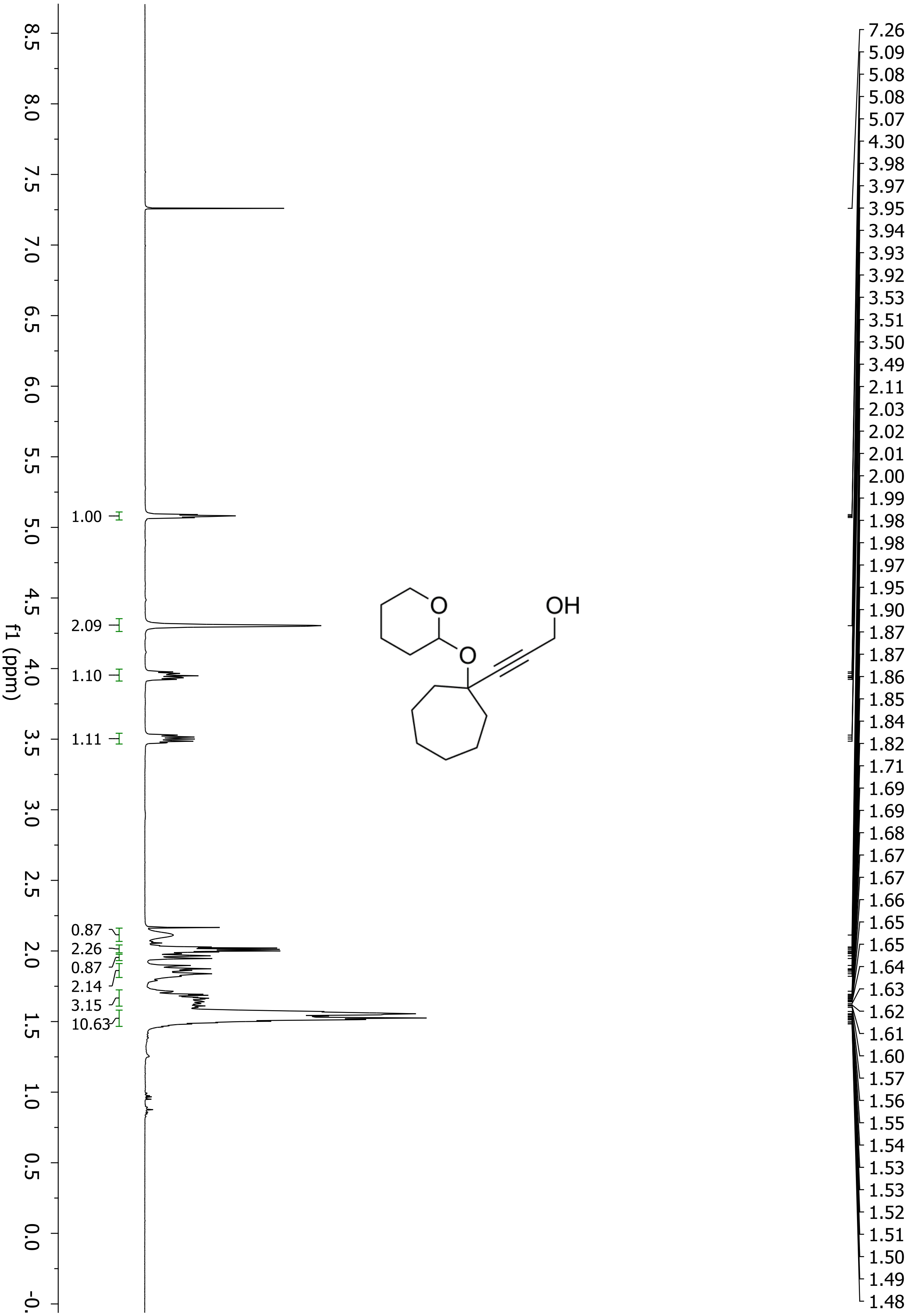

150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
96.34
87.26
82.77
77.48
77.16
76.84
71.27
63.54
51.87
32.10
30.79
29.85
25.92
20.73
-4.92
O
O
O
Si

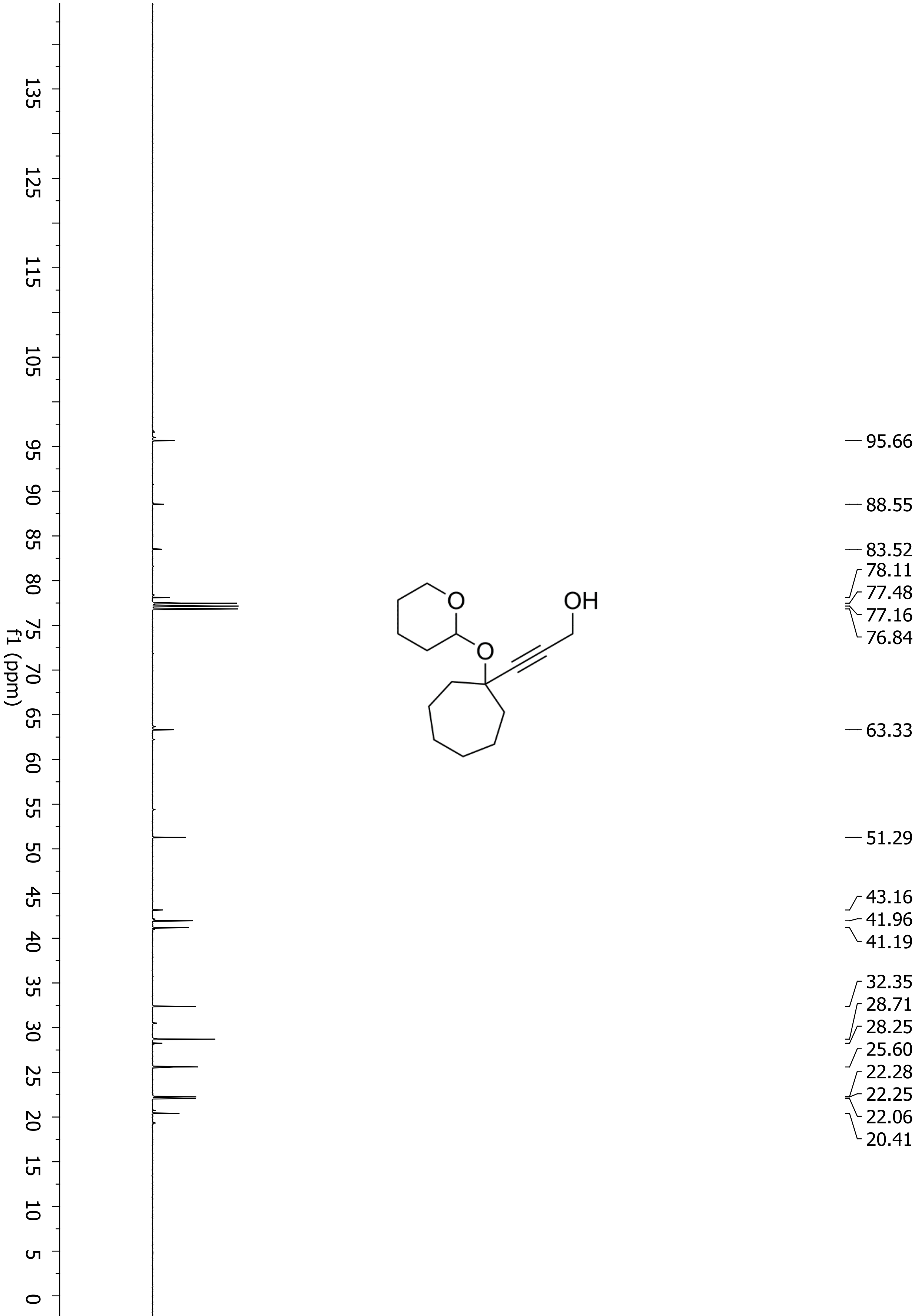

7.26
5.06
5.05
5.05
5.04
4.29
4.28
3.92
3.53
3.52
3.50
2.19
2.18
2.16
1.97
1.97
1.96
1.95
1.93
1.92
1.91
1.85
1.84
1.83
1.83
1.82
1.81
1.81
1.80
1.80
1.79
1.79
1.78
1.77
1.77
1.76
1.75
1.74
1.74
1.73
1.72
1.72
1.72
1.71
1.71
1.70
1.70
1.69
1.68
1.68
1.67
1.56
1.55
1.55
1.54
1.52
1.51
1.50
1.00
2.10
1.11
1.14
0.96
1.17
2.10
4.27
3.33
4.36
f1 (ppm)
OH
O
O

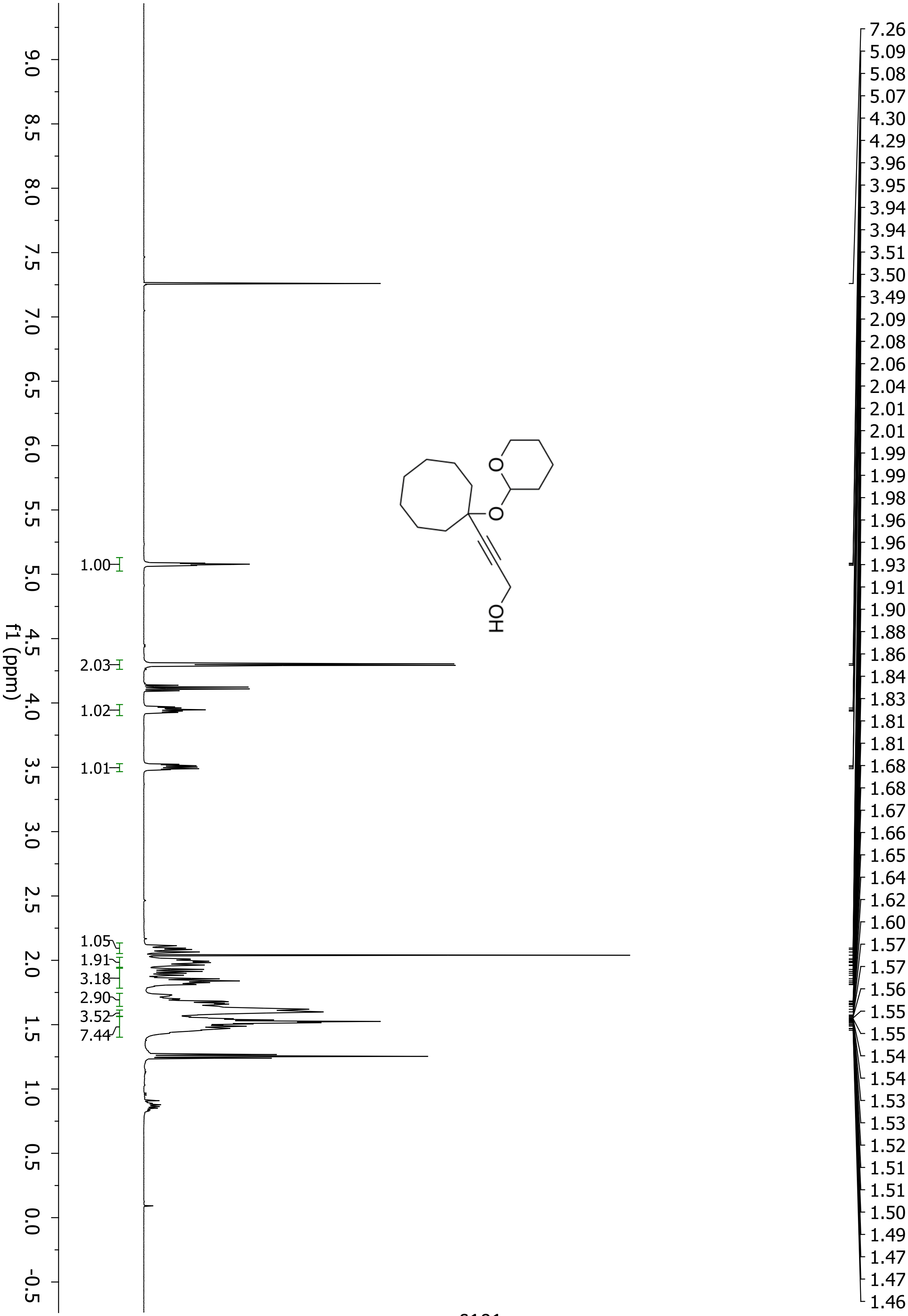

96.29
87.44
83.06
80.72
77.48
77.16
76.84
63.27
51.19
41.24
40.29
32.03
25.55
23.45
23.02
20.15
f1 (ppm)
O
O
OH

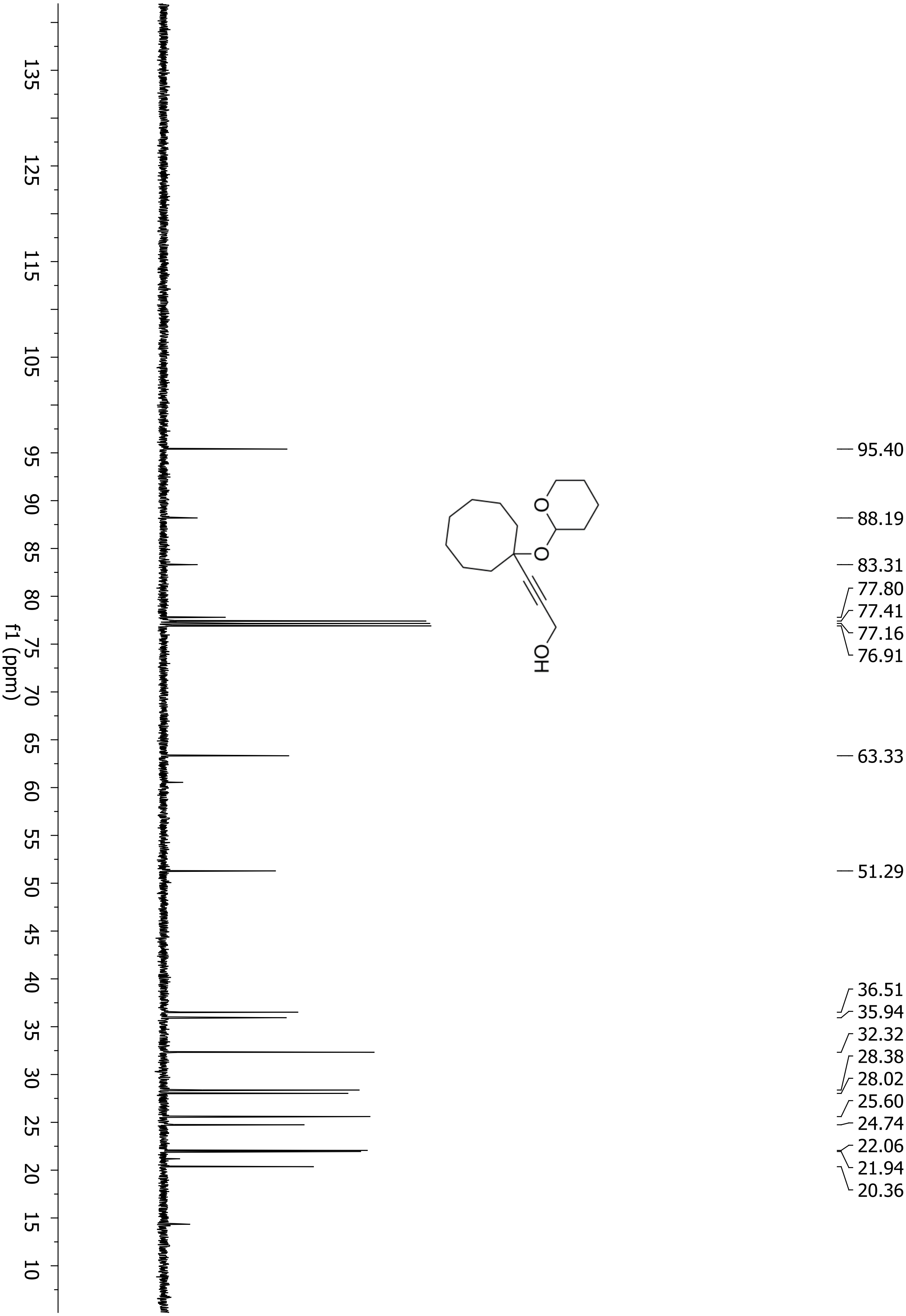


10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
1.00
1.82
1.03
1.12
1.85
2.16
5.60
8.09
O
O
OH

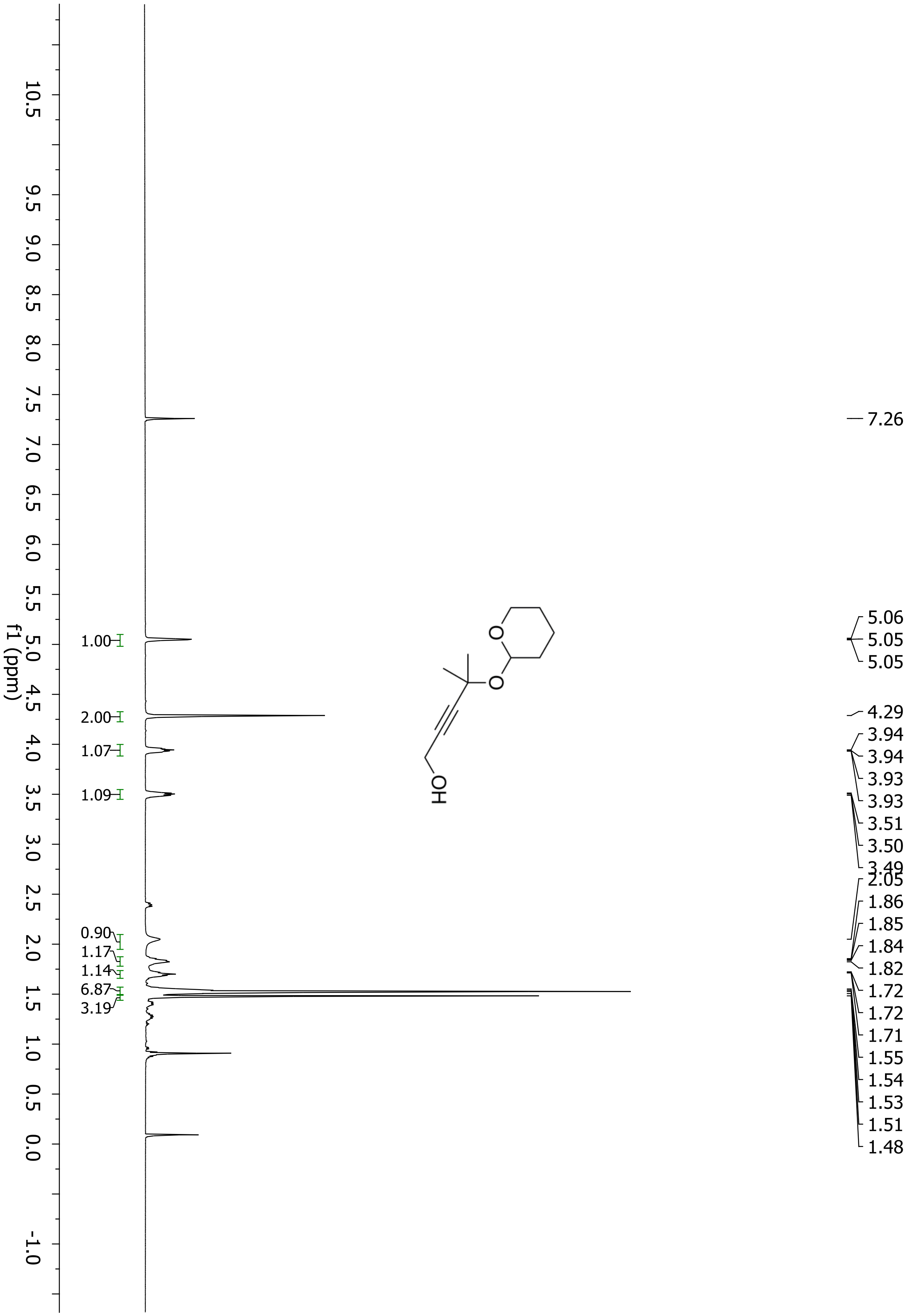

7.26
5.09
5.08
5.08
5.07
4.30
3.98
3.97
3.95
3.94
3.93
3.92
3.53
3.51
3.50
3.49
2.11
2.03
2.02
2.01
2.00
1.99
1.98
1.98
1.97
1.95
1.90
1.87
1.87
1.86
1.85
1.84
1.82
1.71
1.69
1.69
1.68
1.67
1.67
1.66
1.65
1.65
1.64
1.63
1.62
1.61
1.60
1.57
1.56
1.55
1.54
1.53
1.53
1.52
1.51
1.50
1.49
1.48
1.00
2.09
1.10
1.11
0.87
2.26
0.87
2.14
3.15
10.63
f1 (ppm)
OH
O
O


95.66
88.55
83.52
78.11
77.48
77.16
76.84
63.33
51.29
43.16
41.96
41.19
32.35
28.71
28.25
25.60
22.28
22.25
22.06
20.41
OH
O
O
f1 (ppm)

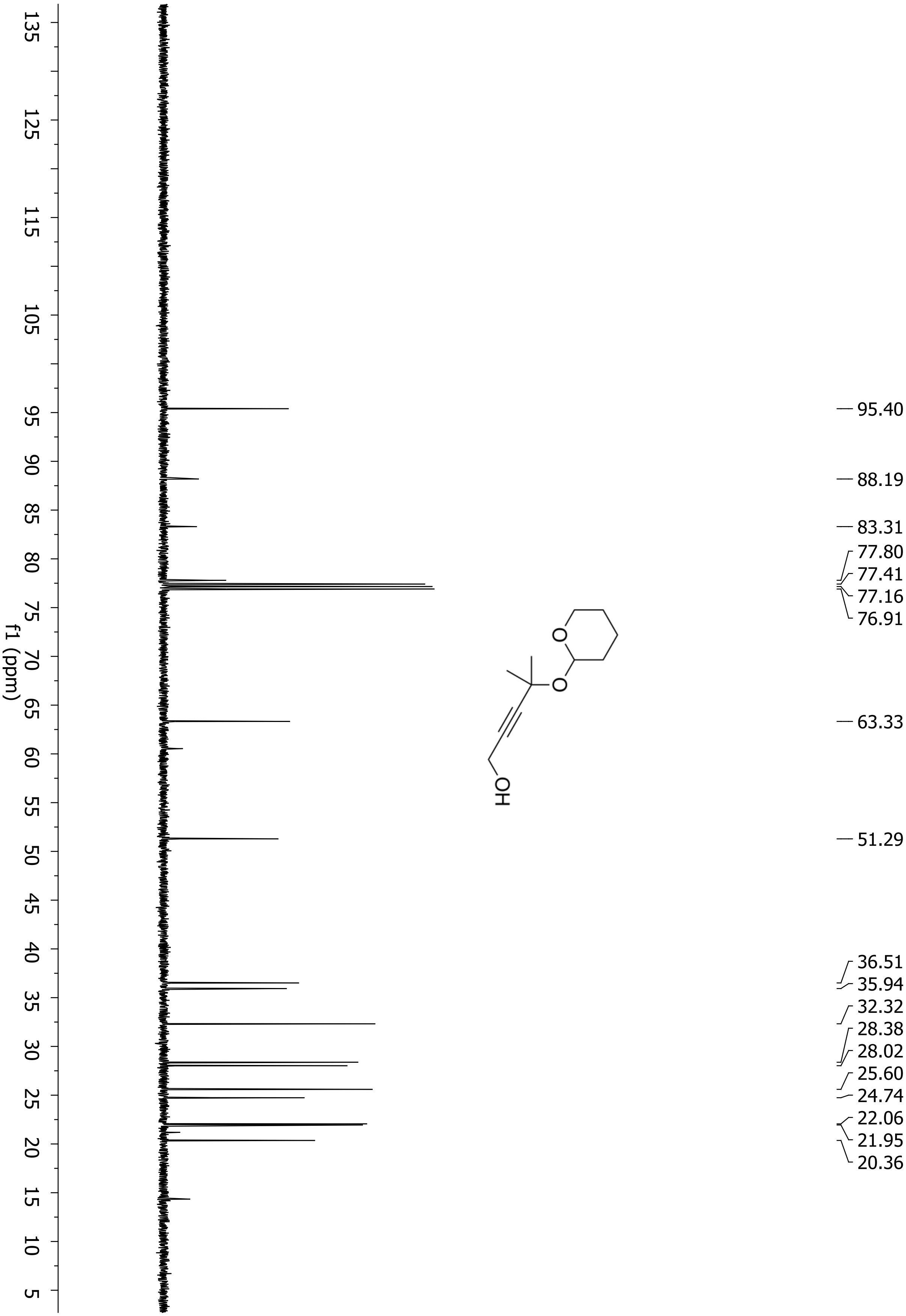

7.26
5.09
5.08
5.07
4.30
4.29
3.96
3.95
3.94
3.94
3.51
3.50
3.49
2.09
2.08
2.06
2.04
2.01
2.01
1.99
1.99
1.98
1.96
1.96
1.93
1.91
1.90
1.88
1.86
1.84
1.83
1.81
1.81
1.68
1.68
1.67
1.66
1.65
1.64
1.62
1.60
1.57
1.57
1.56
1.55
1.55
1.54
1.54
1.53
1.53
1.52
1.51
1.51
1.50
1.49
1.47
1.47
1.46
1.00
2.03
1.02
1.01
1.05
1.91
3.18
2.90
3.52
7.44
O
O
OH
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5



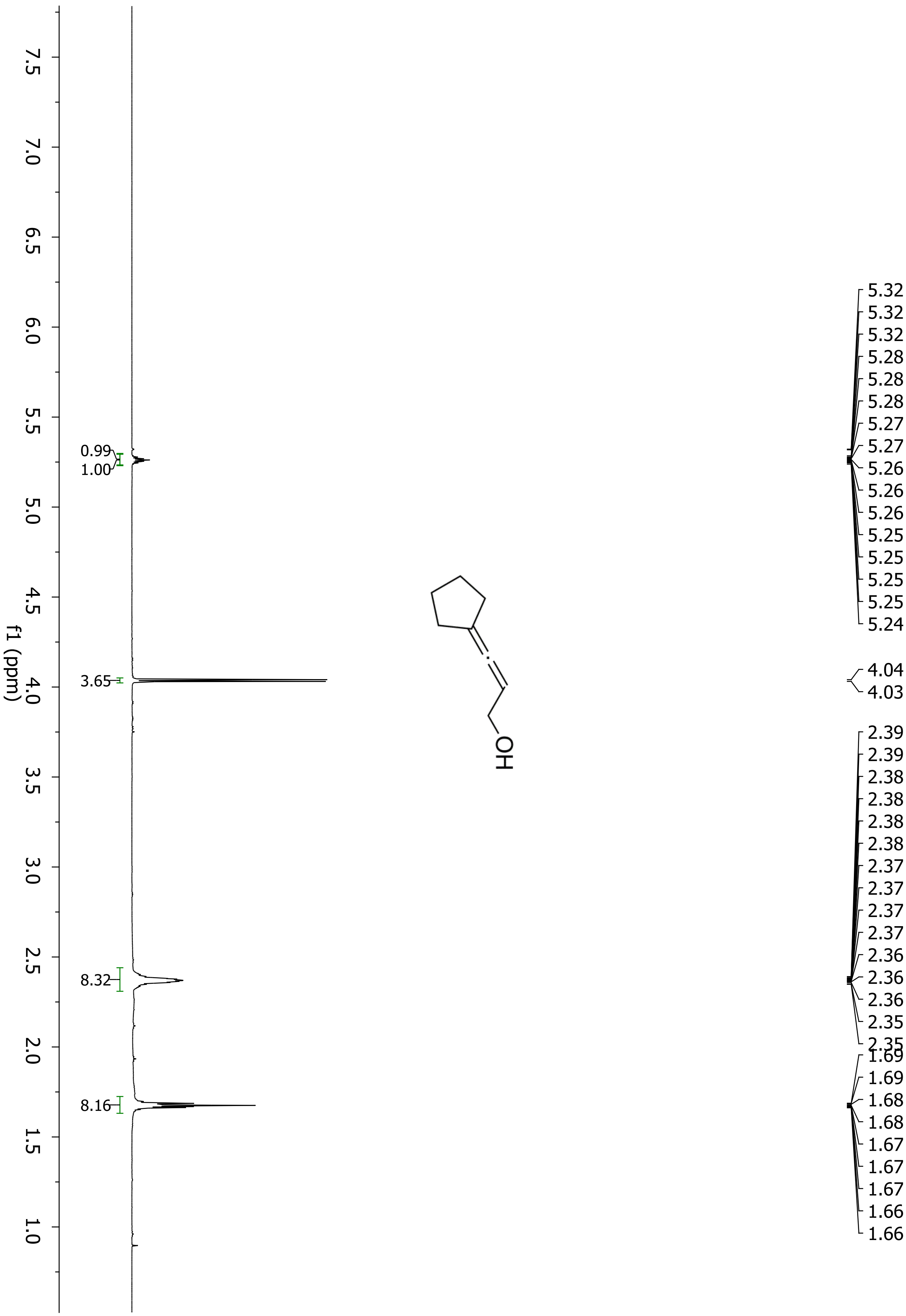
95.40
88.19
83.31
77.80
77.41
77.16
76.91
63.33
51.29
36.51
35.94
32.32
28.38
28.02
25.60
24.74
22.06
21.94
20.36
f1 (ppm)
OH
O
O

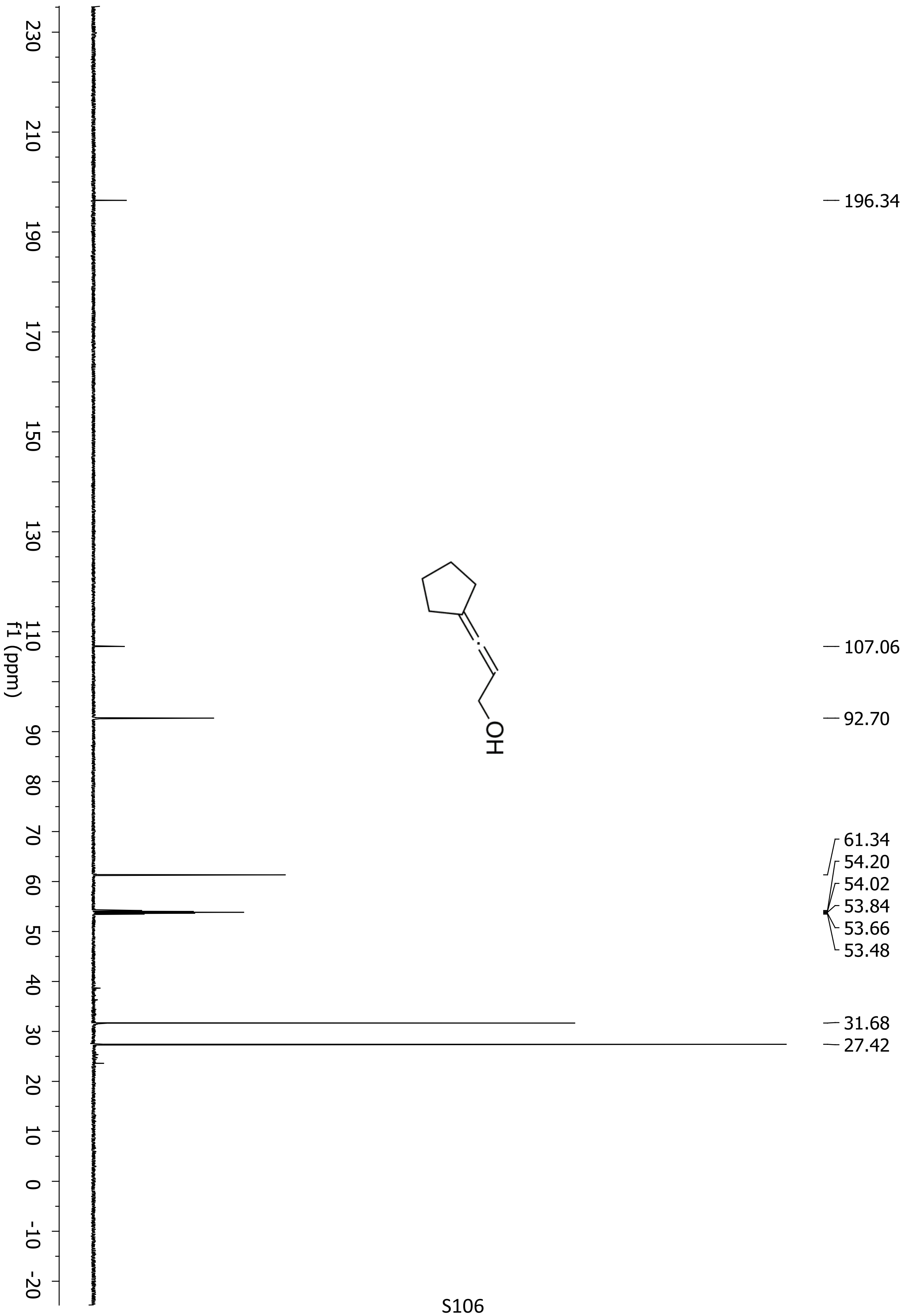


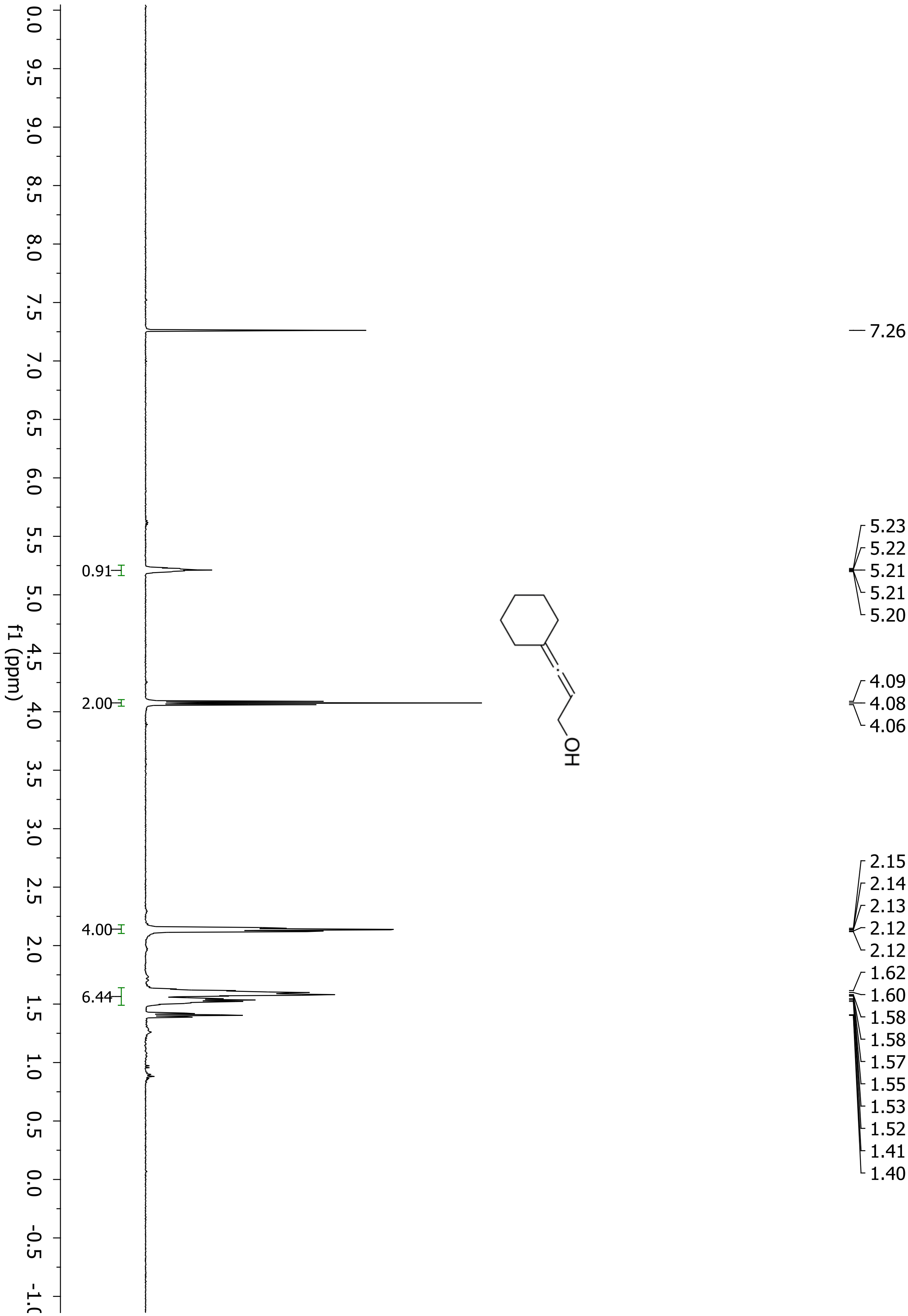
7.26
5.06
5.05
5.05
4.29
3.94
3.94
3.93
3.93
3.51
3.50
3.49
2.05
1.86
1.85
1.84
1.82
1.72
1.72
1.71
1.55
1.54
1.53
1.51
1.48
1.00
2.00
1.07
1.09
0.90
1.17
1.14
6.87
3.19
f1 (ppm)
OH
O
O



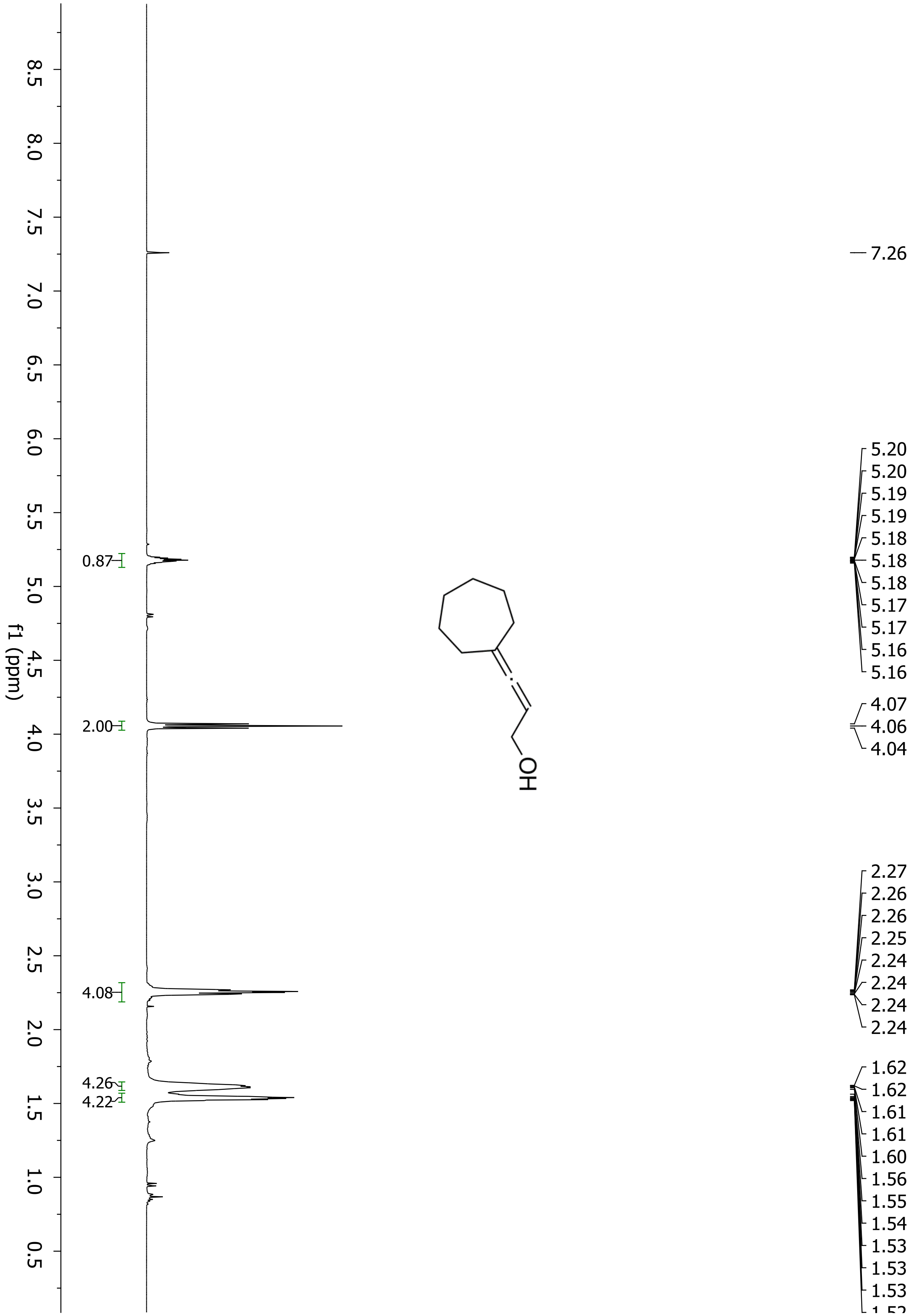
95.40
88.19
83.31
77.80
77.41
77.16
76.91
63.33
51.29
36.51
35.94
32.32
28.38
28.02
25.60
24.74
22.06
21.95
20.36
OH
O
O
f1 (ppm)

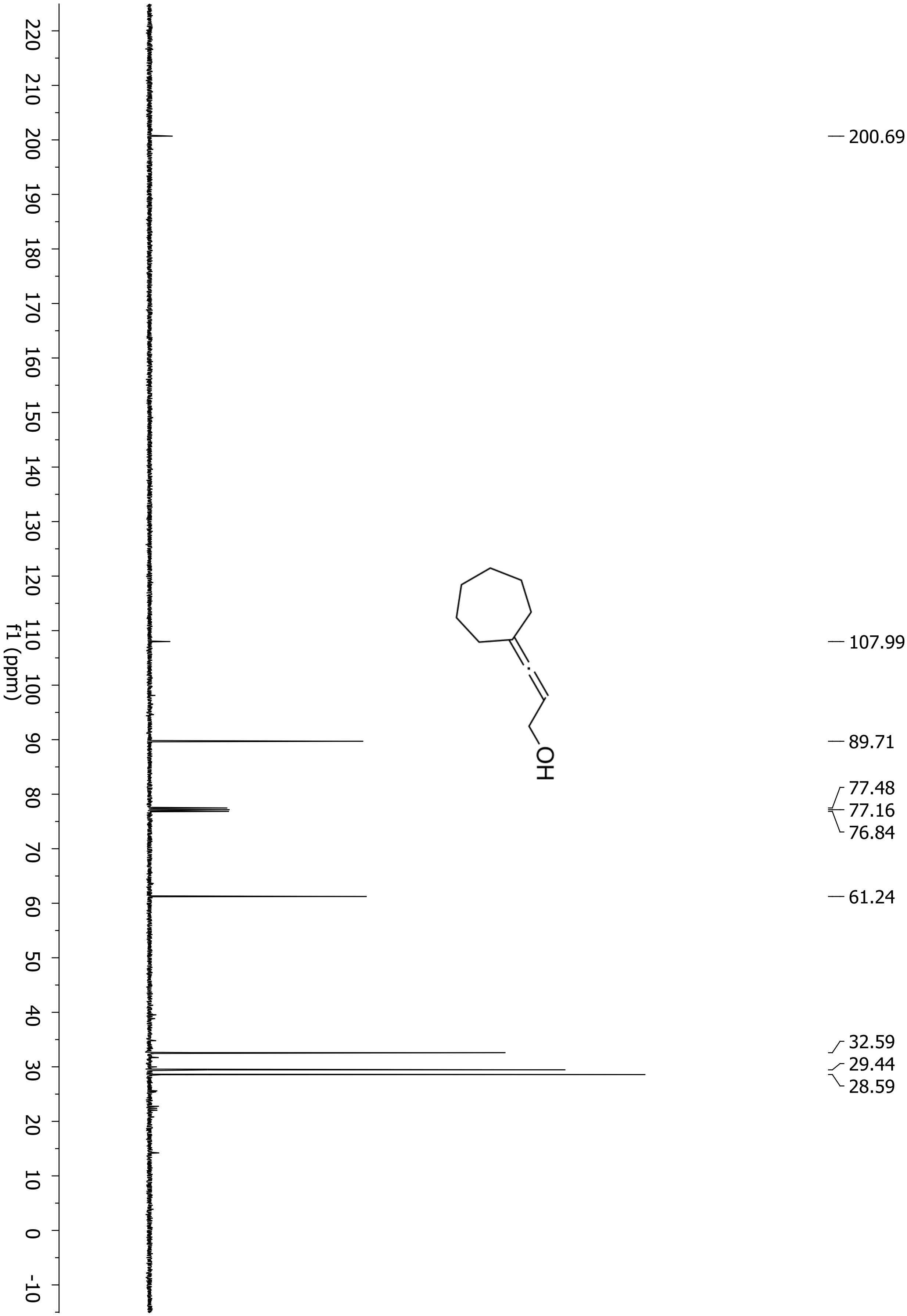

5.32
5.32
5.32
5.28
5.28
5.28
5.27
5.27
5.26
5.26
5.26
5.25
5.25
5.25
5.25
5.24
4.04
4.03
2.39
2.39
2.38
2.38
2.38
2.38
2.37
2.37
2.37
2.37
2.36
2.36
2.36
2.35
2.35
1.69
1.69
1.68
1.68
1.67
1.67
1.67
1.66
1.66
0.99
1.00
3.65
8.32
8.16
OH
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

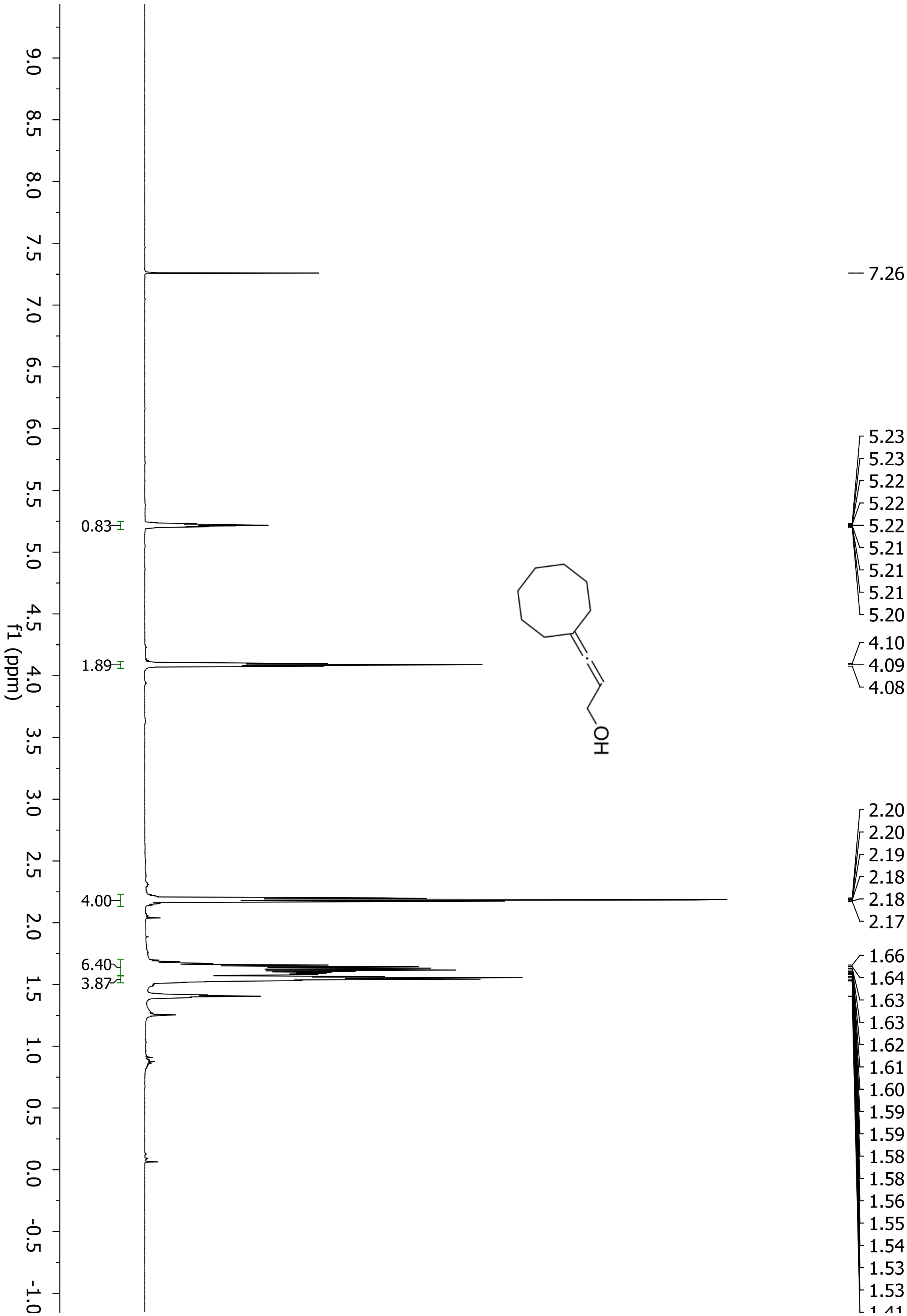

196.34
107.06
92.70
61.34
54.20
54.02
53.84
53.66
53.48
31.68
27.42
OH
f1 (ppm)



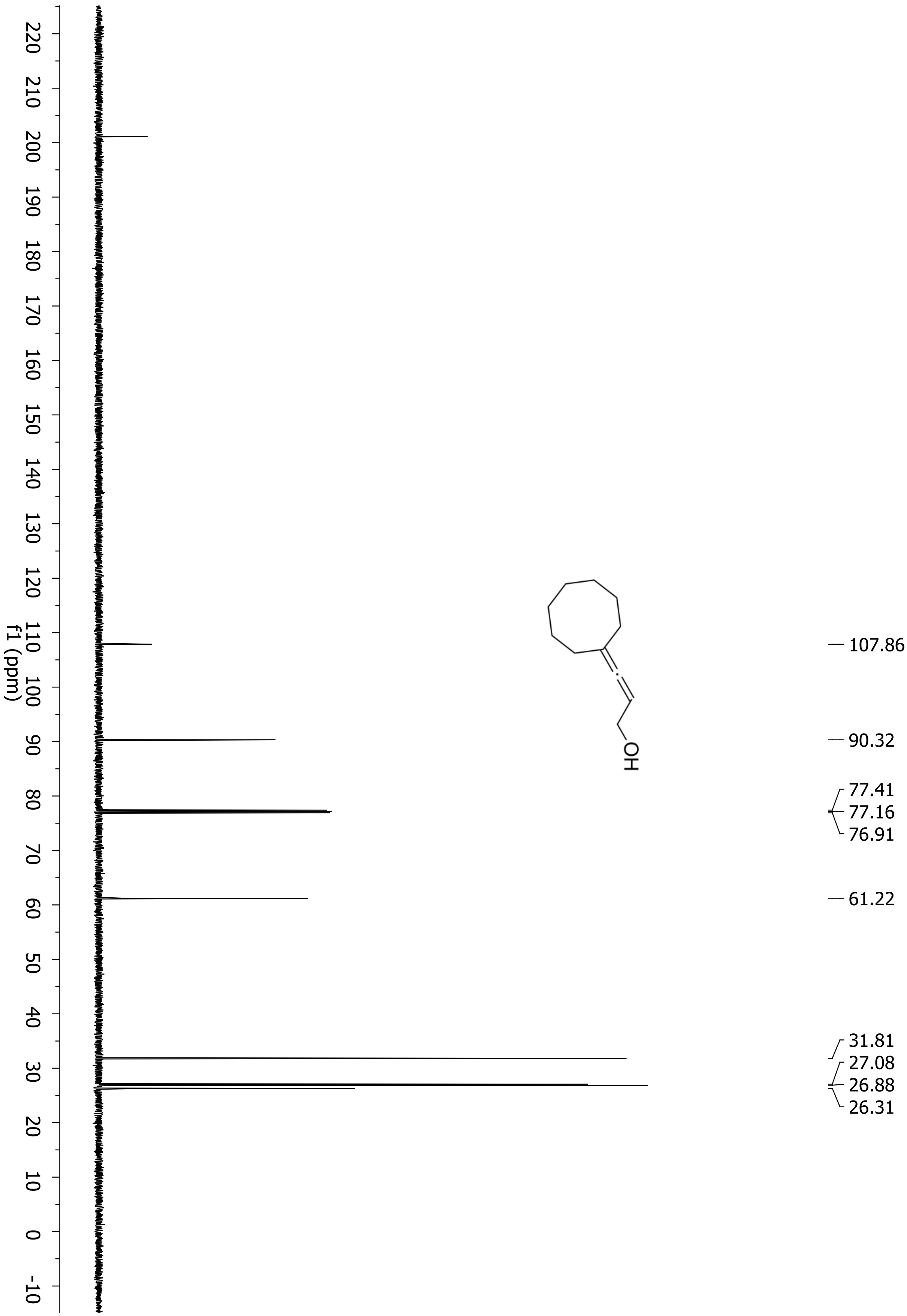
7.26
5.23
5.22
5.21
5.21
5.20
4.09
4.08
4.06
2.15
2.14
2.13
2.12
2.12
1.62
1.60
1.58
1.58
1.57
1.55
1.53
1.52
1.41
1.40
0.91
2.00
4.00
6.44
OH
f1 (ppm)

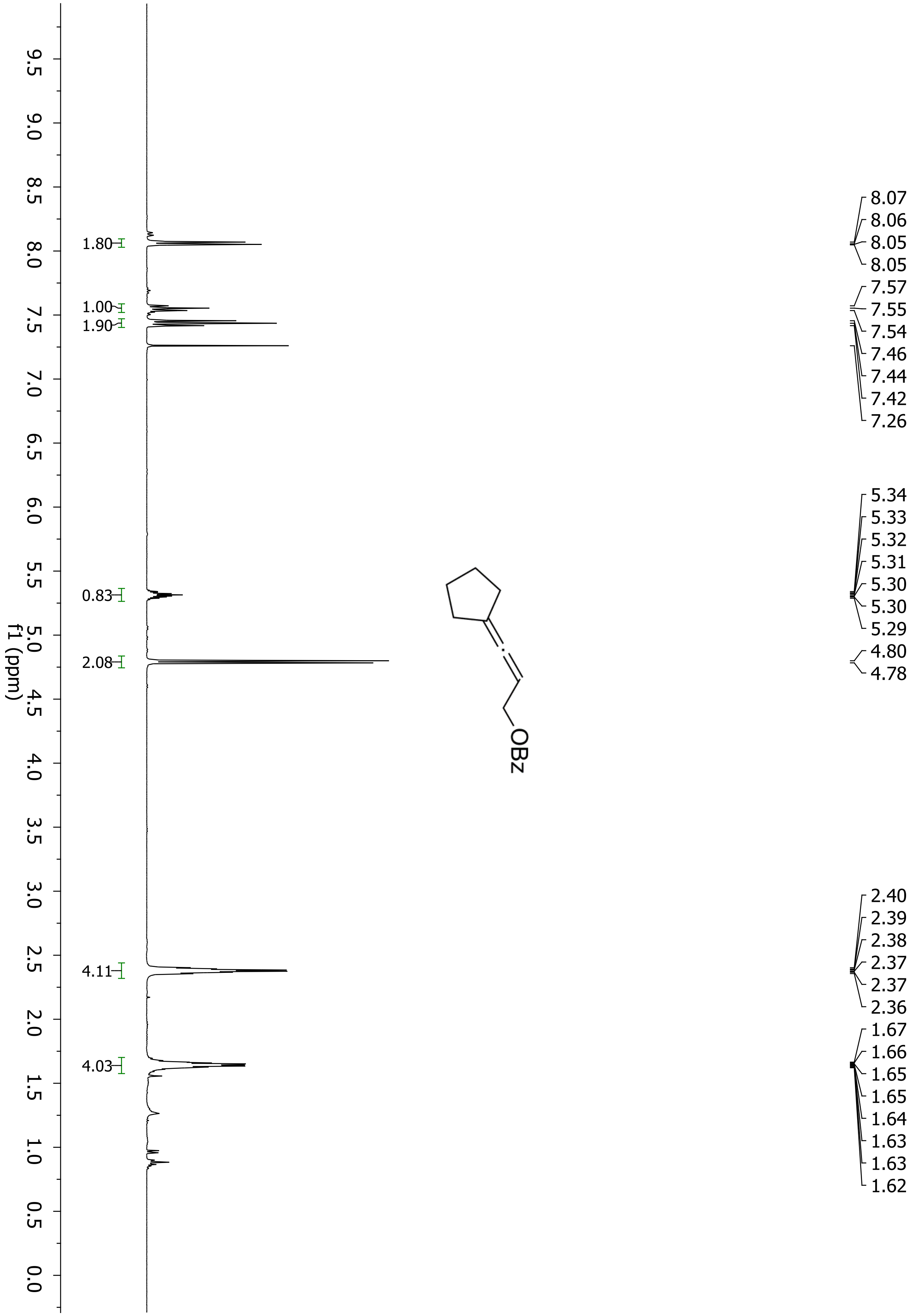

8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
0.87
2.00
4.08
4.26
4.22
OH
7.26
5.20
5.20
5.19
5.19
5.18
5.18
5.18
5.17
5.17
5.16
5.16
4.07
4.06
4.04
2.27
2.26
2.26
2.25
2.24
2.24
2.24
2.24
1.62
1.62
1.61
1.61
1.60
1.56
1.55
1.54
1.53
1.53
1.53

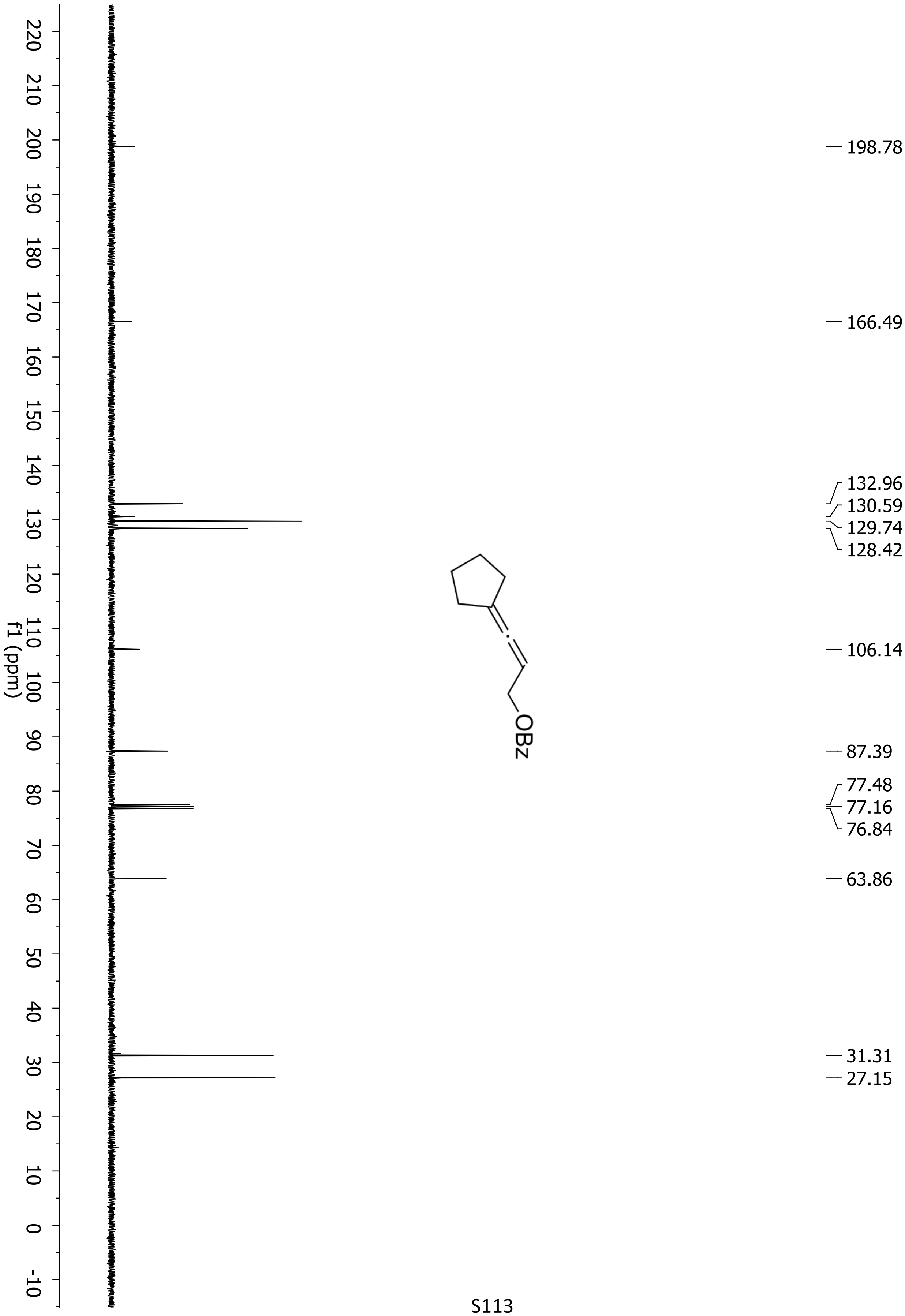

200.69
107.99
89.71
77.48
77.16
76.84
61.24
32.59
29.44
28.59
f1 (ppm)
OH



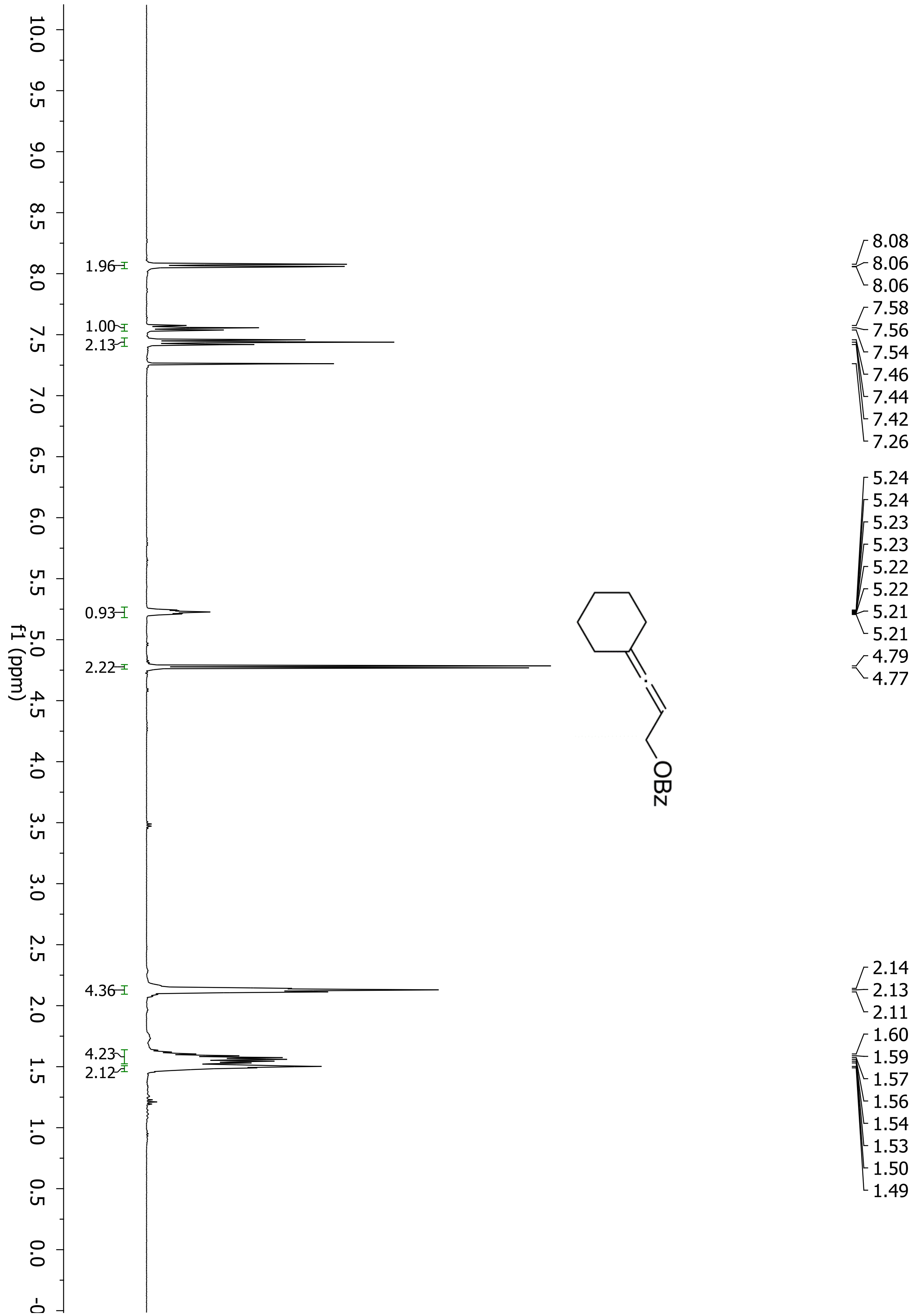
7.26
5.23
5.23
5.22
5.22
5.22
5.21
5.21
5.21
5.20
4.10
4.09
4.08
2.20
2.20
2.19
2.18
2.18
2.17
1.66
1.64
1.63
1.63
1.62
1.61
1.60
1.59
1.59
1.58
1.58
1.56
1.55
1.54
1.53
1.53
OH
0.83
1.89
4.00
6.40
3.87
f1 (ppm)

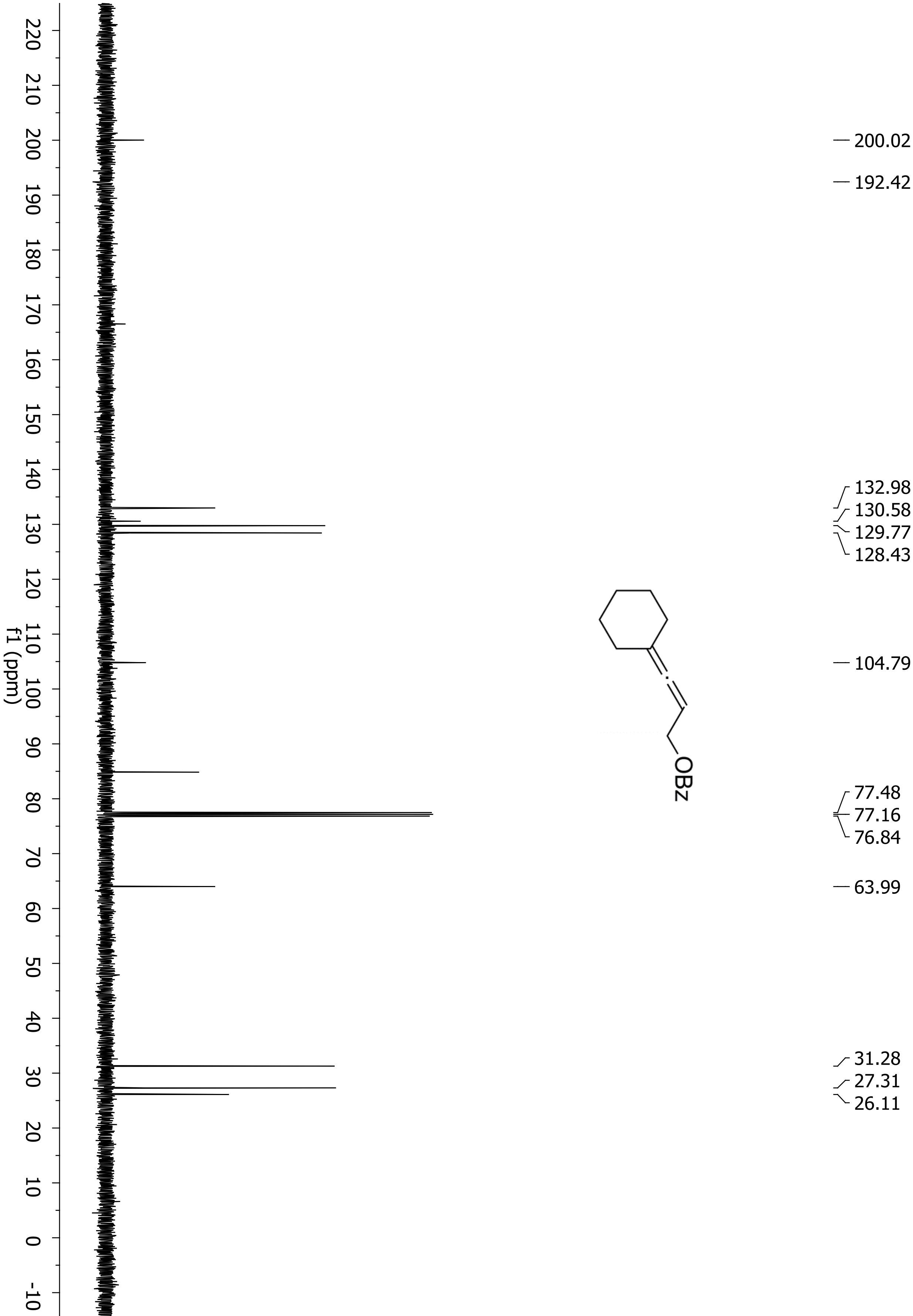

107.86
90.32
77.41
77.16
76.91
61.22
31.81
27.08
26.88
26.31
OH
f1 (ppm)

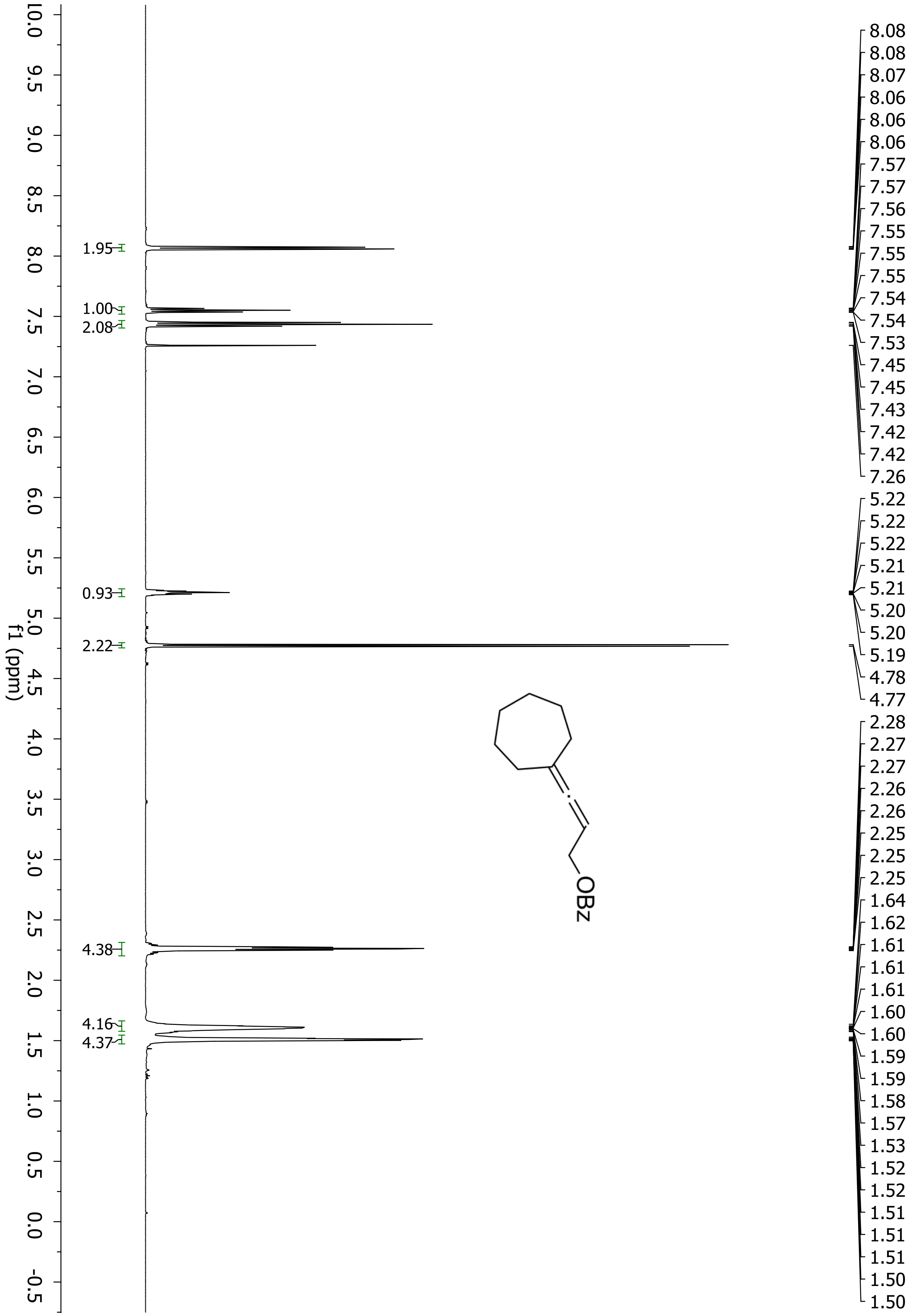

8.07
8.06
8.05
8.05
7.57
7.55
7.54
7.46
7.44
7.42
7.26
5.34
5.33
5.32
5.31
5.30
5.30
5.29
4.80
4.78
2.40
2.39
2.38
2.37
2.37
2.36
1.67
1.66
1.65
1.65
1.64
1.63
1.63
1.62
1.80
1.00
1.90
0.83
2.08
4.11
4.03
OBz
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

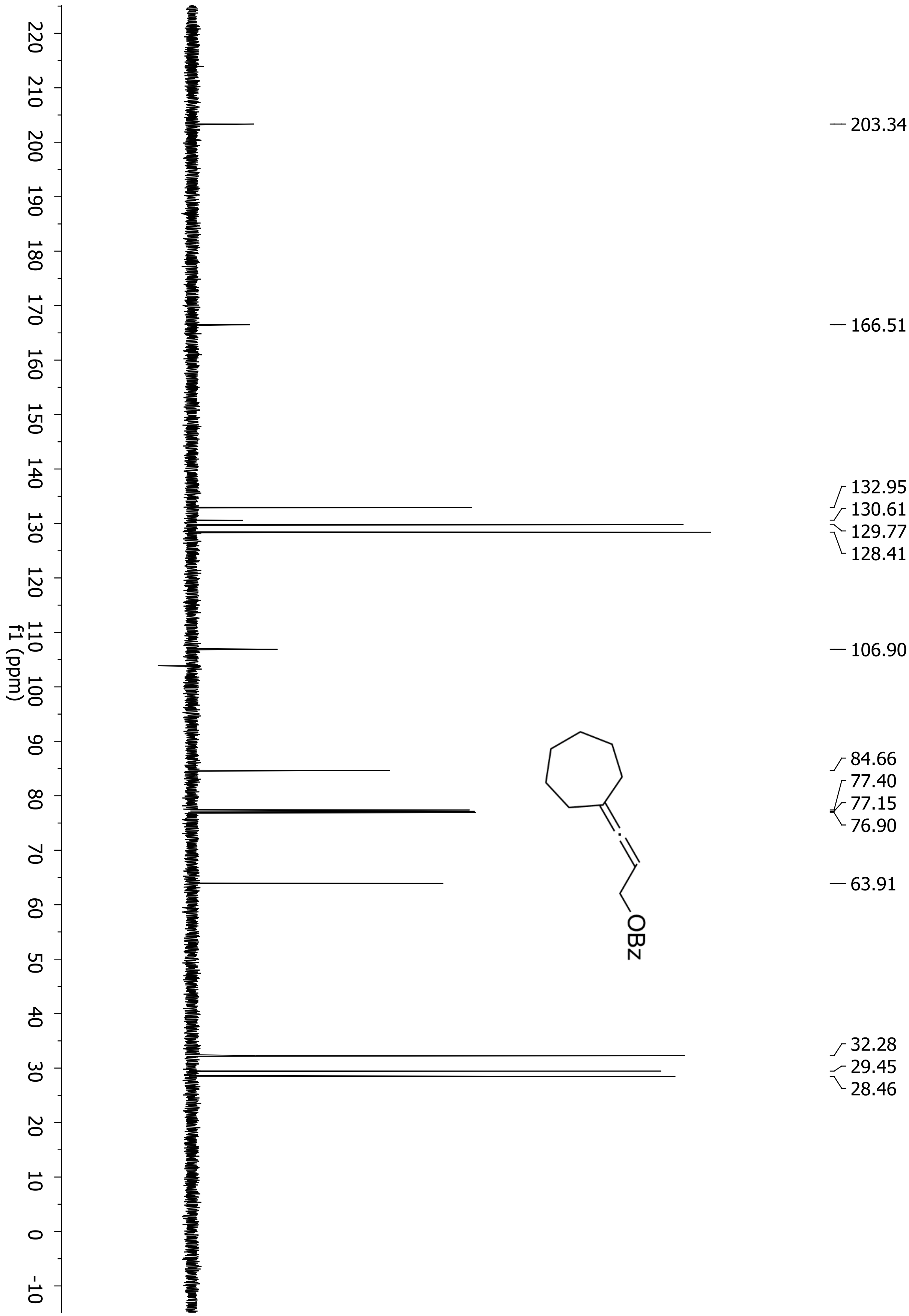


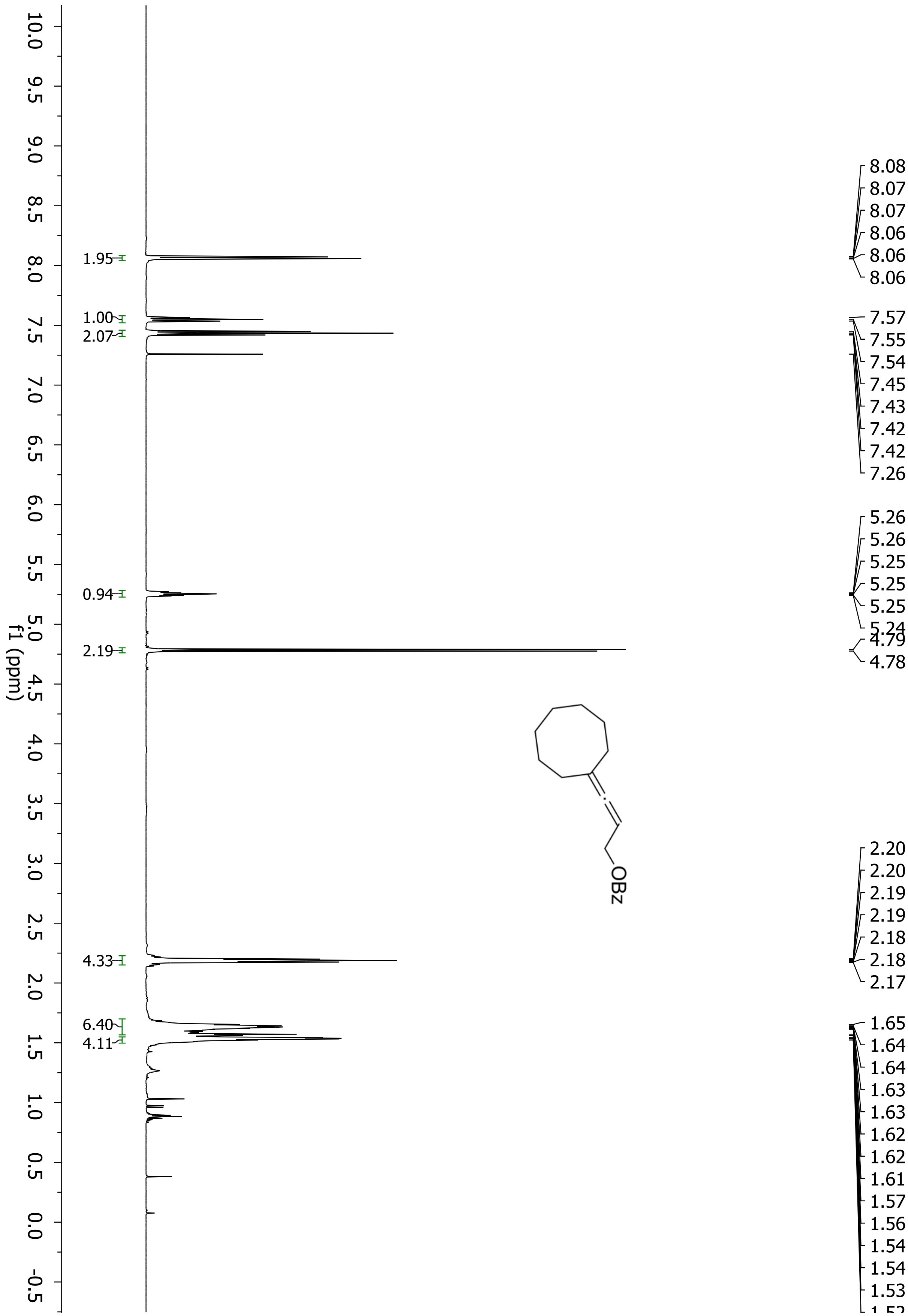
198.78
166.49
132.96
130.59
129.74
128.42
106.14
87.39
77.48
77.16
76.84
63.86
31.31
27.15
OBz
f1 (ppm)


8.08
8.06
8.06
7.58
7.56
7.54
7.46
7.44
7.42
7.26
5.24
5.24
5.23
5.23
5.22
5.22
5.21
5.21
4.79
4.77
2.14
2.13
2.11
1.60
1.59
1.57
1.56
1.54
1.53
1.50
1.49
1.96
1.00
2.13
0.93
2.22
4.36
4.23
2.12
OBz
f1 (ppm)

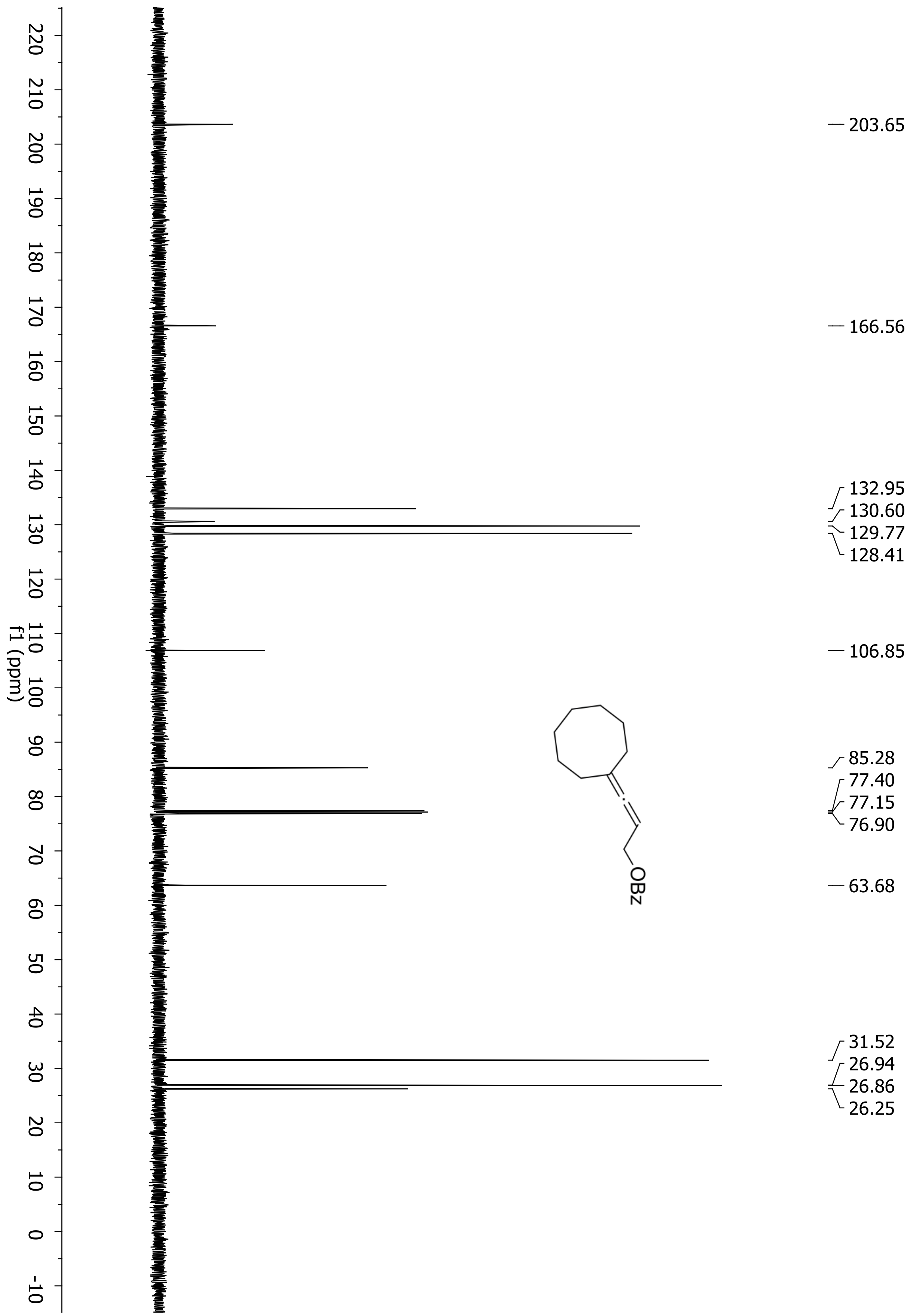

200.02
192.42
132.98
130.58
129.77
128.43
104.79
77.48
77.16
76.84
63.99
31.28
27.31
26.11
OBz
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

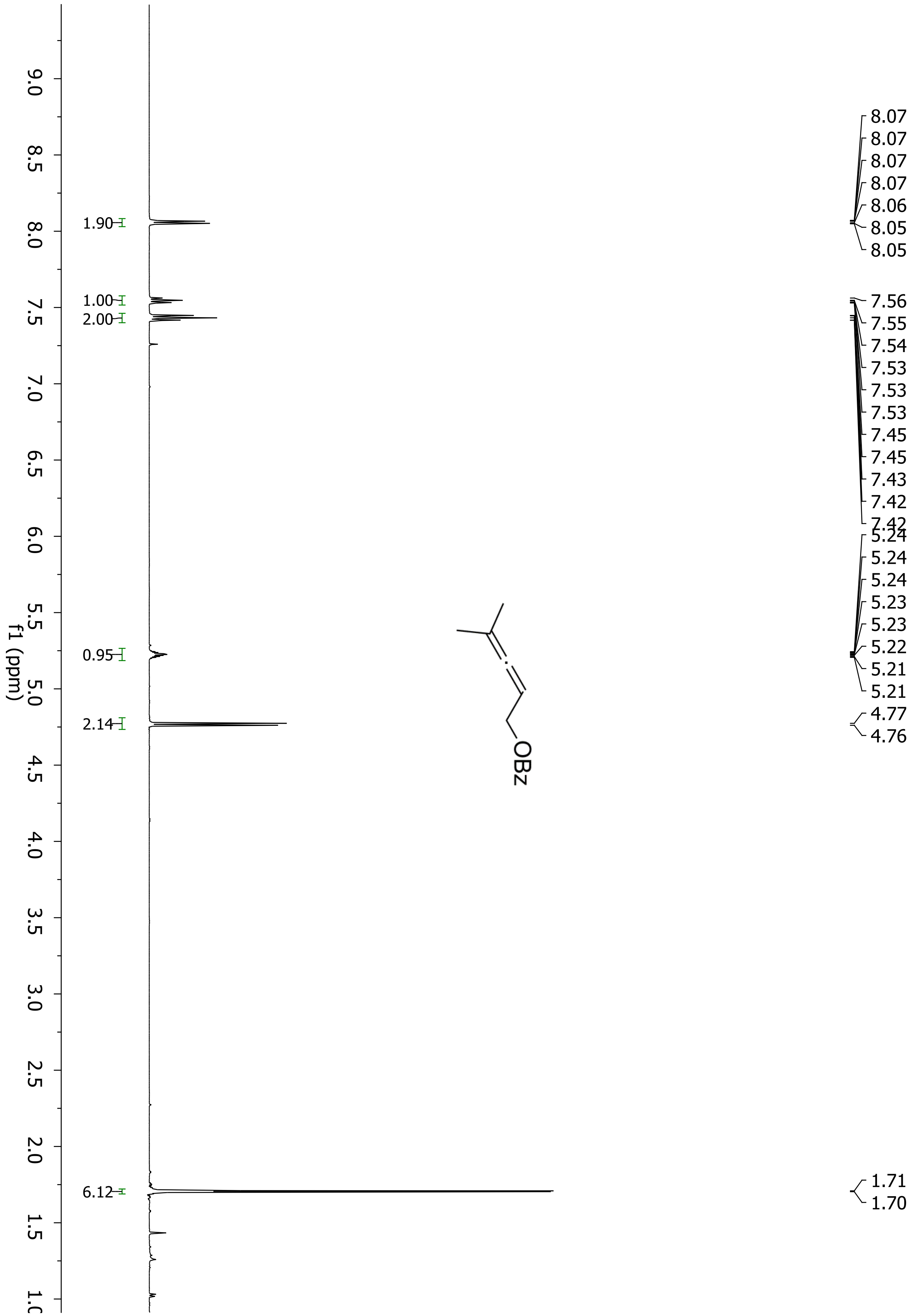

8.08
8.08
8.07
8.06
8.06
8.06
7.57
7.57
7.56
7.55
7.55
7.55
7.54
7.54
7.53
7.45
7.45
7.43
7.42
7.42
7.26
5.22
5.22
5.22
5.21
5.21
5.20
5.20
5.19
4.78
4.77
2.28
2.27
2.27
2.26
2.26
2.25
2.25
2.25
1.64
1.62
1.61
1.61
1.61
1.60
1.60
1.59
1.59
1.58
1.57
1.53
1.52
1.52
1.51
1.51
1.51
1.50
1.50
1.95
1.00
2.08
0.93
2.22
4.38
4.16
4.37
OBz
f1 (ppm)


203.34
166.51
132.95
130.61
129.77
128.41
106.90
84.66
77.40
77.15
76.90
63.91
32.28
29.45
28.46
OBz
f1 (ppm)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

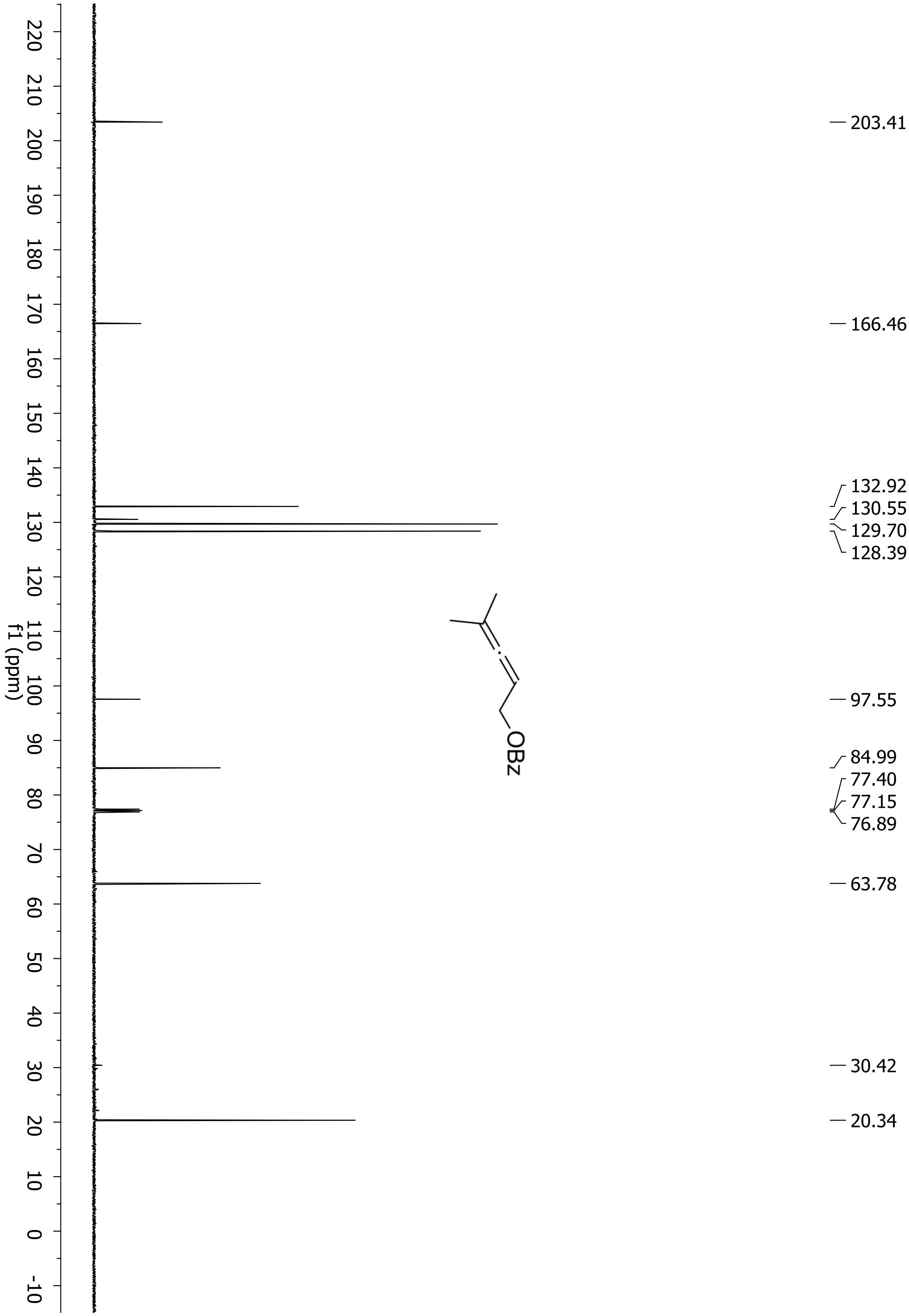


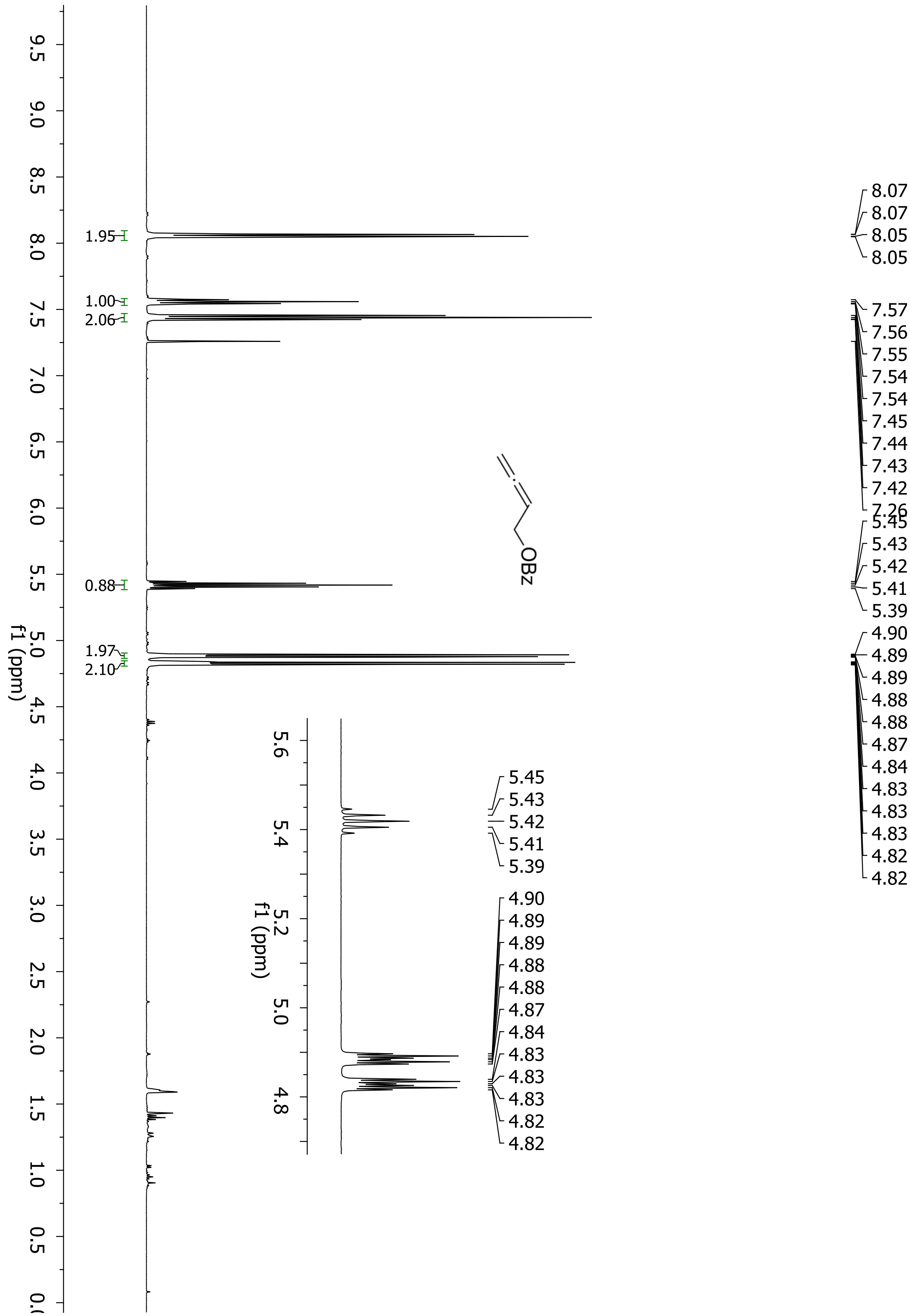
8.08
8.07
8.07
8.06
8.06
8.06
7.57
7.55
7.54
7.45
7.43
7.42
7.42
7.26
5.26
5.26
5.25
5.25
5.25
5.24
4.79
4.78
2.20
2.20
2.19
2.19
2.18
2.18
2.17
1.65
1.64
1.64
1.63
1.63
1.62
1.62
1.61
1.57
1.56
1.54
1.54
1.53
1.95
1.00
2.07
0.94
2.19
4.33
6.40
4.11
OBz
f1 (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


203.65
166.56
132.95
130.60
129.77
128.41
106.85
85.28
77.40
77.15
76.90
63.68
31.52
26.94
26.86
26.25
OBz
f1 (ppm)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

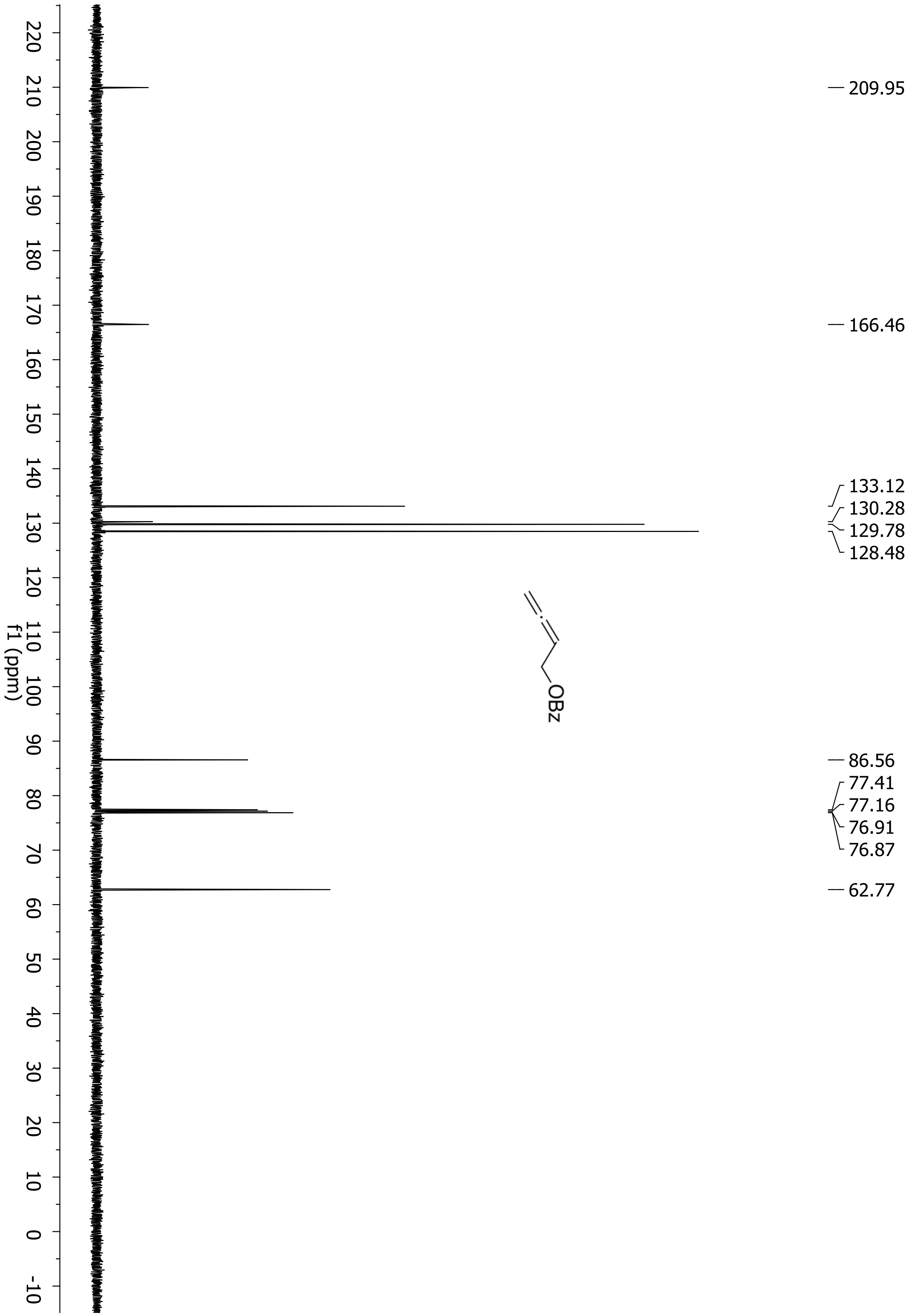


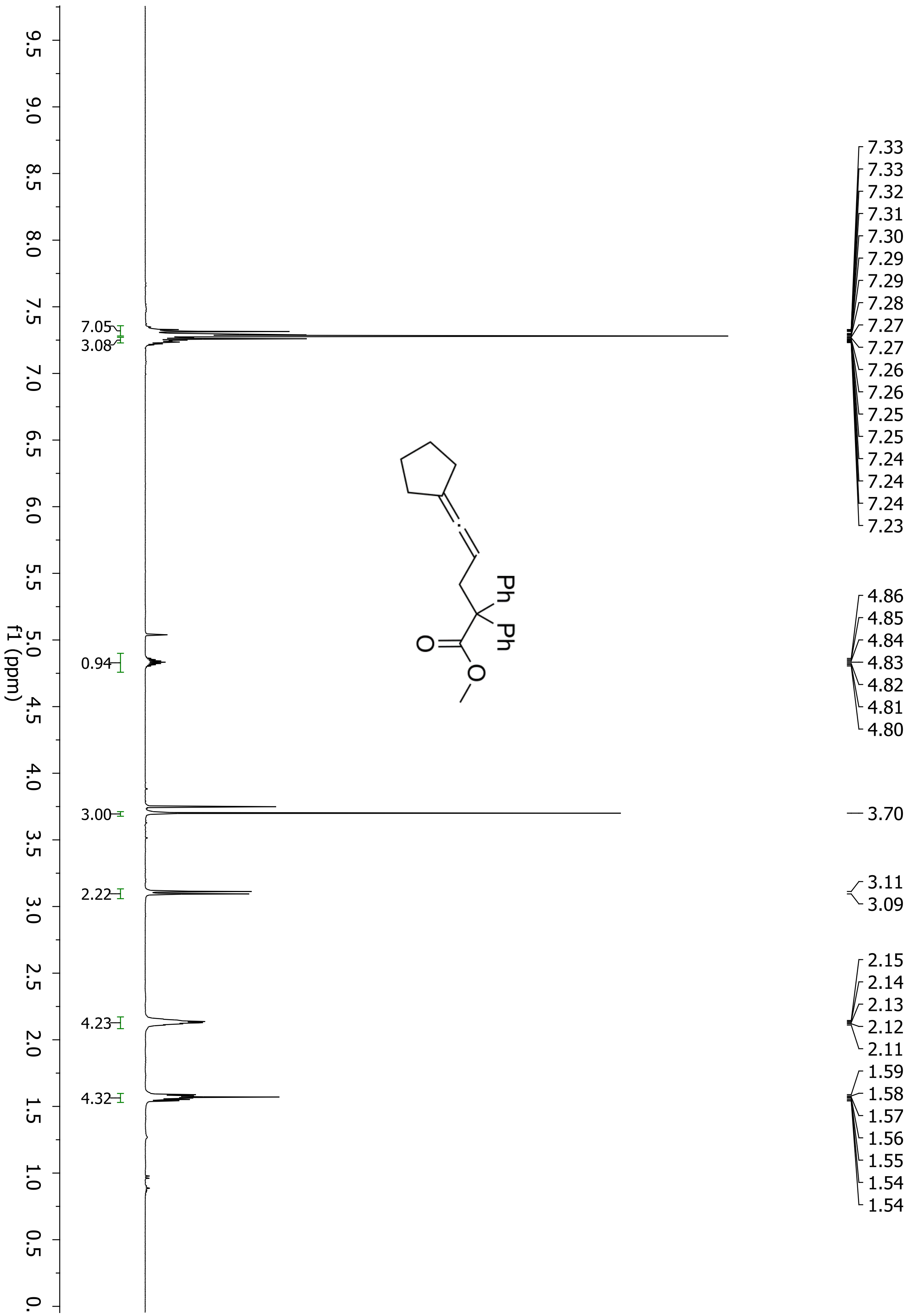
OBz
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
1.90
1.00
2.00
0.95
2.14
6.12
8.07
8.07
8.07
8.07
8.06
8.05
8.05
7.56
7.55
7.54
7.53
7.53
7.53
7.45
7.45
7.43
7.42
7.42
5.24
5.24
5.24
5.23
5.23
5.22
5.21
5.21
4.77
4.76
1.71
1.70


203.41
166.46
132.92
130.55
129.70
128.39
97.55
84.99
77.40
77.15
76.89
63.78
30.42
20.34
OBz
f1 (ppm)

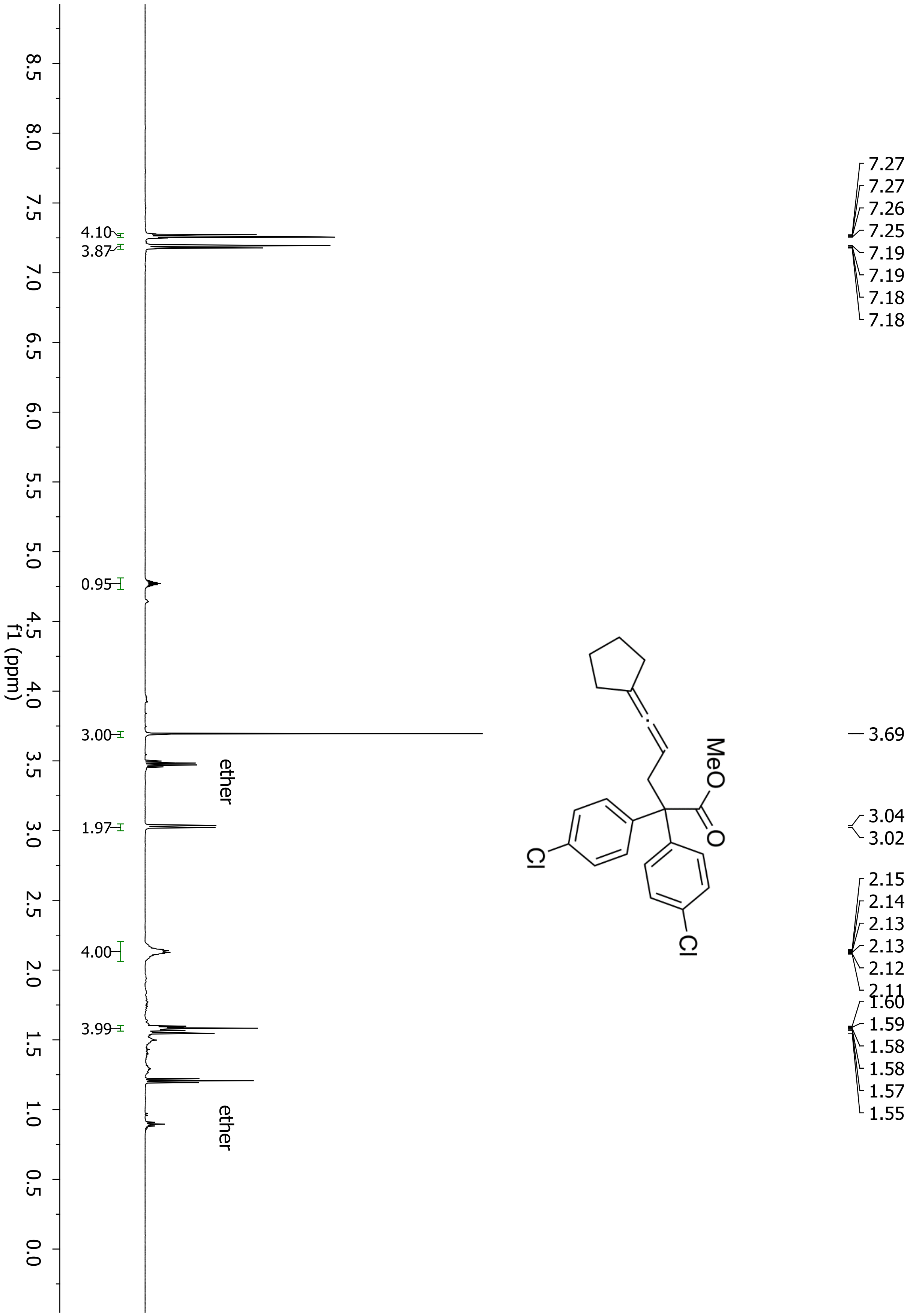


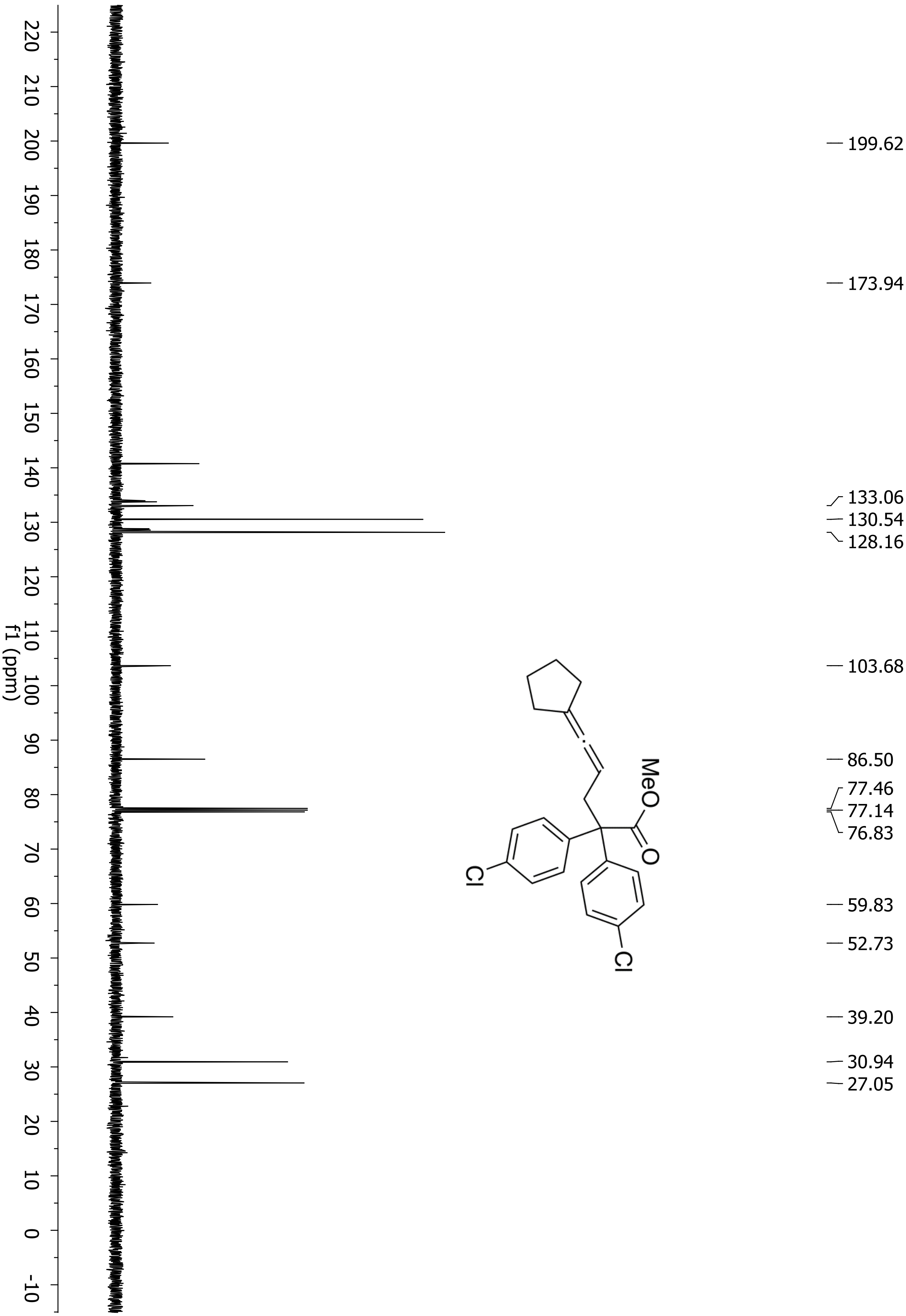
8.07
8.07
8.05
8.05
7.57
7.56
7.55
7.54
7.54
7.45
7.44
7.43
7.42
7.26
5.45
5.43
5.42
5.41
5.39
4.90
4.89
4.89
4.88
4.88
4.87
4.84
4.83
4.83
4.83
4.82
4.82
OBz
f1 (ppm)
1.95
1.00
2.06
0.88
1.97
2.10


209.95
166.46
133.12
130.28
129.78
128.48
86.56
77.41
77.16
76.91
76.87
62.77
OBz
f1 (ppm)

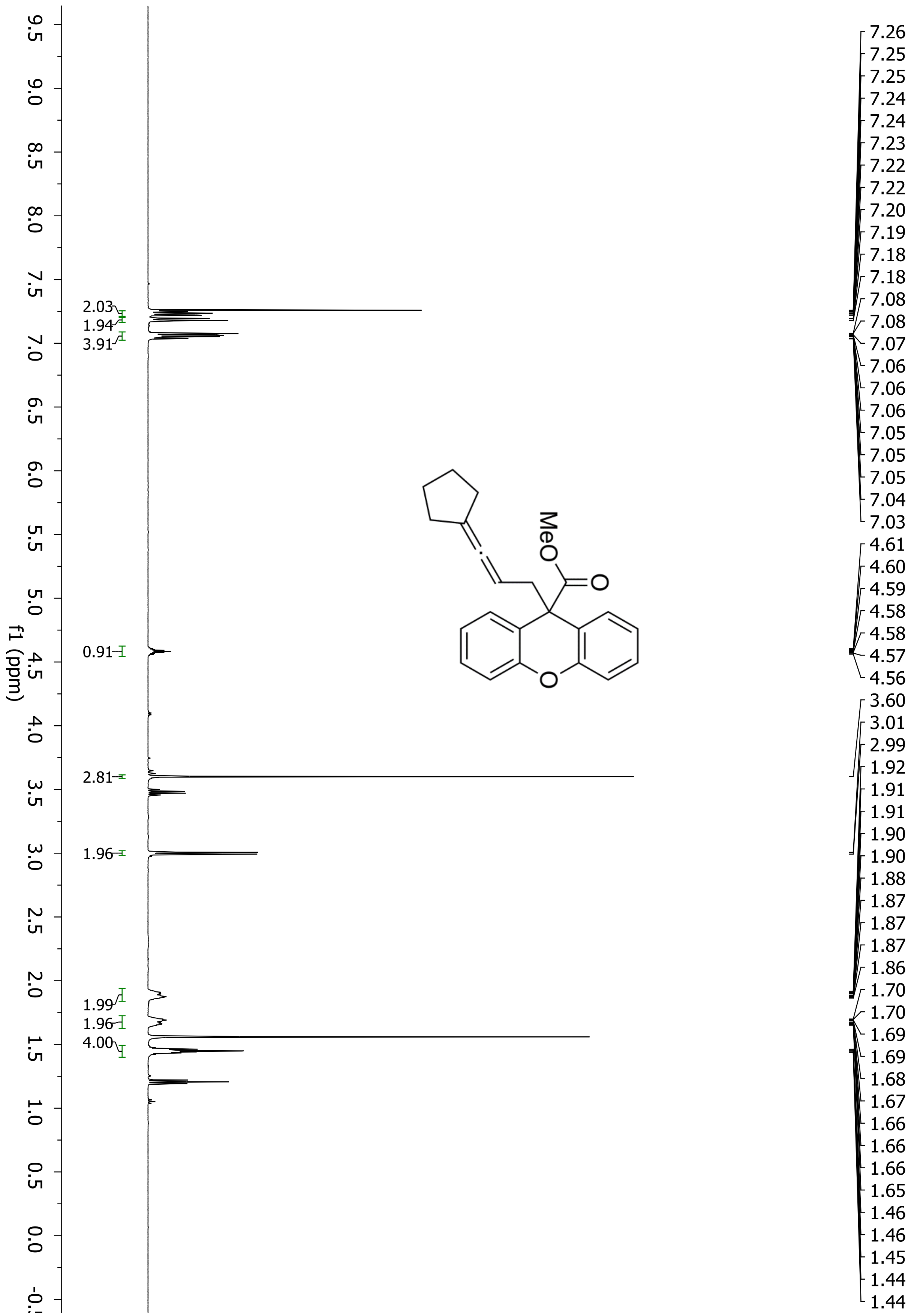


f1 (ppm)
7.33
7.33
7.32
7.31
7.30
7.29
7.29
7.28
7.27
7.27
7.26
7.26
7.25
7.25
7.24
7.24
7.24
7.23
4.86
4.85
4.84
4.83
4.82
4.81
4.80
3.70
3.11
3.09
2.15
2.14
2.13
2.12
2.11
1.59
1.58
1.57
1.56
1.55
1.54
1.54
7.05
3.08
0.94
3.00
2.22
4.23
4.32
Ph
Ph
O
O

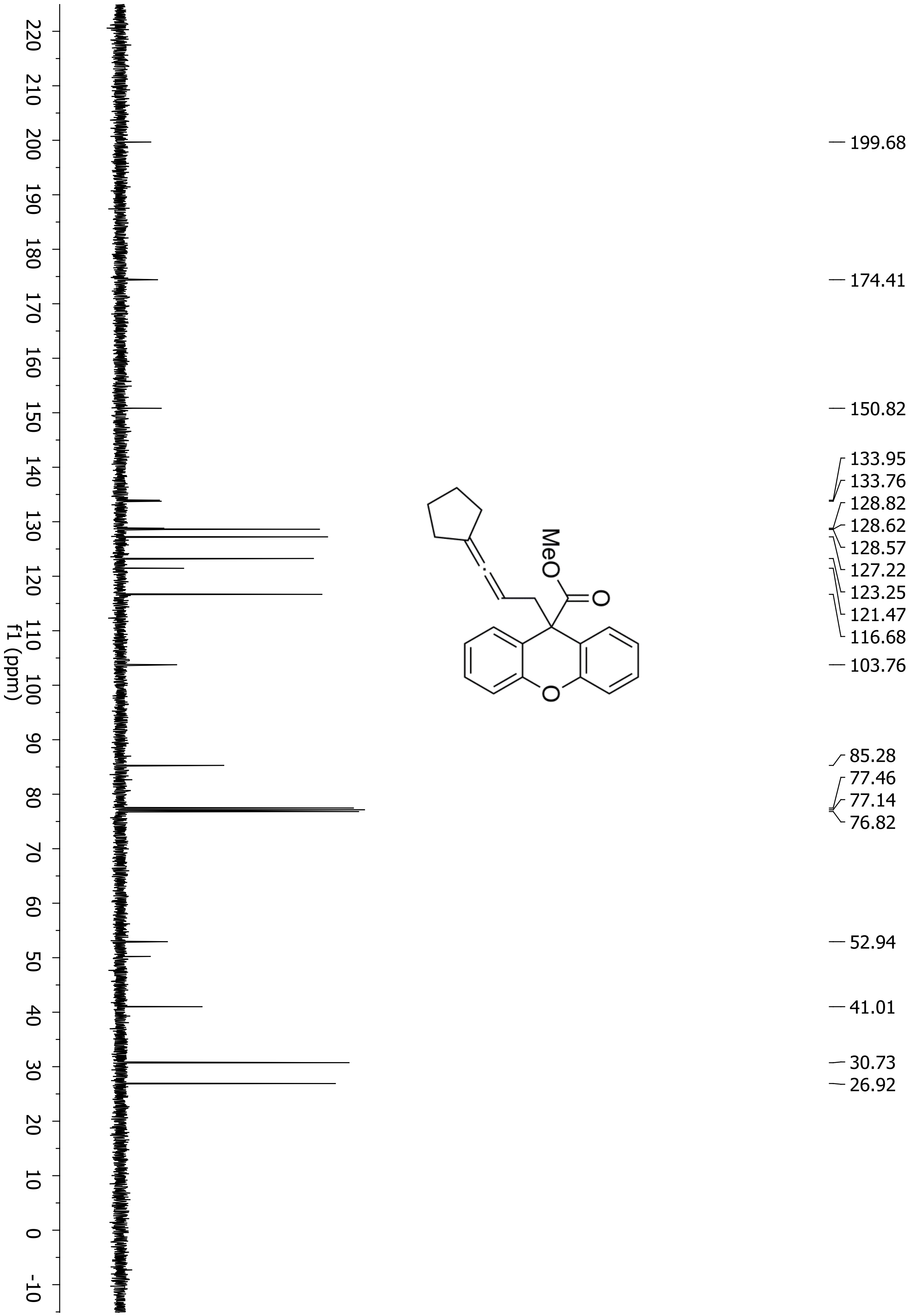

7.27
7.27
7.26
7.25
7.19
7.19
7.18
7.18
3.69
3.04
3.02
2.15
2.14
2.13
2.13
2.12
2.11
1.60
1.59
1.58
1.58
1.57
1.55
4.10
3.87
0.95
3.00
1.97
4.00
3.99
ether
ether
MeO
O
Cl
Cl
f1 (ppm)

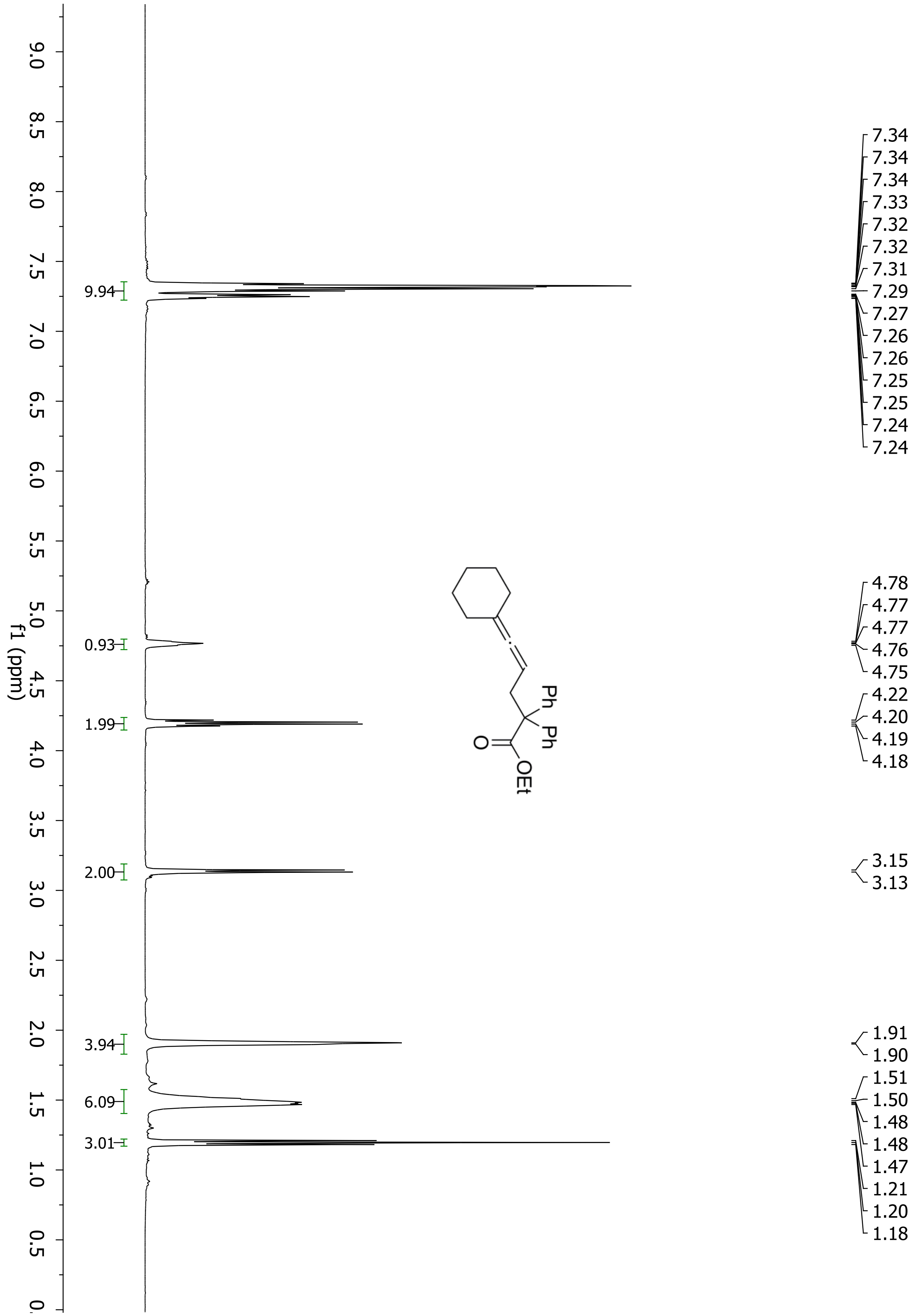


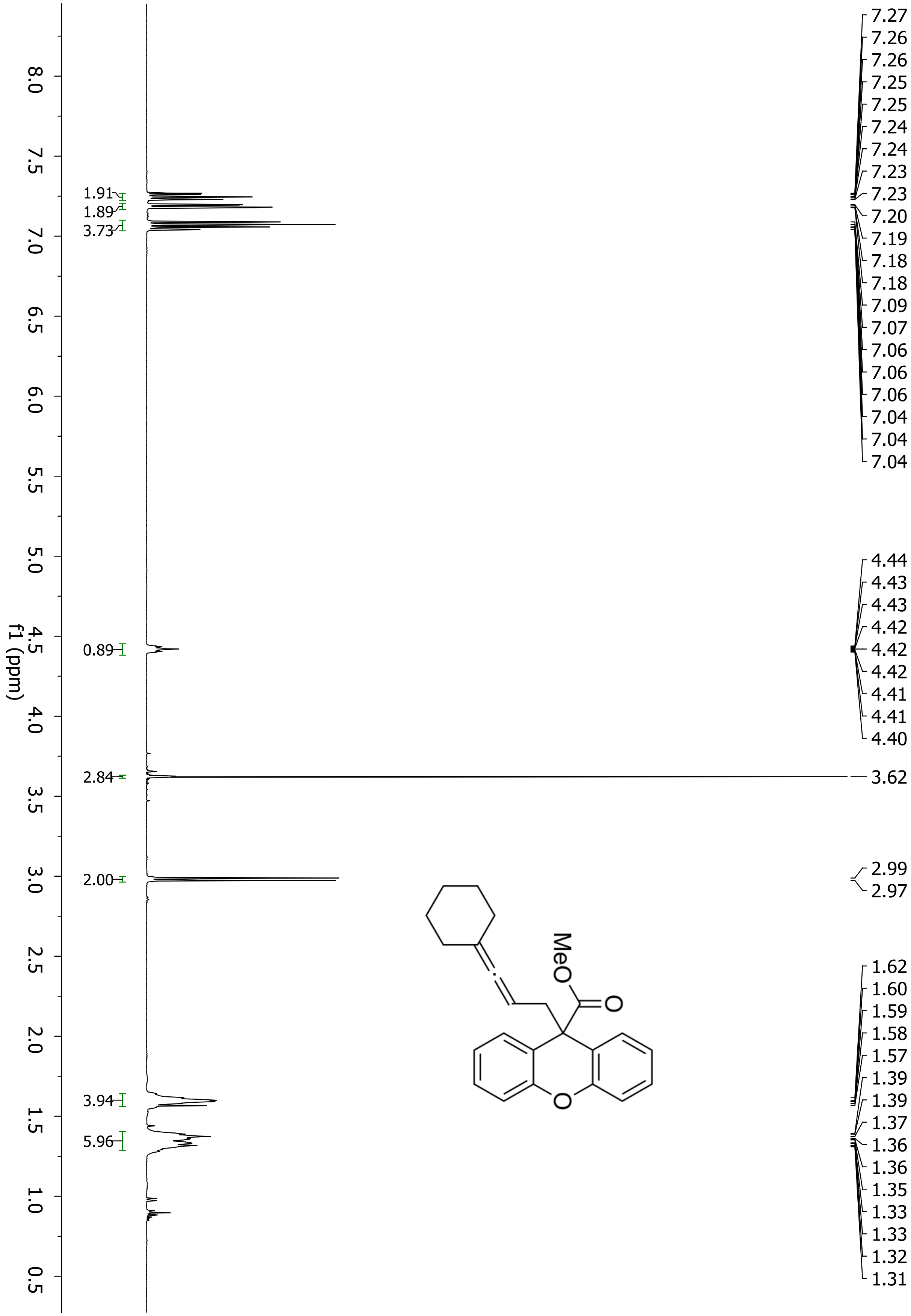
199.62
173.94
133.06
130.54
128.16
103.68
86.50
77.46
77.14
76.83
59.83
52.73
39.20
30.94
27.05
f1 (ppm)
MeO
O
Cl
Cl

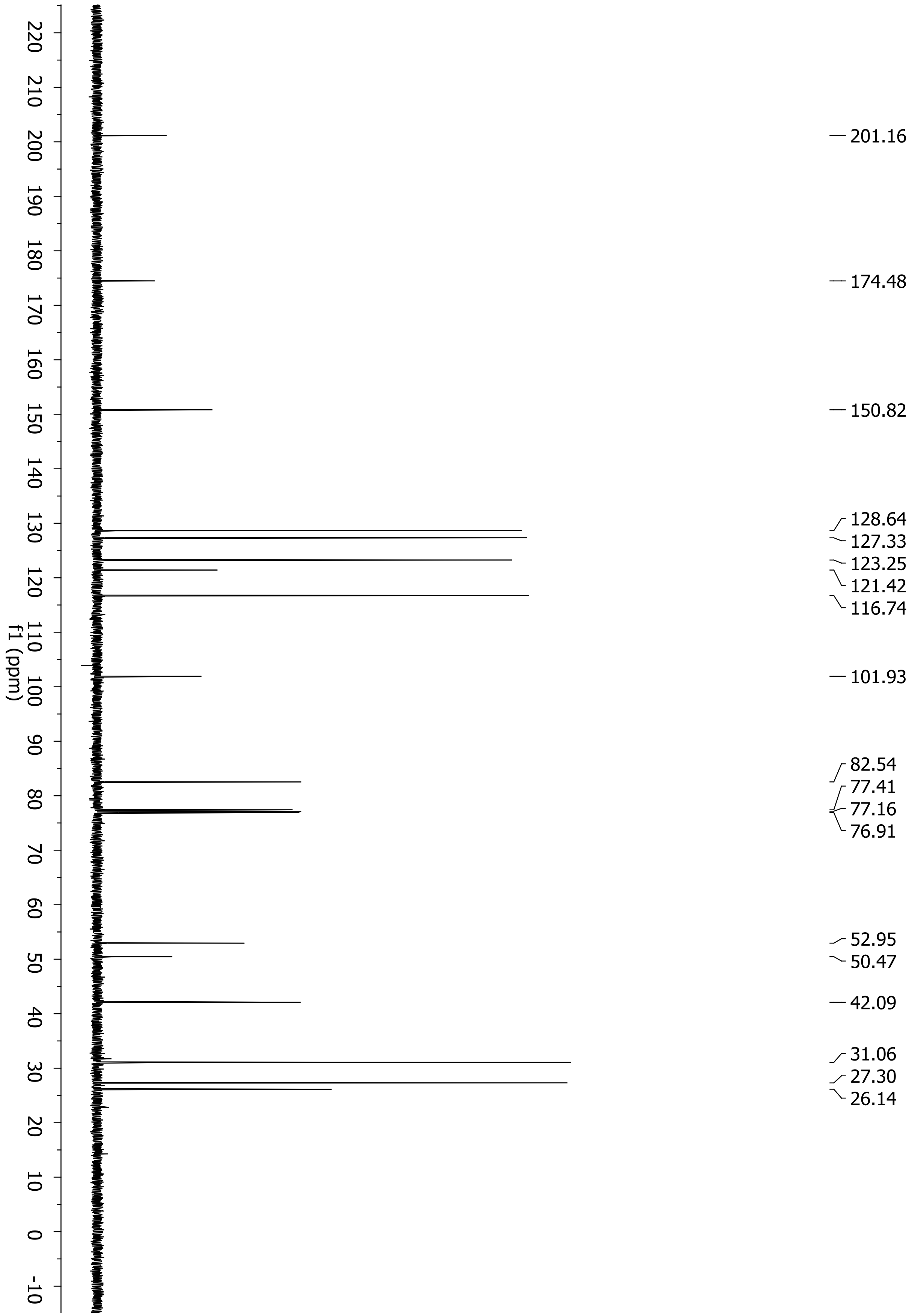


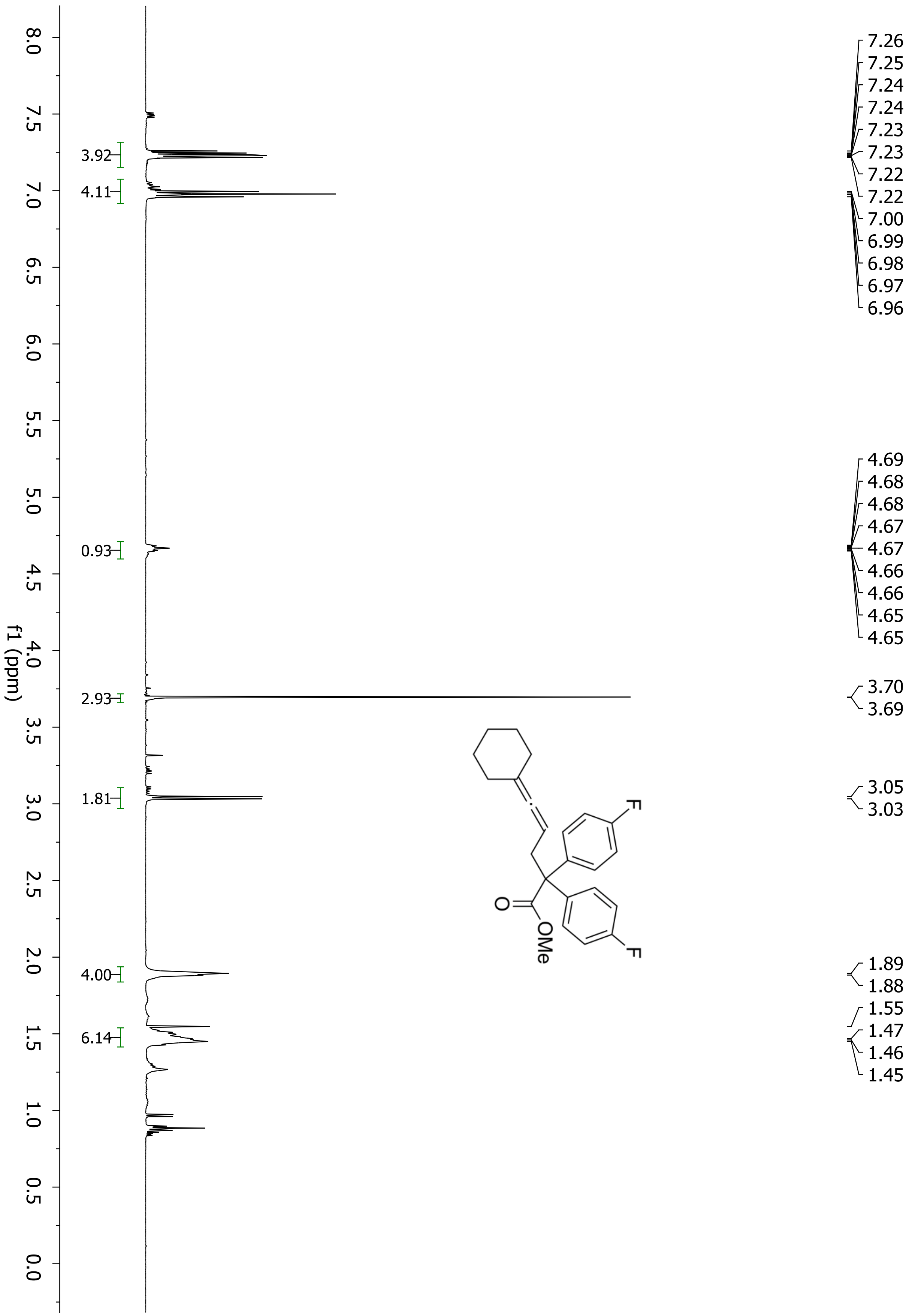
7.26
7.25
7.25
7.24
7.24
7.23
7.22
7.22
7.20
7.19
7.18
7.18
7.08
7.08
7.07
7.06
7.06
7.06
7.05
7.05
7.05
7.04
7.03
4.61
4.60
4.59
4.58
4.58
4.57
4.56
3.60
3.01
2.99
1.92
1.91
1.91
1.90
1.90
1.88
1.87
1.87
1.87
1.86
1.70
1.70
1.69
1.69
1.68
1.67
1.66
1.66
1.66
1.65
1.46
1.46
1.45
1.44
1.44
MeO
O
O
2.03
1.94
3.91
0.91
2.81
1.96
1.99
1.96
4.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

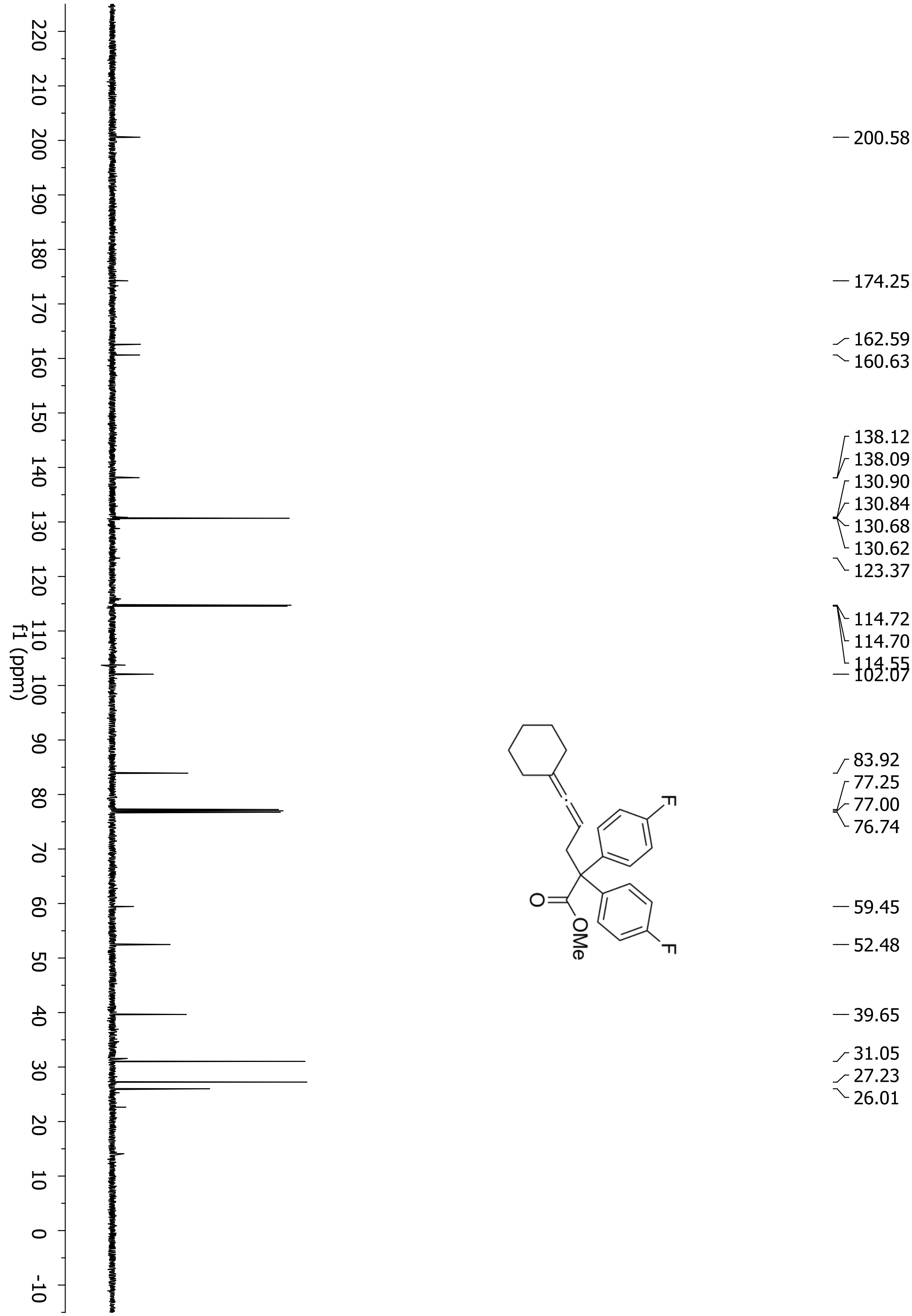

199.68
174.41
150.82
133.95
133.76
128.82
128.62
128.57
127.22
123.25
121.47
116.68
103.76
85.28
77.46
77.14
76.82
52.94
41.01
30.73
26.92
MeO
O
f1 (ppm)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

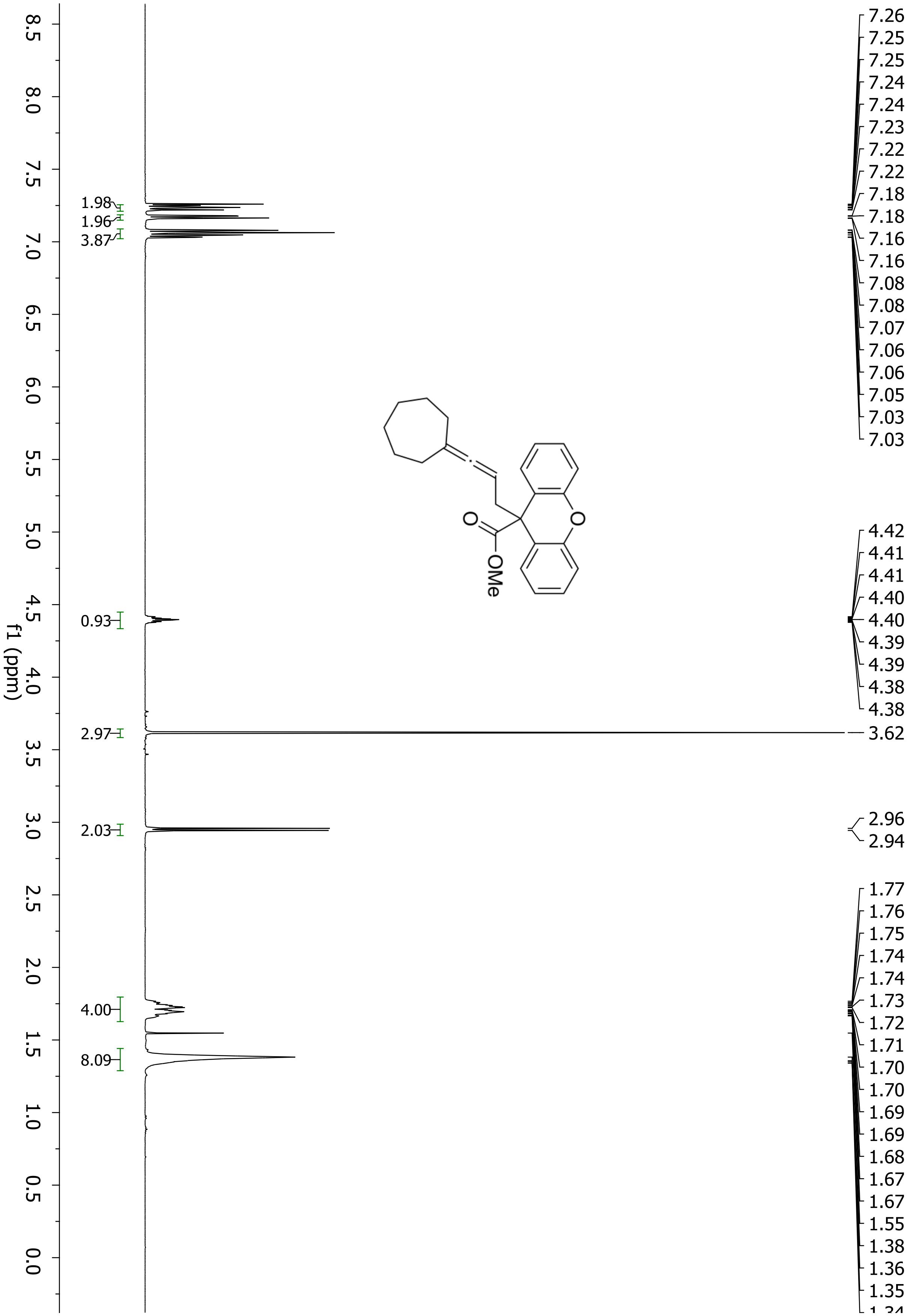

Ph
Ph
O
OEt
7.34
7.34
7.34
7.33
7.32
7.32
7.31
7.29
7.27
7.26
7.26
7.25
7.25
7.24
7.24
4.78
4.77
4.77
4.76
4.75
4.22
4.20
4.19
4.18
3.15
3.13
1.91
1.90
1.51
1.50
1.48
1.48
1.47
1.21
1.20
1.18
9.94
0.93
1.99
2.00
3.94
6.09
3.01
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.

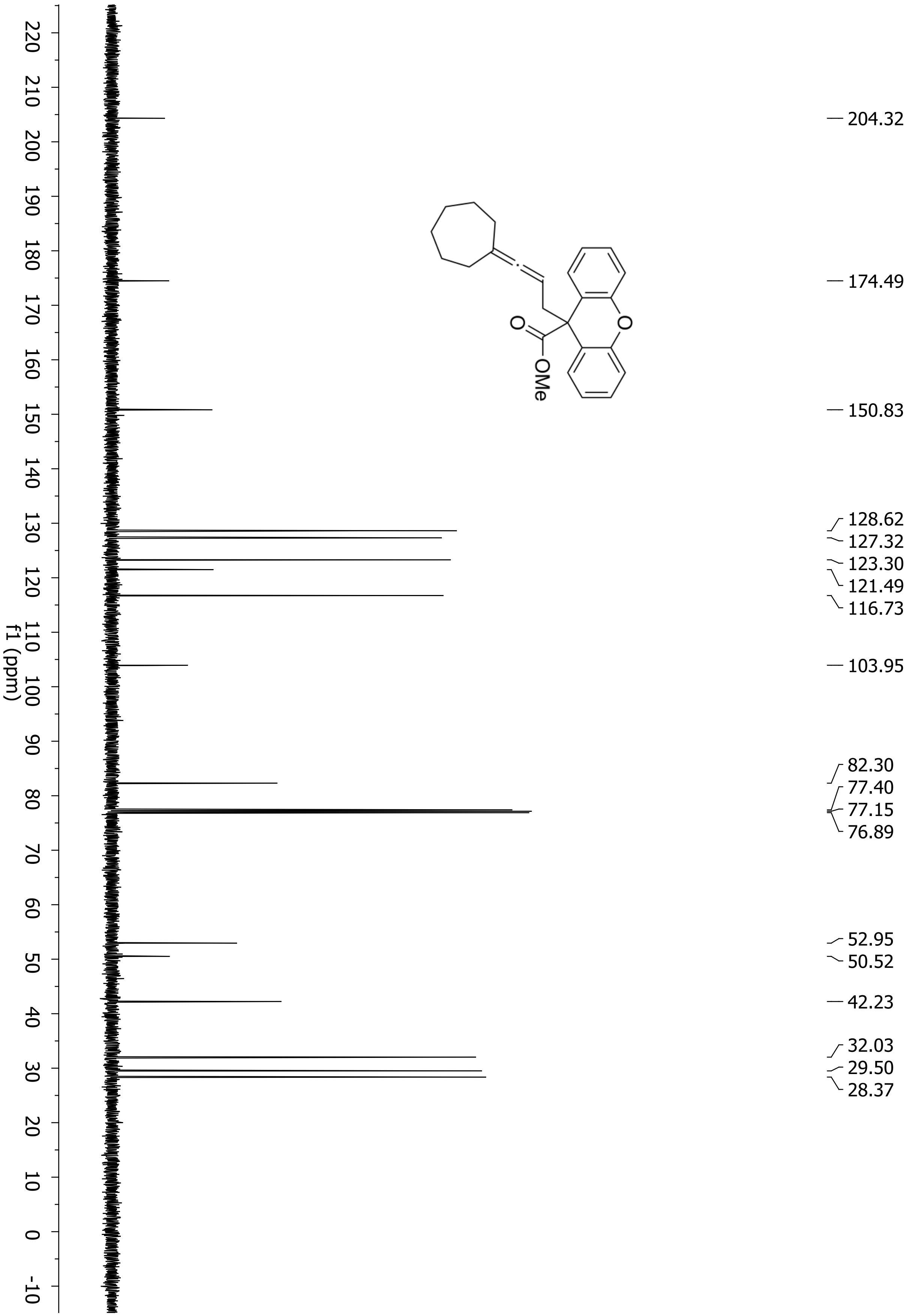

7.27
7.26
7.26
7.25
7.25
7.24
7.24
7.23
7.23
7.20
7.19
7.18
7.18
7.09
7.07
7.06
7.06
7.06
7.04
7.04
7.04
4.44
4.43
4.43
4.42
4.42
4.42
4.41
4.41
4.40
3.62
2.99
2.97
1.62
1.60
1.59
1.58
1.57
1.39
1.39
1.37
1.36
1.36
1.35
1.33
1.33
1.32
1.31
1.91
1.89
3.73
0.89
2.84
2.00
3.94
5.96
MeO
O
O
f1 (ppm)


201.16
174.48
150.82
128.64
127.33
123.25
121.42
116.74
101.93
82.54
77.41
77.16
76.91
52.95
50.47
42.09
31.06
27.30
26.14
f1 (ppm)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

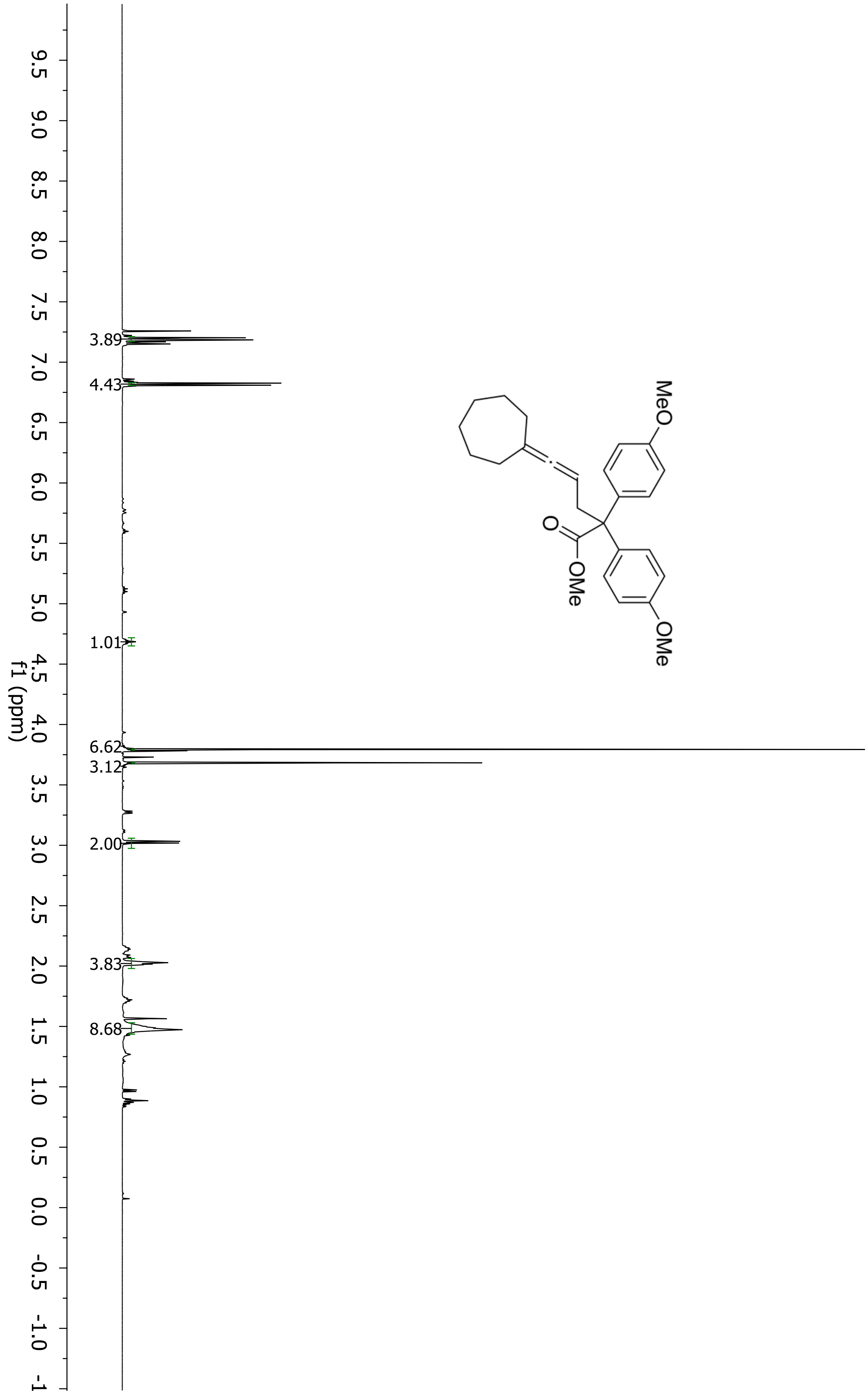

7.26
7.25
7.24
7.24
7.23
7.23
7.22
7.22
7.00
6.99
6.98
6.97
6.96
4.69
4.68
4.68
4.67
4.67
4.66
4.66
4.65
4.65
3.70
3.69
3.05
3.03
1.89
1.88
1.55
1.47
1.46
1.45
3.92
4.11
0.93
2.93
1.81
4.00
6.14
f1 (ppm)
F
F
O
OMe

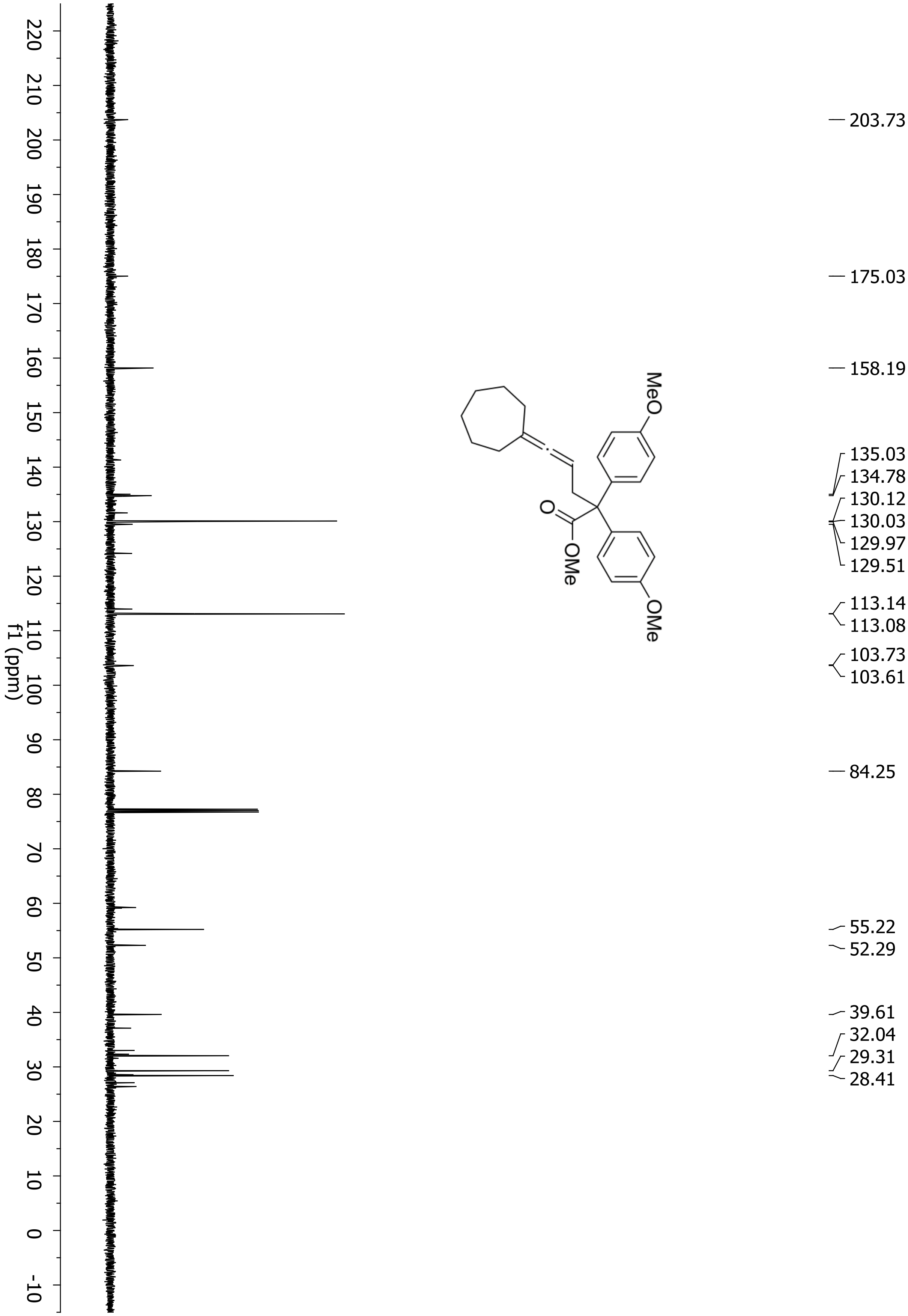

200.58
174.25
162.59
160.63
138.12
138.09
130.90
130.84
130.68
130.62
123.37
114.72
114.70
114.55
102.07
83.92
77.25
77.00
76.74
59.45
52.48
39.65
31.05
27.23
26.01
f1 (ppm)
F
F
O
OMe

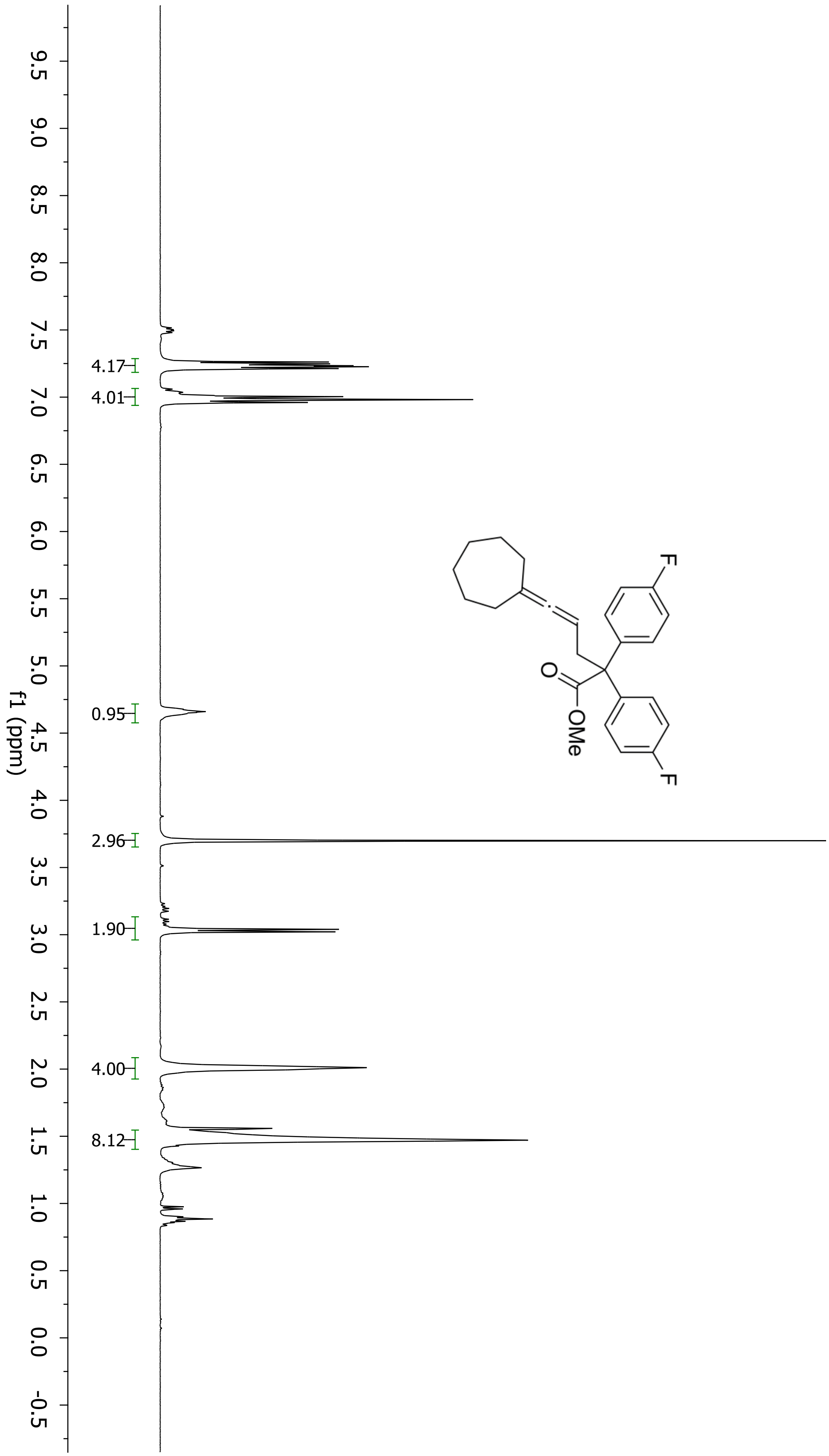

7.26
7.25
7.25
7.24
7.24
7.23
7.22
7.22
7.18
7.18
7.16
7.16
7.08
7.08
7.07
7.06
7.06
7.05
7.03
7.03
4.42
4.41
4.41
4.40
4.40
4.39
4.39
4.38
4.38
3.62
2.96
2.94
1.77
1.76
1.75
1.74
1.74
1.73
1.72
1.71
1.70
1.70
1.69
1.69
1.68
1.67
1.67
1.55
1.38
1.36
1.35
1.98
1.96
3.87
0.93
2.97
2.03
4.00
8.09
O
O
OMe
f1 (ppm)

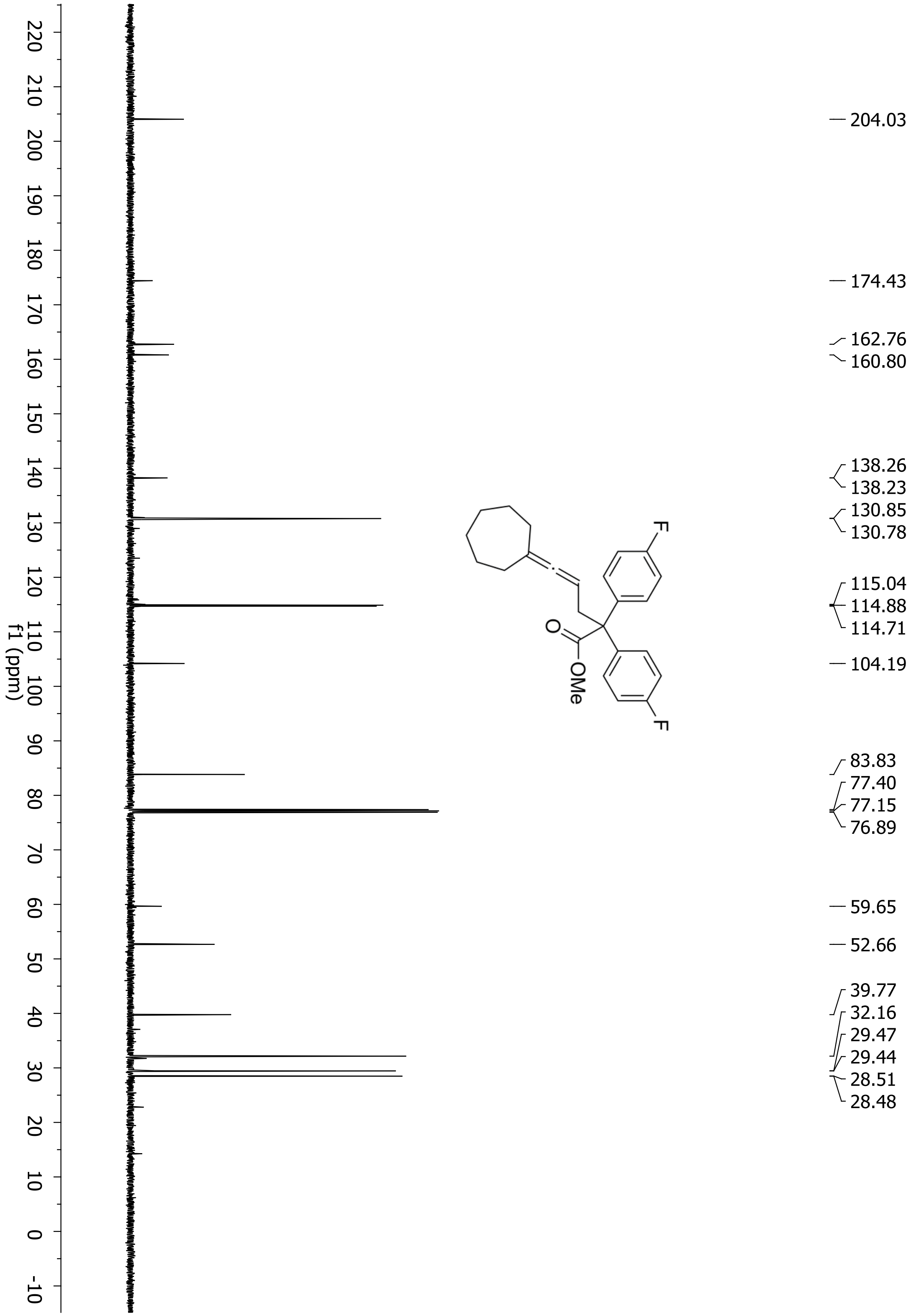


204.32
174.49
150.83
128.62
127.32
123.30
121.49
116.73
103.95
82.30
77.40
77.15
76.89
52.95
50.52
42.23
32.03
29.50
28.37
f1 (ppm)
O
O
OMe

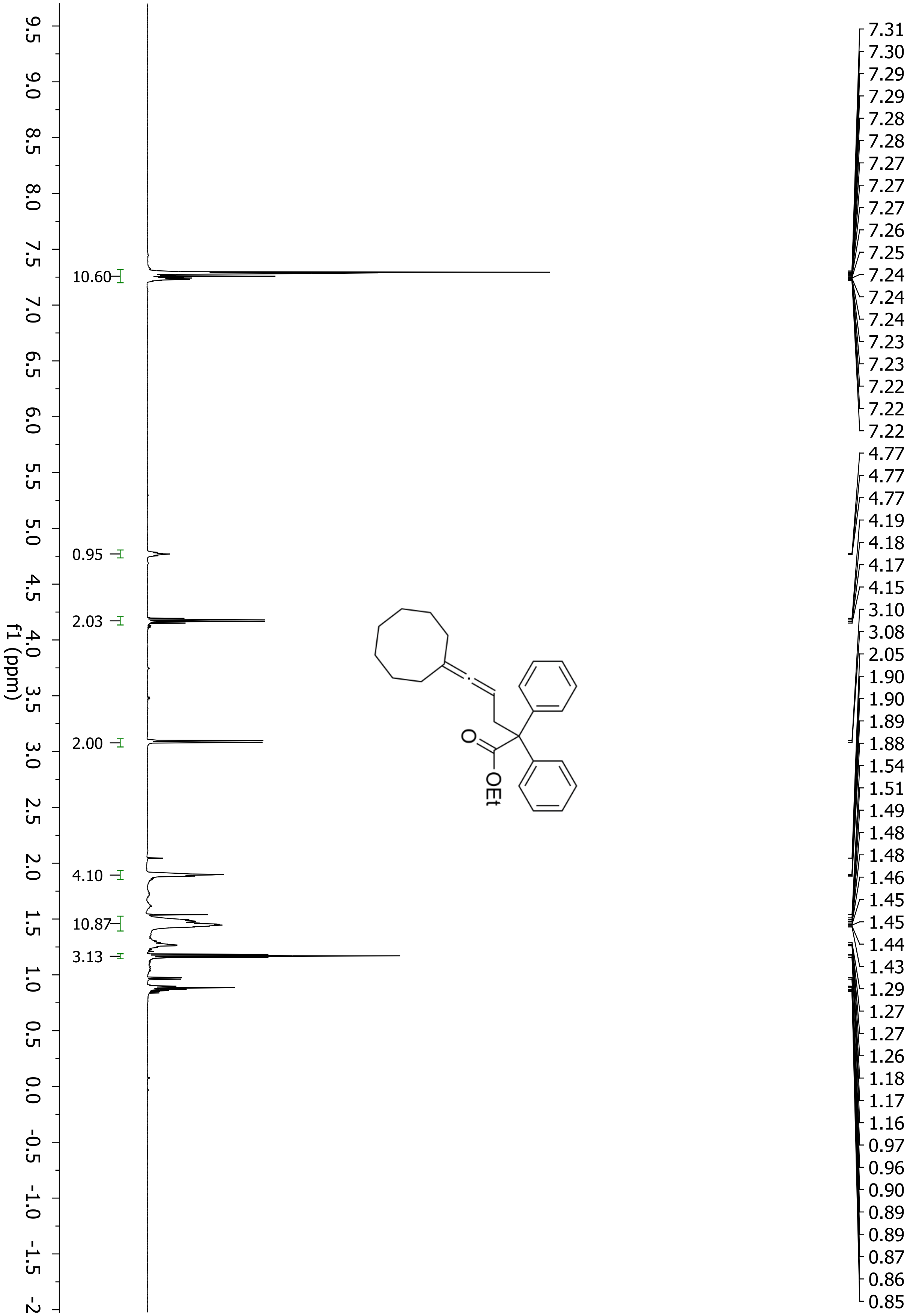

3.89
4.43
1.01
6.62
3.12
2.00
3.83
8.68
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1
f1 (ppm)
MeO
O
OMe
OMe

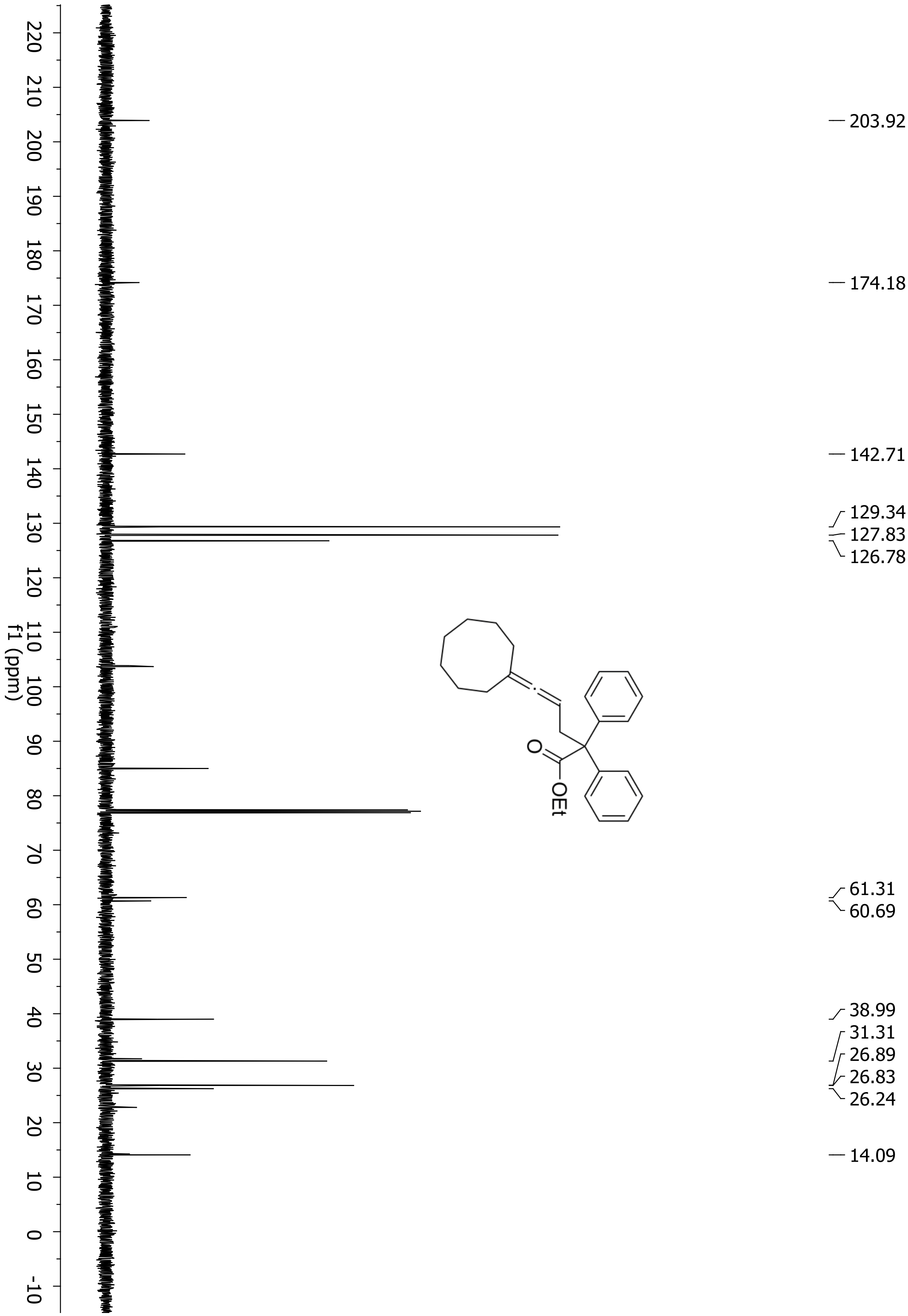

203.73
175.03
158.19
135.03
134.78
130.12
130.03
129.97
129.51
113.14
113.08
103.73
103.61
84.25
55.22
52.29
39.61
32.04
29.31
28.41
MeO
OMe
OMe
O
f1 (ppm)

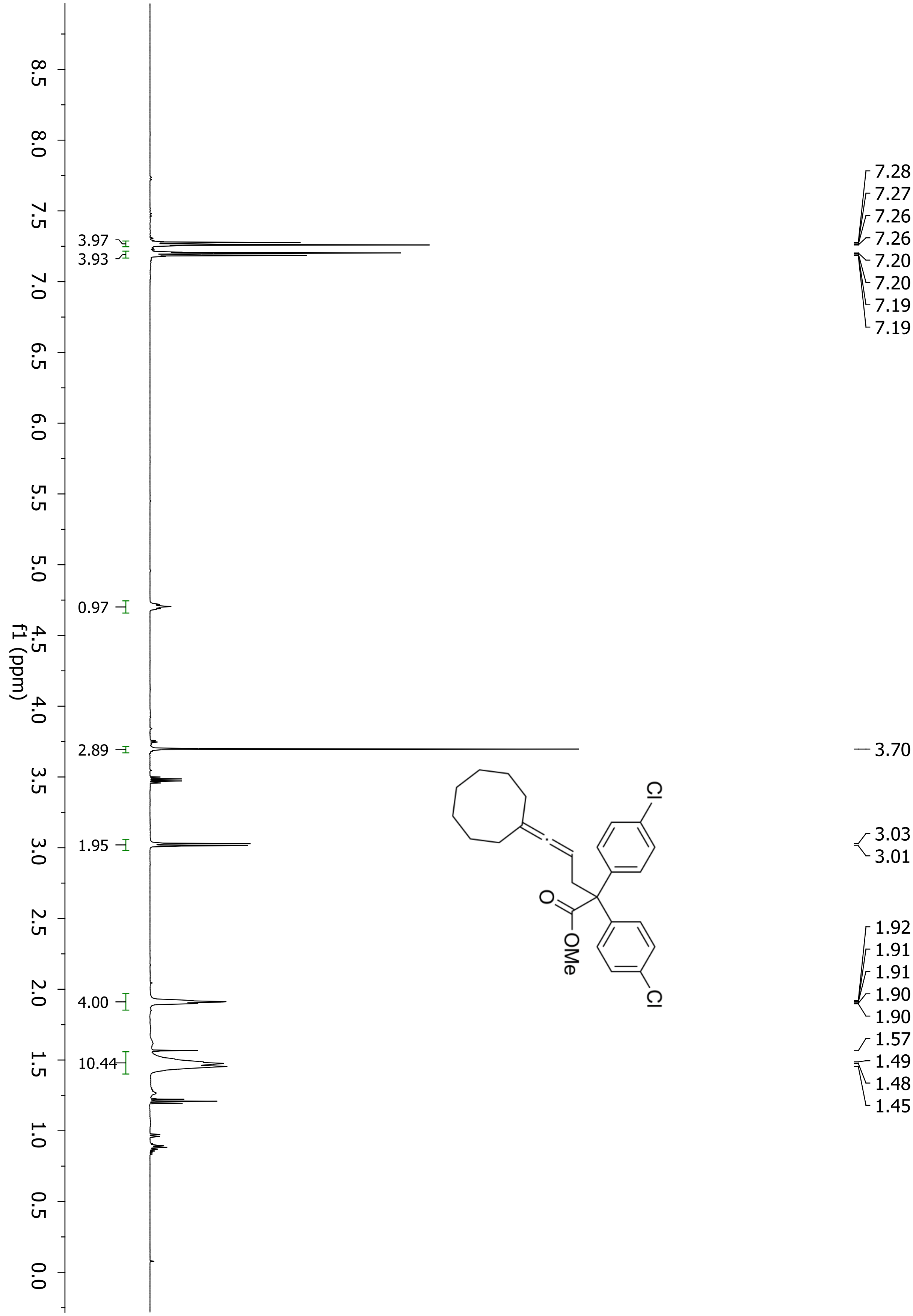

9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
4.17
4.01
0.95
2.96
1.90
4.00
8.12
F
F
O
OMe

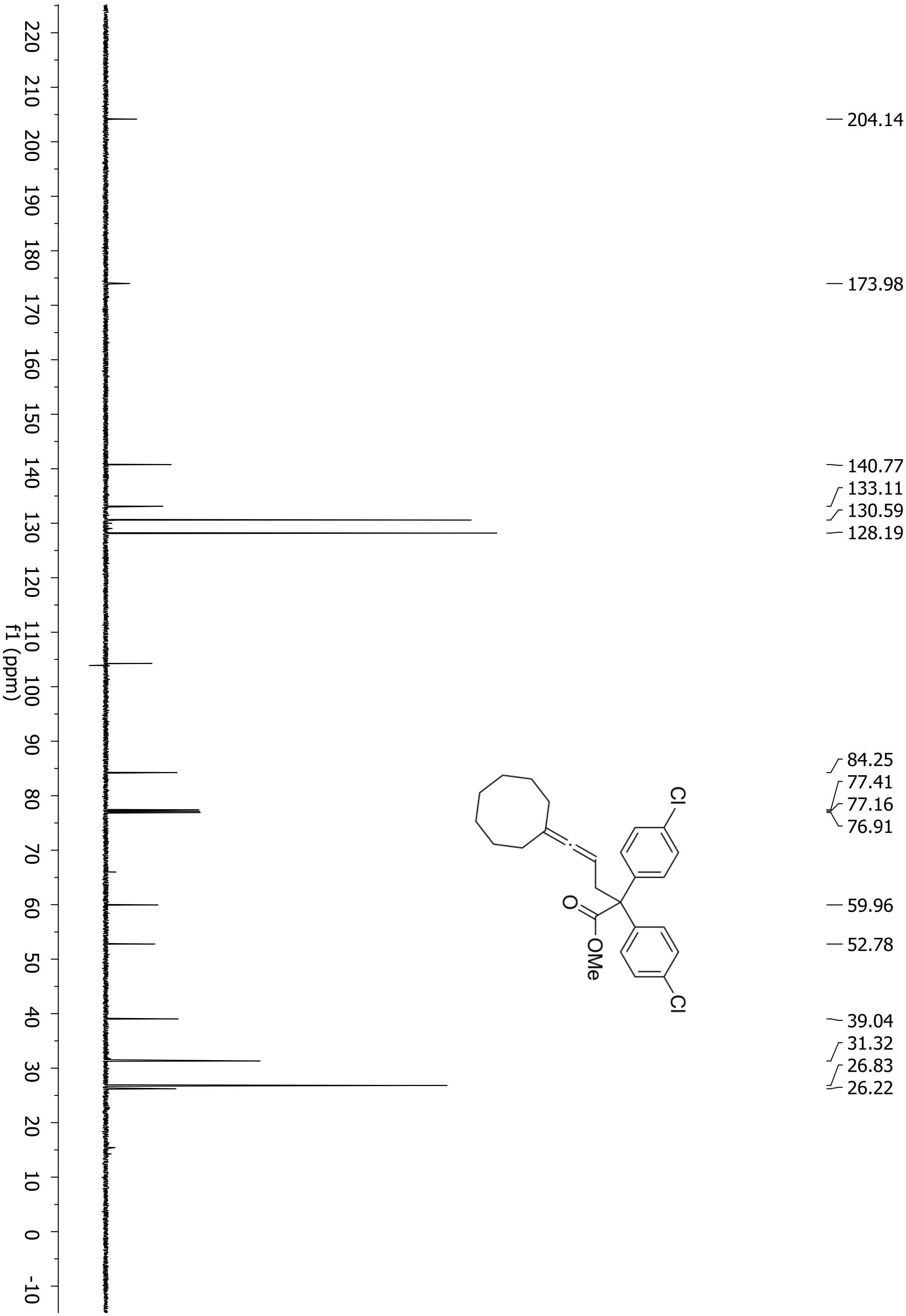


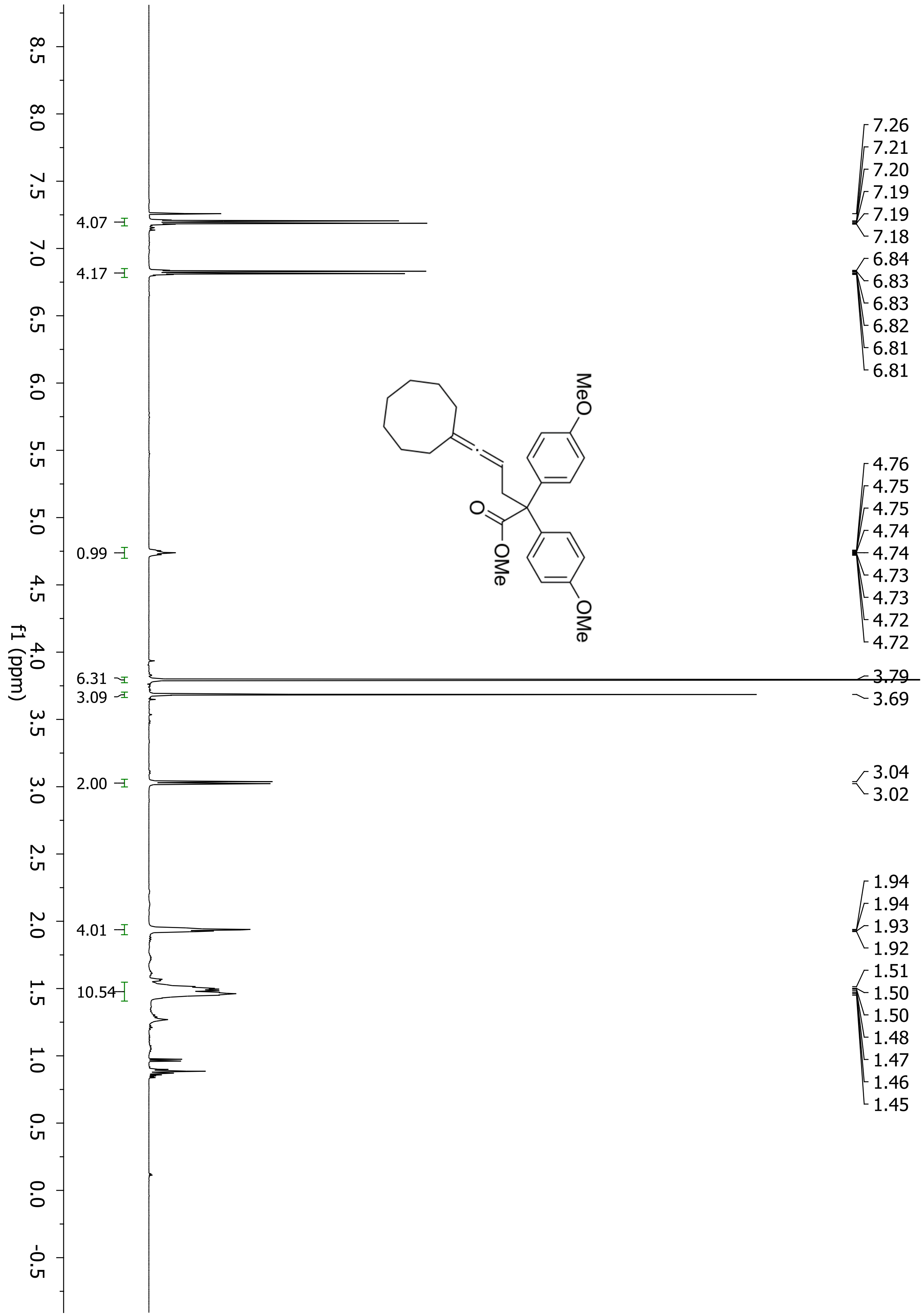
204.03
174.43
162.76
160.80
138.26
138.23
130.85
130.78
115.04
114.88
114.71
104.19
83.83
77.40
77.15
76.89
59.65
52.66
39.77
32.16
29.47
29.44
28.51
28.48
f1 (ppm)
OMe
O
F
F


7.31
7.30
7.29
7.29
7.28
7.28
7.27
7.27
7.27
7.26
7.25
7.24
7.24
7.24
7.23
7.23
7.22
7.22
7.22
4.77
4.77
4.77
4.19
4.18
4.17
4.15
3.10
3.08
2.05
1.90
1.90
1.89
1.88
1.54
1.51
1.49
1.48
1.48
1.46
1.45
1.45
1.44
1.43
1.29
1.27
1.27
1.26
1.18
1.17
1.16
0.97
0.96
0.90
0.89
0.89
0.87
0.86
0.85
10.60
0.95
2.03
2.00
4.10
10.87
3.13
O
OEt
f1 (ppm)

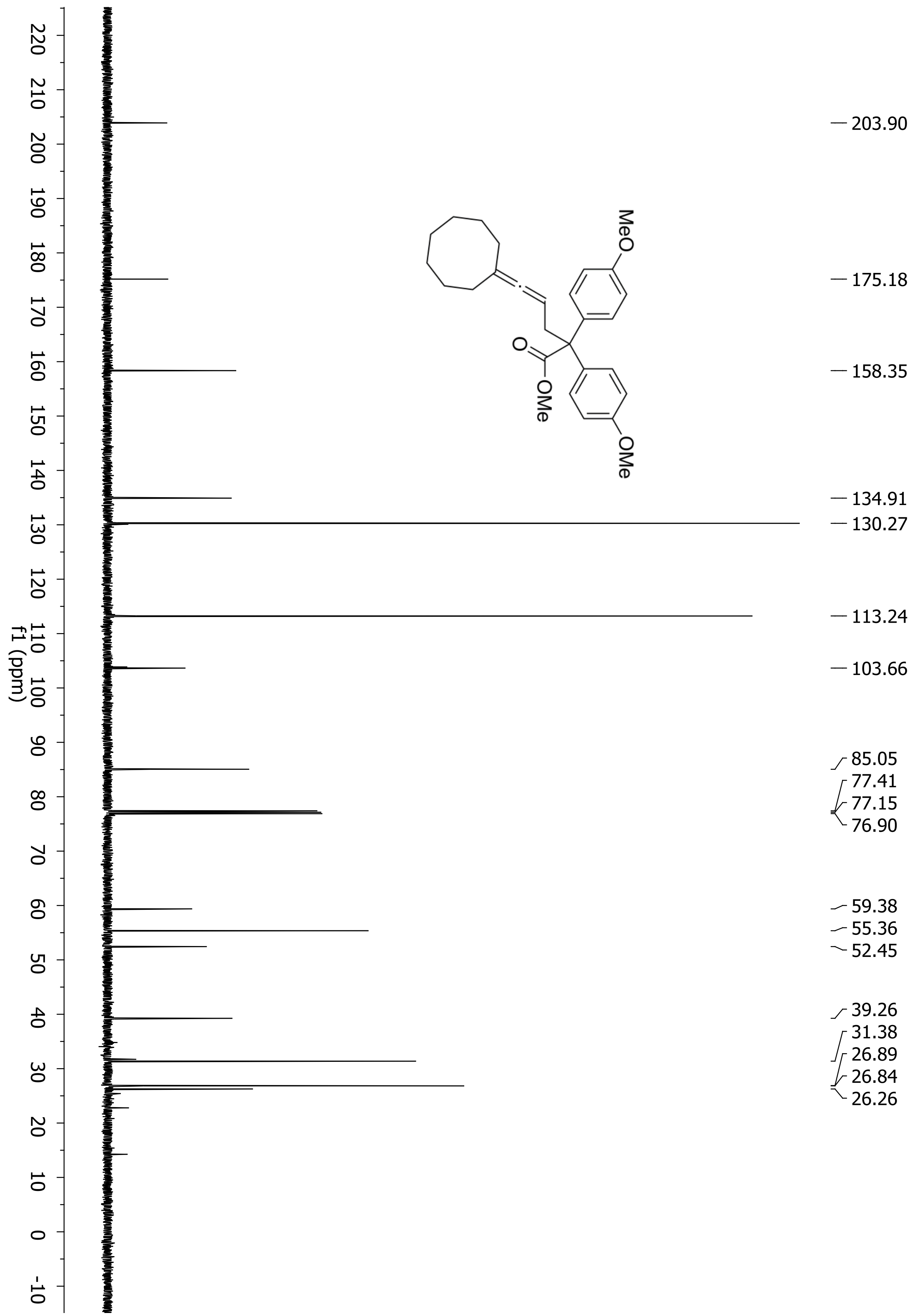

203.92
174.18
142.71
129.34
127.83
126.78
61.31
60.69
38.99
31.31
26.89
26.83
26.24
14.09
f1 (ppm)
O
OEt

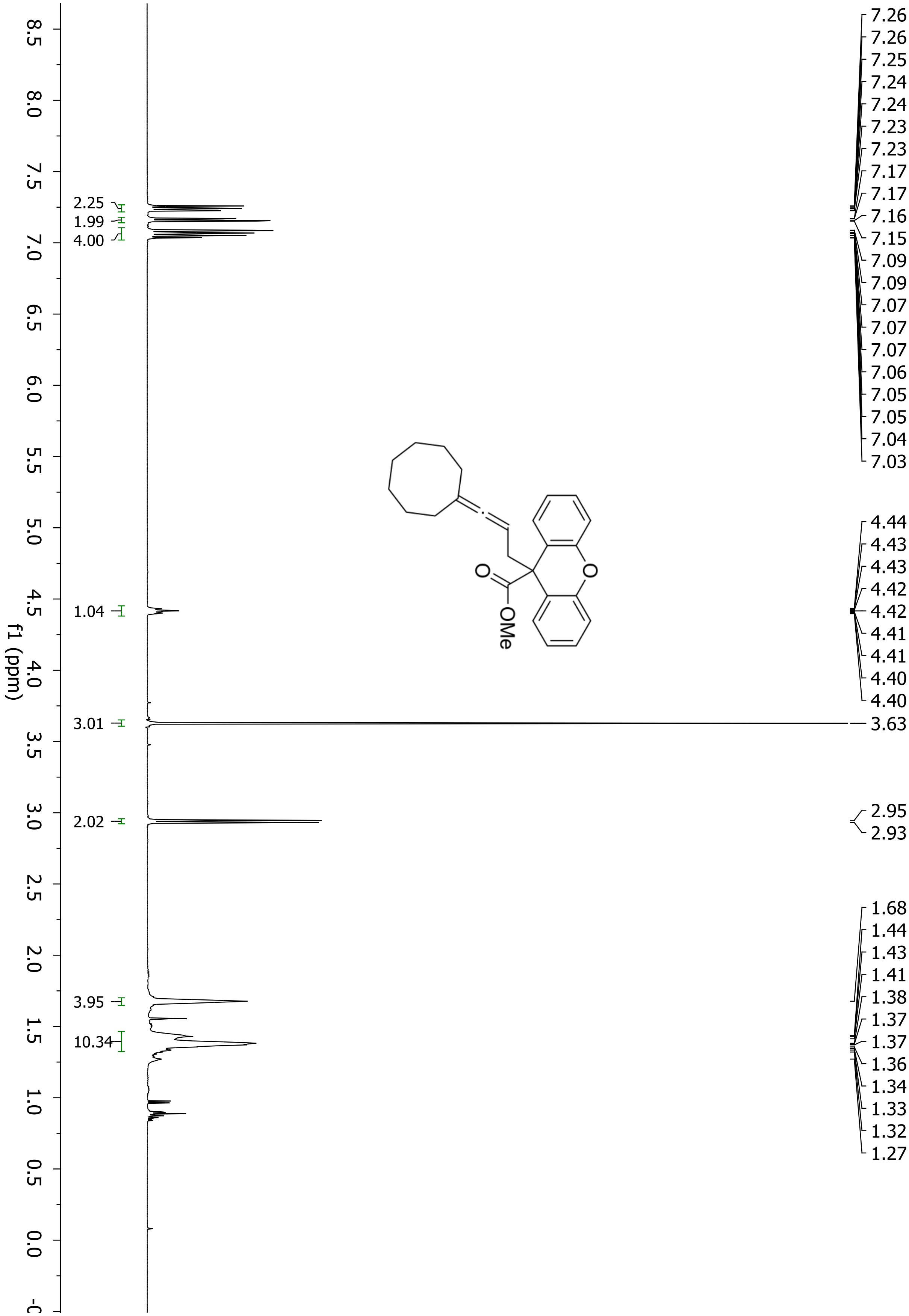

7.28
7.27
7.26
7.26
7.20
7.20
7.19
7.19
3.70
3.03
3.01
1.92
1.91
1.91
1.90
1.90
1.57
1.49
1.48
1.45
3.97
3.93
0.97
2.89
1.95
4.00
10.44
f1 (ppm)
Cl
Cl
O
OMe

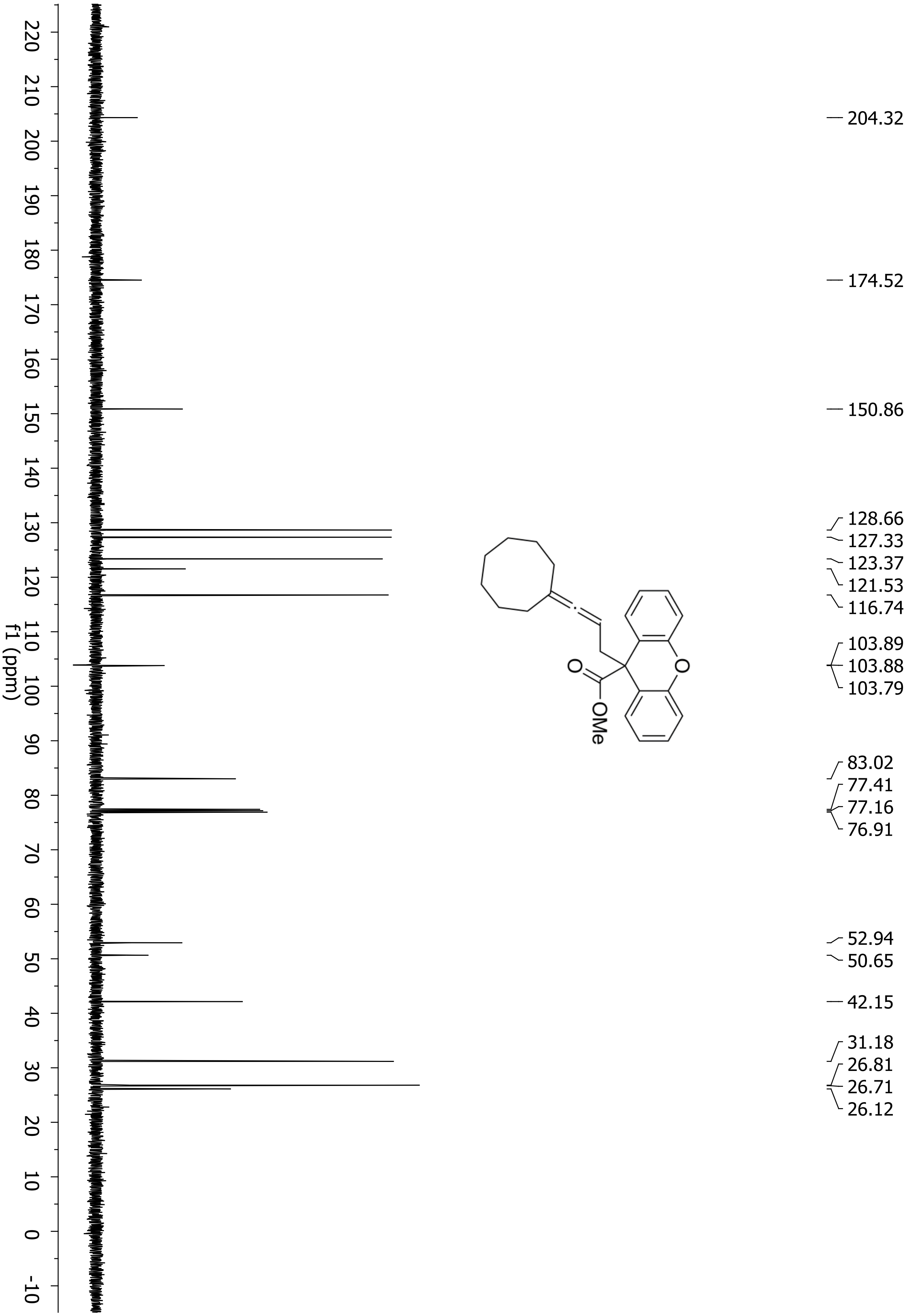

204.14
173.98
140.77
133.11
130.59
128.19
84.25
77.41
77.16
76.91
59.96
52.78
39.04
31.32
26.83
26.22
f1 (ppm)
Cl
Cl
O
OMe

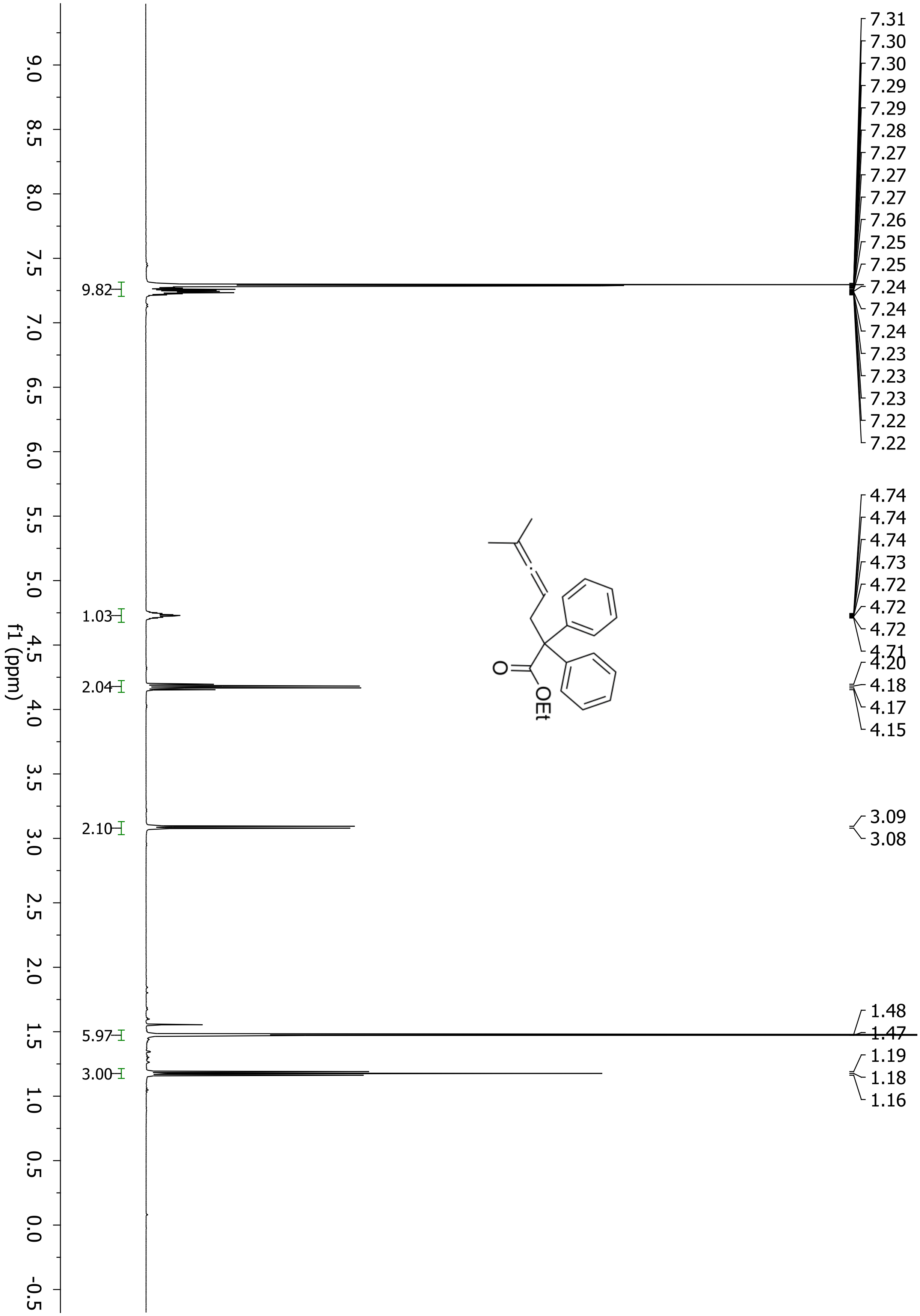


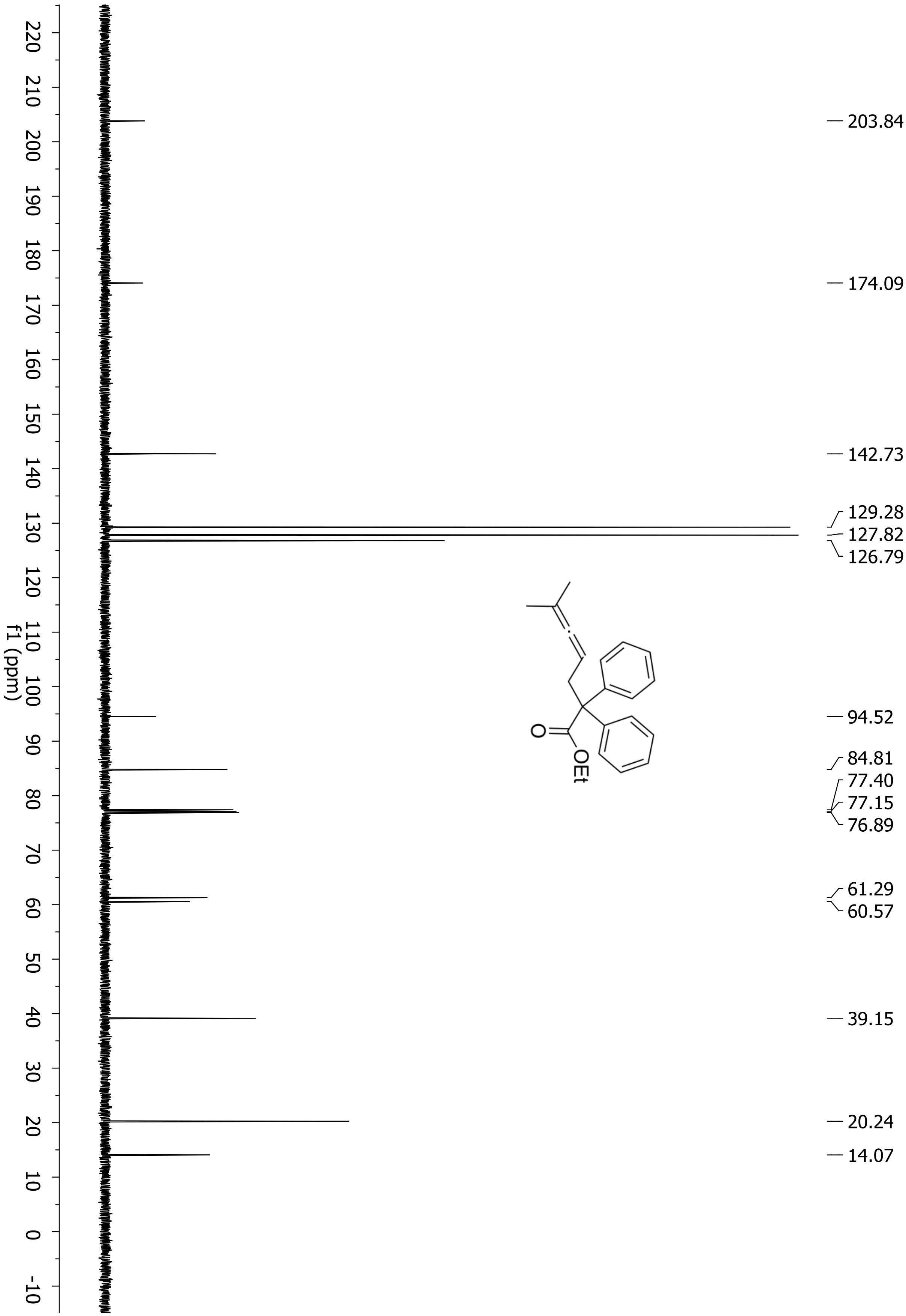
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
4.07
4.17
0.99
6.31
3.09
2.00
4.01
10.54
7.26
7.21
7.20
7.19
7.19
7.18
6.84
6.83
6.83
6.82
6.81
6.81
4.76
4.75
4.75
4.74
4.74
4.73
4.73
4.72
4.72
3.79
3.69
3.04
3.02
1.94
1.94
1.93
1.92
1.51
1.50
1.50
1.48
1.47
1.46
1.45
MeO
O
OMe
OMe

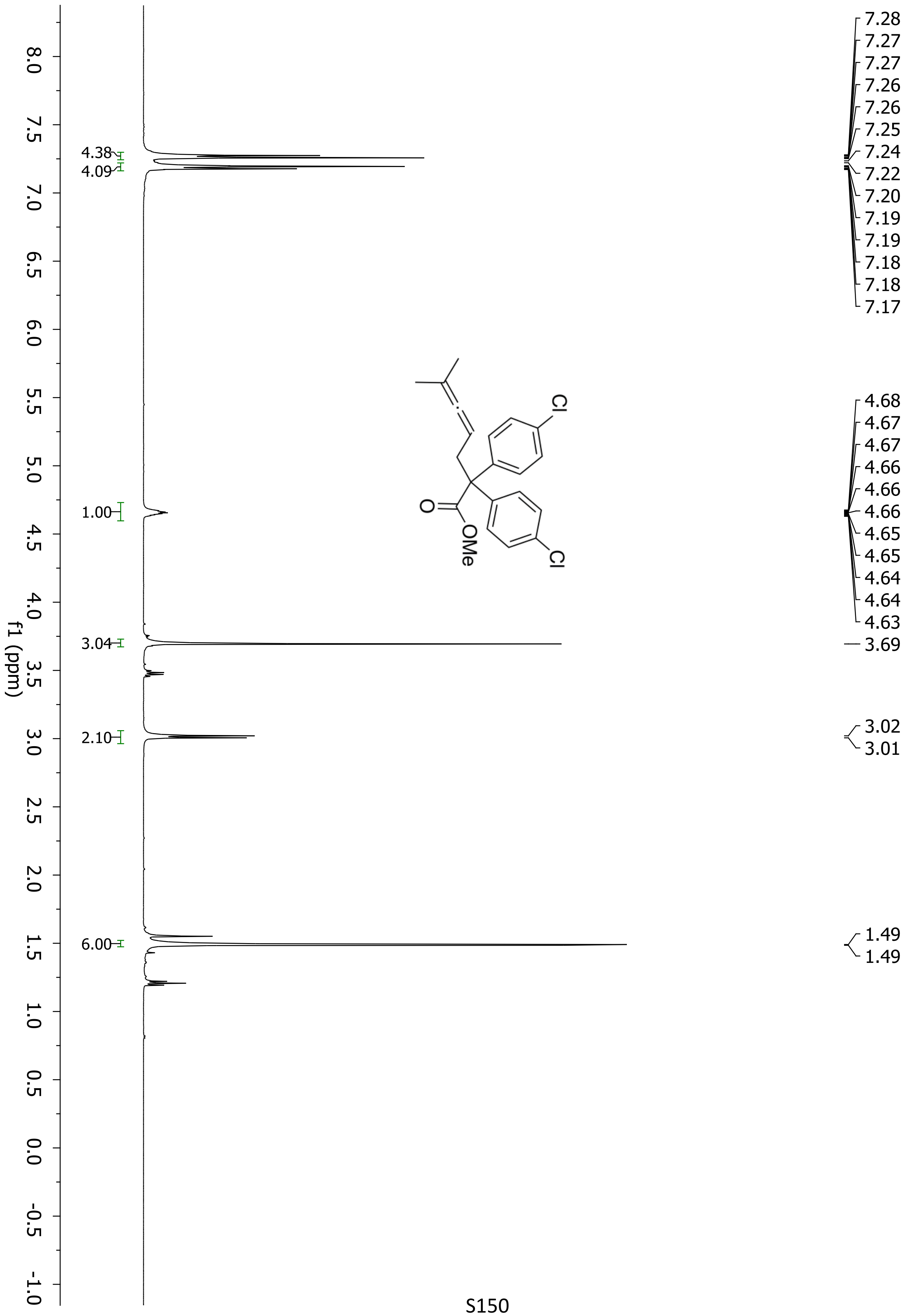

203.90
175.18
158.35
134.91
130.27
113.24
103.66
85.05
77.41
77.15
76.90
59.38
55.36
52.45
39.26
31.38
26.89
26.84
26.26
MeO
O
OMe
OMe
f1 (ppm)

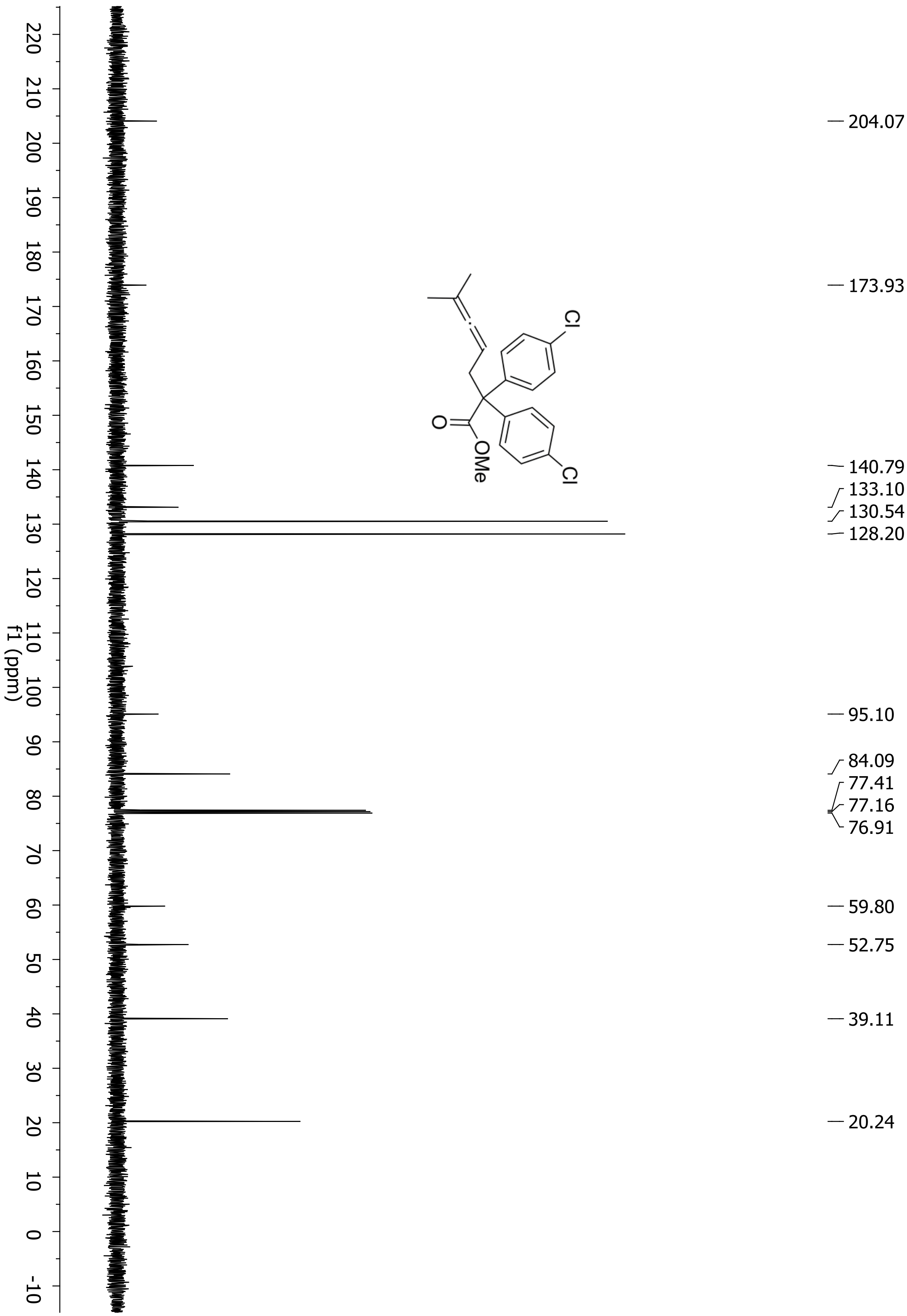

7.26
7.26
7.25
7.24
7.24
7.23
7.23
7.17
7.17
7.16
7.15
7.09
7.09
7.07
7.07
7.07
7.06
7.05
7.05
7.04
7.03
4.44
4.43
4.43
4.42
4.42
4.41
4.41
4.40
4.40
3.63
2.95
2.93
1.68
1.44
1.43
1.41
1.38
1.37
1.37
1.36
1.34
1.33
1.32
1.27
2.25
1.99
4.00
1.04
3.01
2.02
3.95
10.34
O
OMe
f1 (ppm)

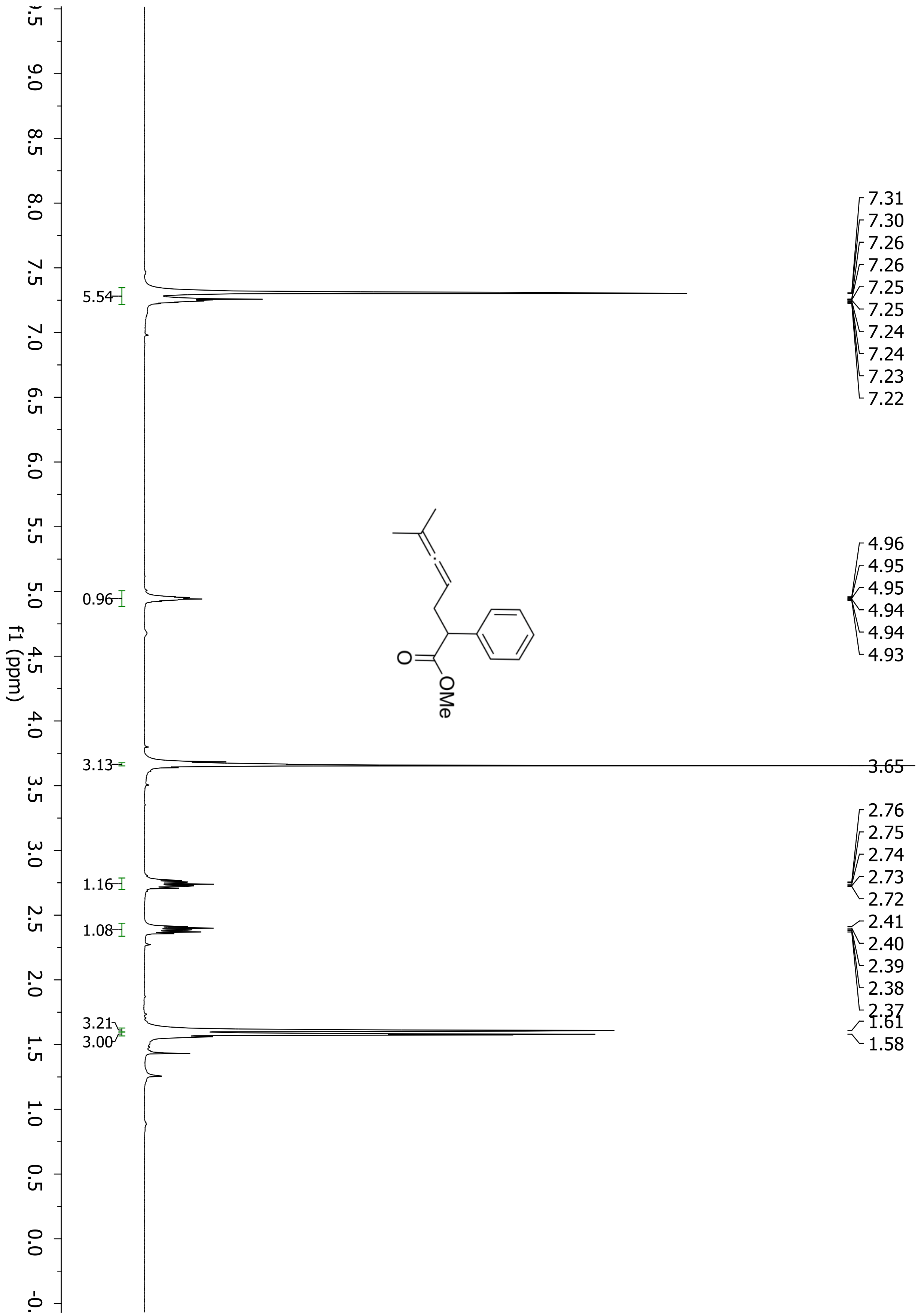

204.32
174.52
150.86
128.66
127.33
123.37
121.53
116.74
103.89
103.88
103.79
83.02
77.41
77.16
76.91
52.94
50.65
42.15
31.18
26.81
26.71
26.12
OMe
f1 (ppm)

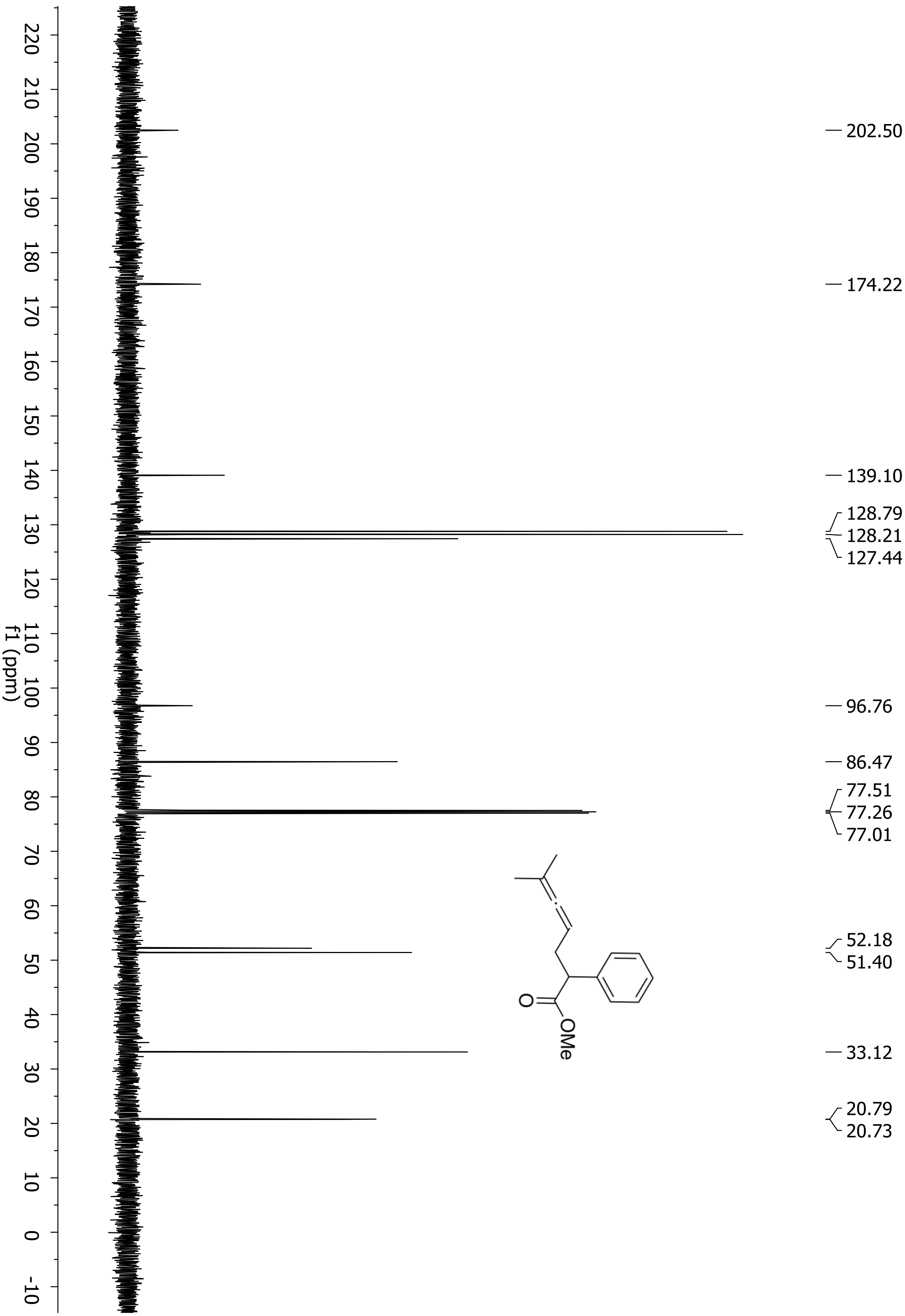

7.31
7.30
7.30
7.29
7.29
7.28
7.27
7.27
7.27
7.26
7.25
7.25
7.24
7.24
7.24
7.23
7.23
7.23
7.22
7.22
4.74
4.74
4.74
4.73
4.72
4.72
4.72
4.71
4.20
4.18
4.17
4.15
3.09
3.08
1.48
1.47
1.19
1.18
1.16
9.82
1.03
2.04
2.10
5.97
3.00
O
OEt
f1 (ppm)

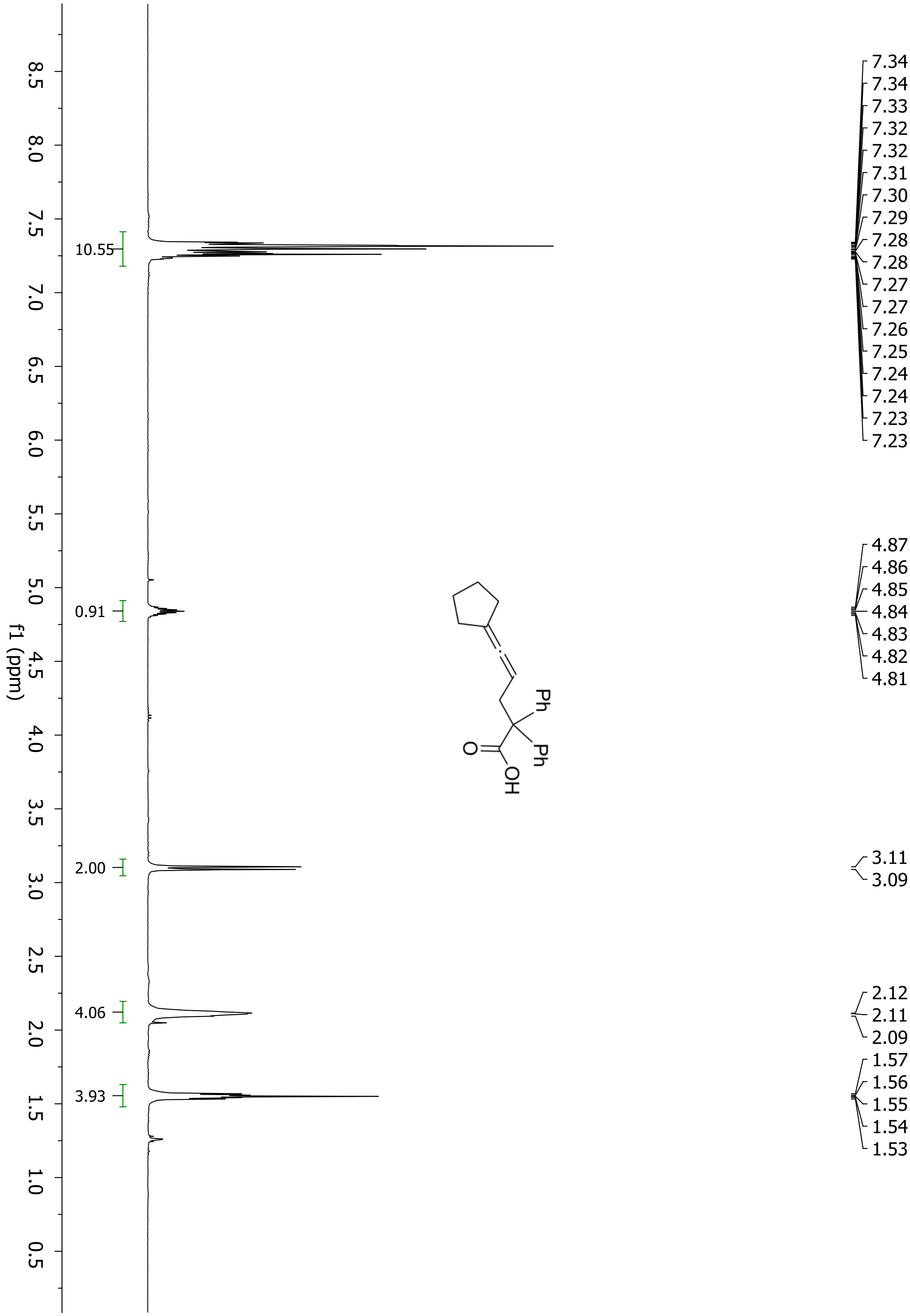

203.84
174.09
142.73
129.28
127.82
126.79
94.52
84.81
77.40
77.15
76.89
61.29
60.57
39.15
20.24
14.07
f1 (ppm)
O
OEt

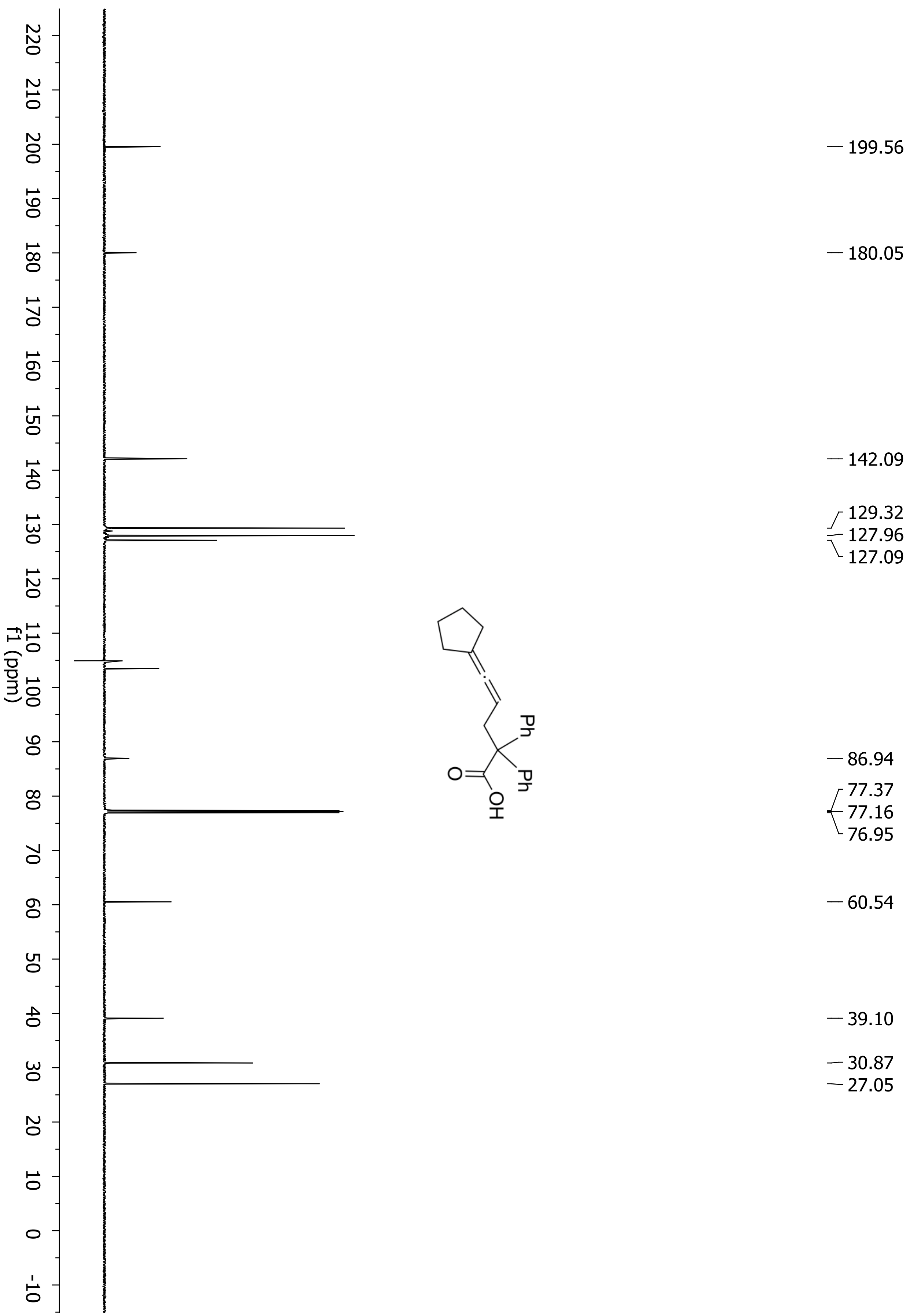

7.28
7.27
7.27
7.26
7.26
7.25
7.24
7.22
7.20
7.19
7.19
7.18
7.18
7.17
4.68
4.67
4.67
4.66
4.66
4.66
4.65
4.65
4.64
4.64
4.63
3.69
3.02
3.01
1.49
1.49
4.38
4.09
1.00
3.04
2.10
6.00
Cl
Cl
O
OMe
f1 (ppm)

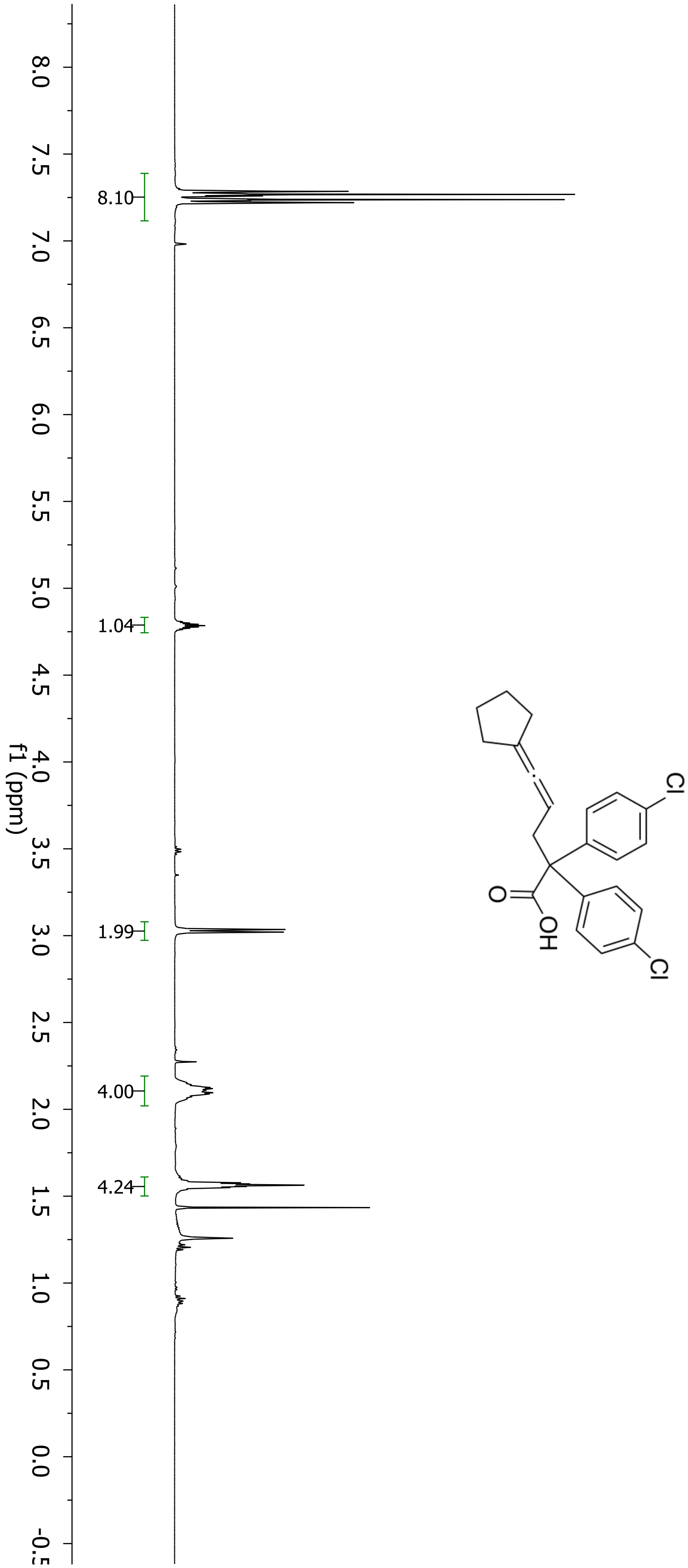

204.07
173.93
140.79
133.10
130.54
128.20
95.10
84.09
77.41
77.16
76.91
59.80
52.75
39.11
20.24
f1 (ppm)
Cl
Cl
O
OMe

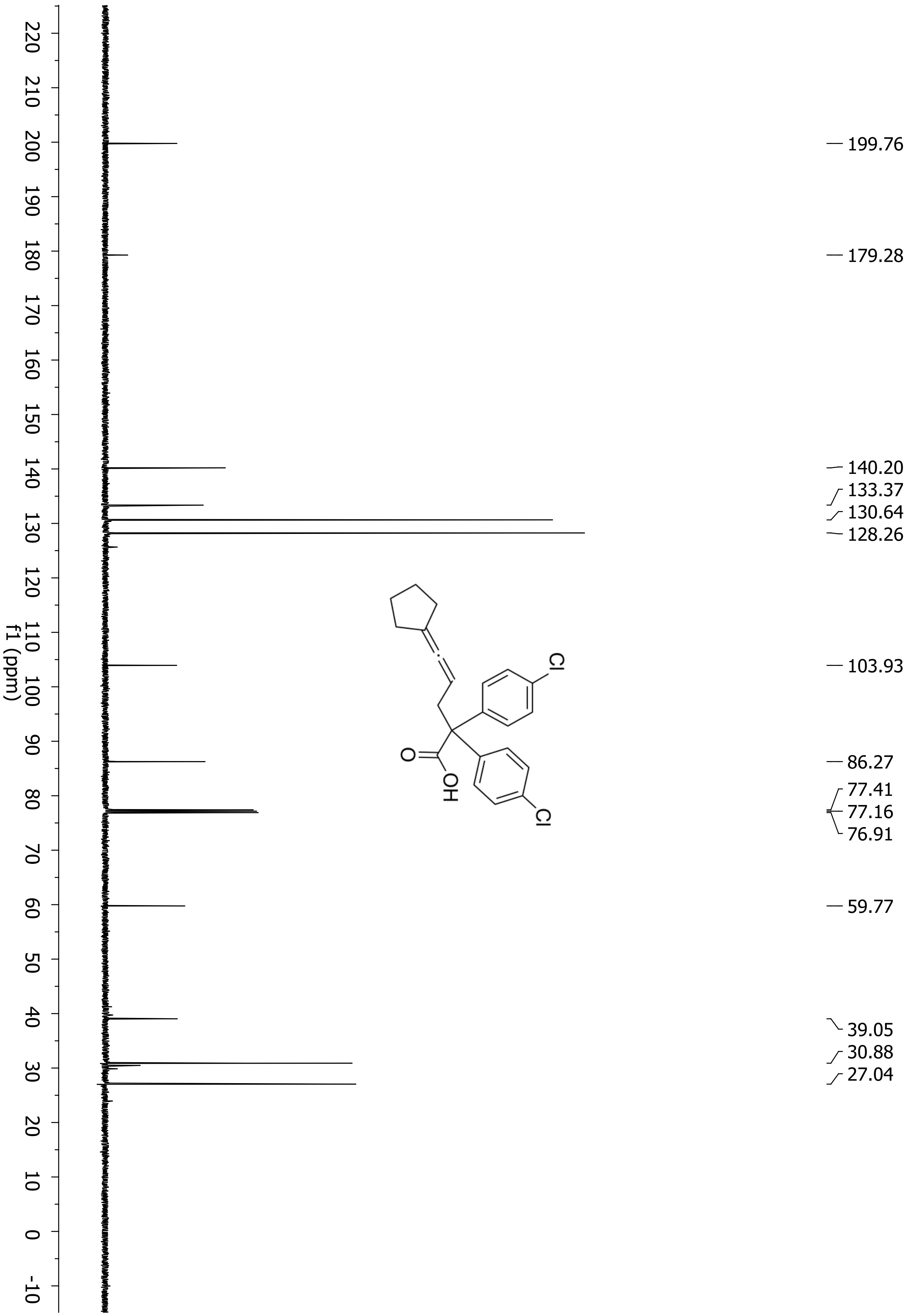

7.31
7.30
7.26
7.26
7.25
7.25
7.24
7.24
7.23
7.22
4.96
4.95
4.95
4.94
4.94
4.93
3.65
2.76
2.75
2.74
2.73
2.72
2.41
2.40
2.39
2.38
2.37
1.61
1.58
5.54
0.96
3.13
1.16
1.08
3.21
3.00
OMe
O
f1 (ppm)

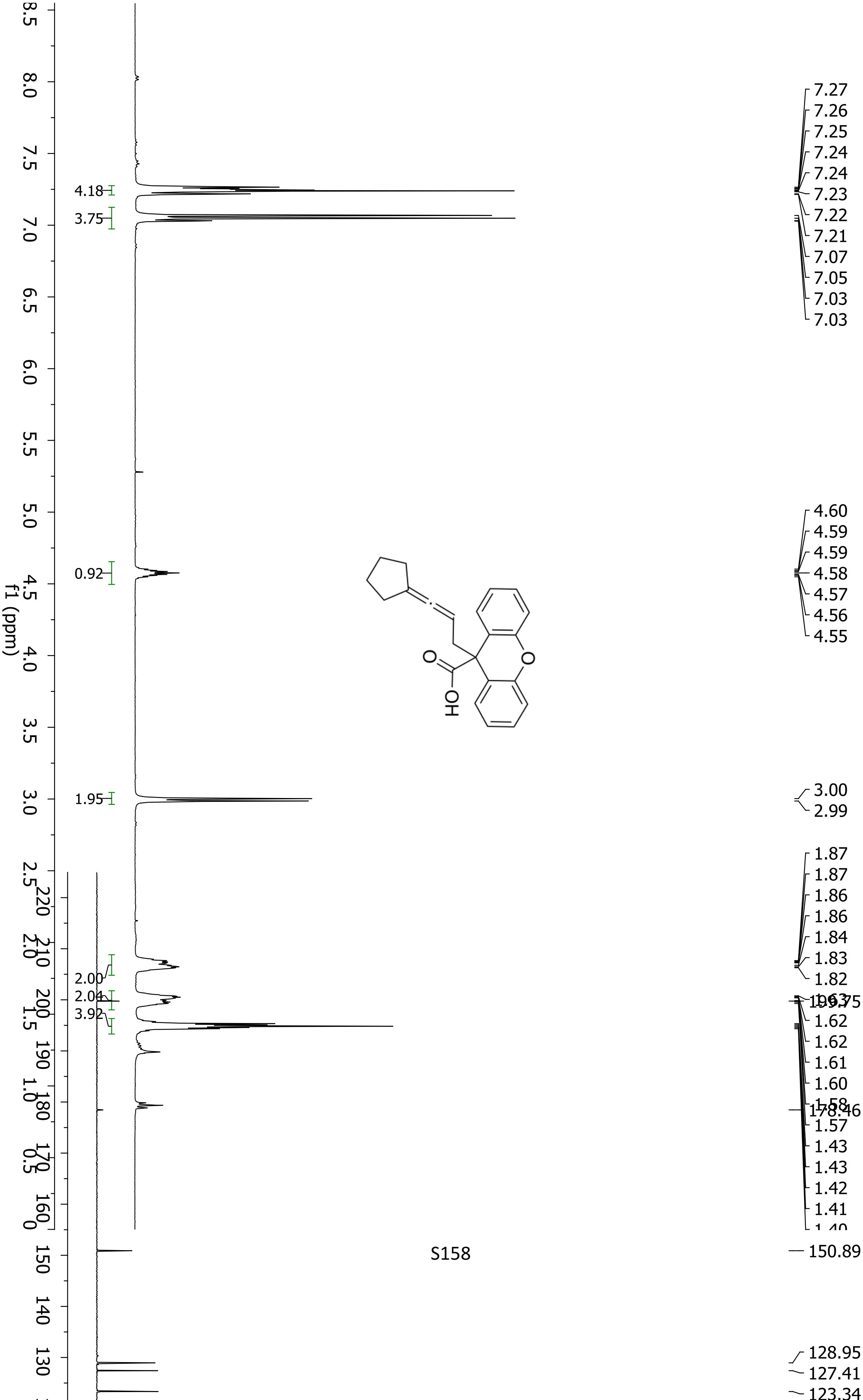

202.50
174.22
139.10
128.79
128.21
127.44
96.76
86.47
77.51
77.26
77.01
52.18
51.40
33.12
20.79
20.73
OMe
O
f1 (ppm)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


f1 (ppm)
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
10.55
0.91
2.00
4.06
3.93
7.34 7.34 7.33 7.32 7.32 7.31 7.30 7.29 7.28 7.28 7.27 7.27 7.26 7.25 7.24 7.24 7.23 7.23
4.87 4.86 4.85 4.84 4.83 4.82 4.81
3.11 3.09
2.12 2.11 2.09
1.57 1.56 1.55 1.54 1.53
Ph
Ph
O
OH

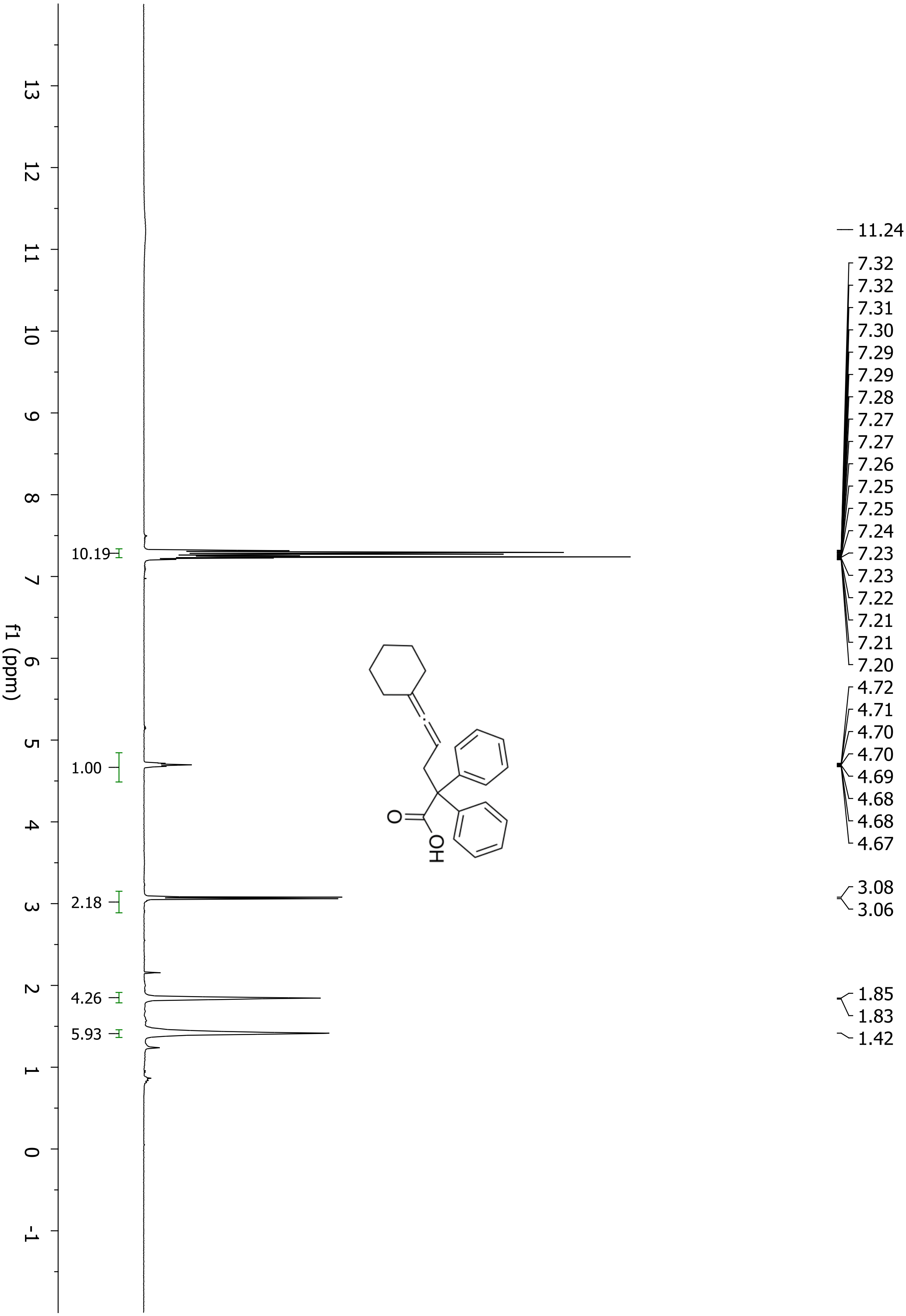

199.56
180.05
142.09
129.32
127.96
127.09
86.94
77.37
77.16
76.95
60.54
39.10
30.87
27.05
Ph
Ph
O
OH
f1 (ppm)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
8.10
1.04
1.99
4.00
4.24
Cl
Cl
O
OH

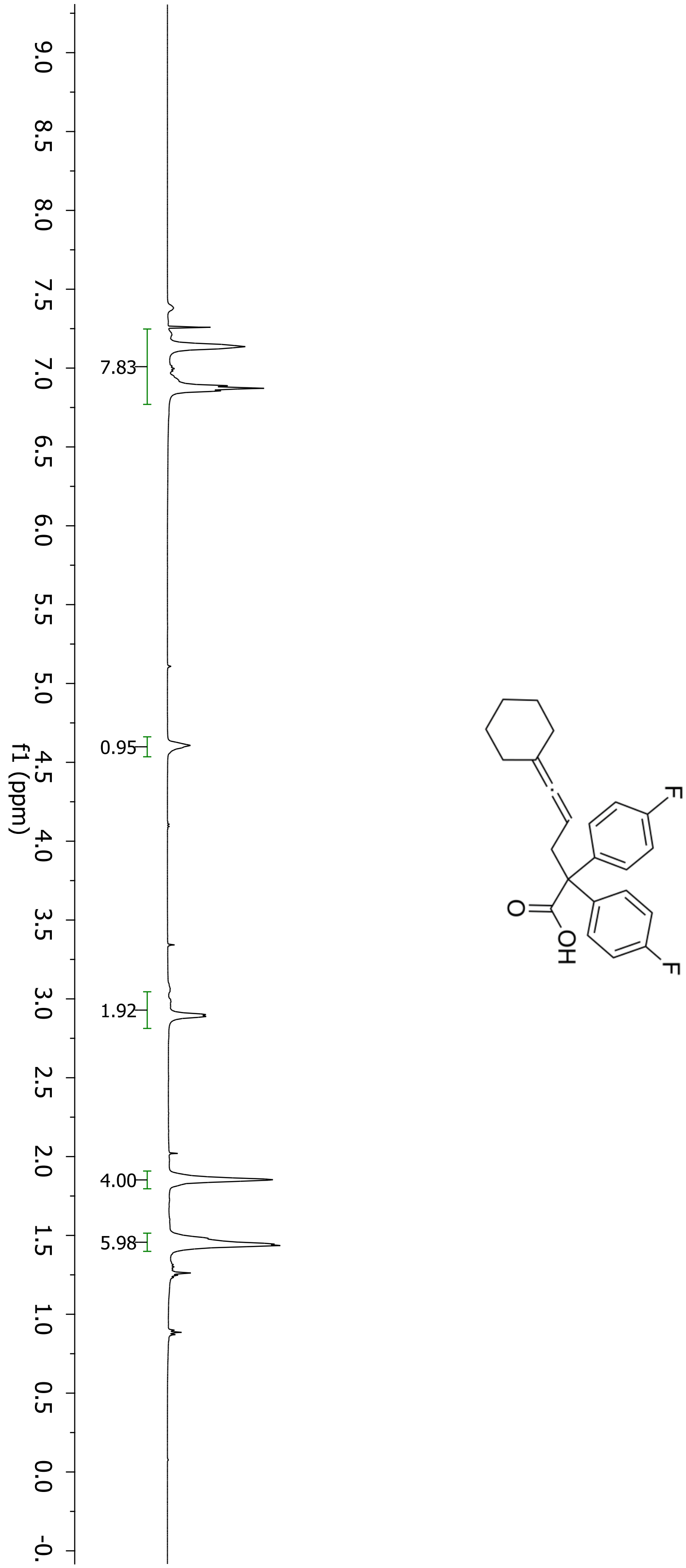

199.76
179.28
140.20
133.37
130.64
128.26
103.93
86.27
77.41
77.16
76.91
59.77
39.05
30.88
27.04
f1 (ppm)
Cl
Cl
O
OH

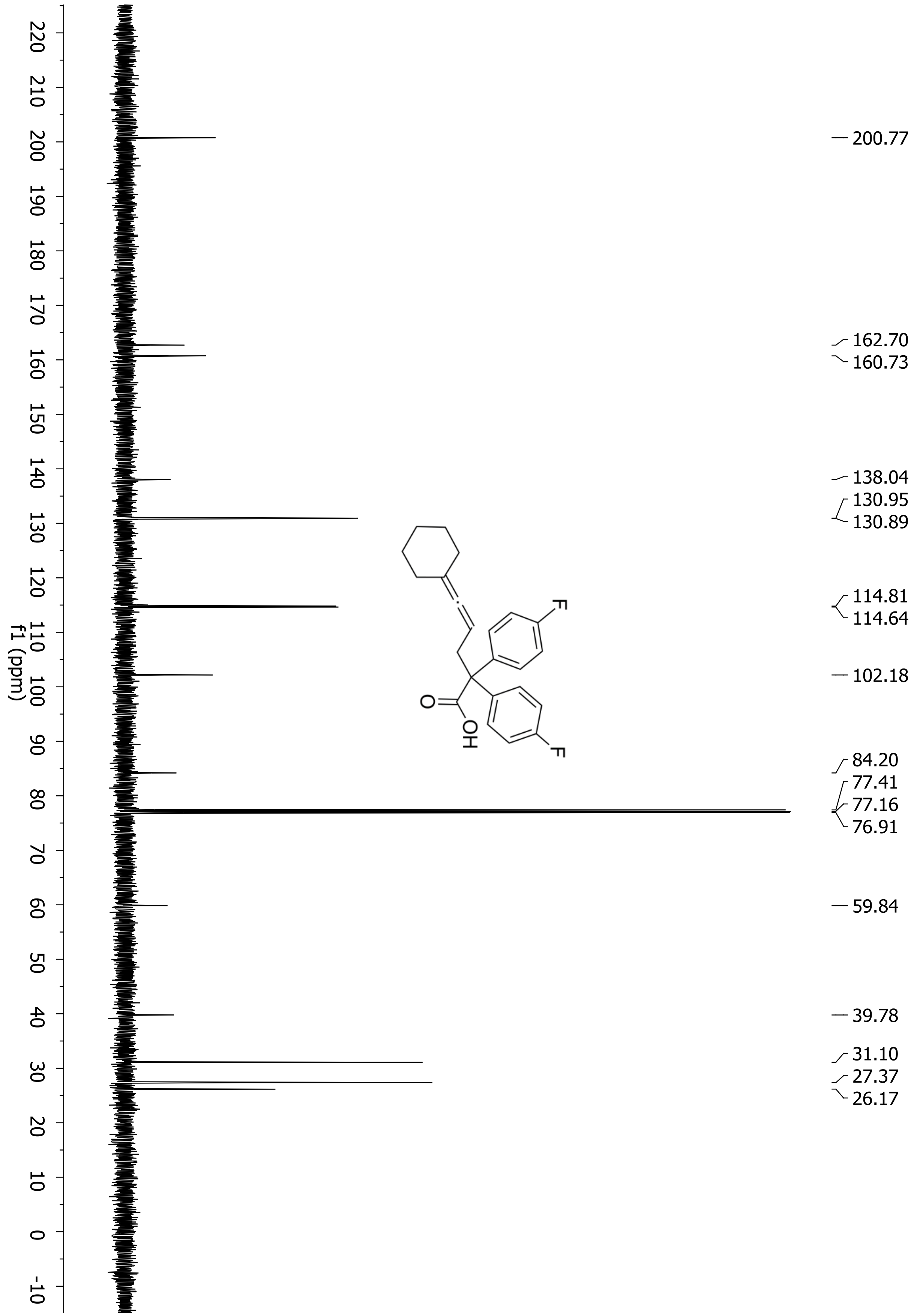


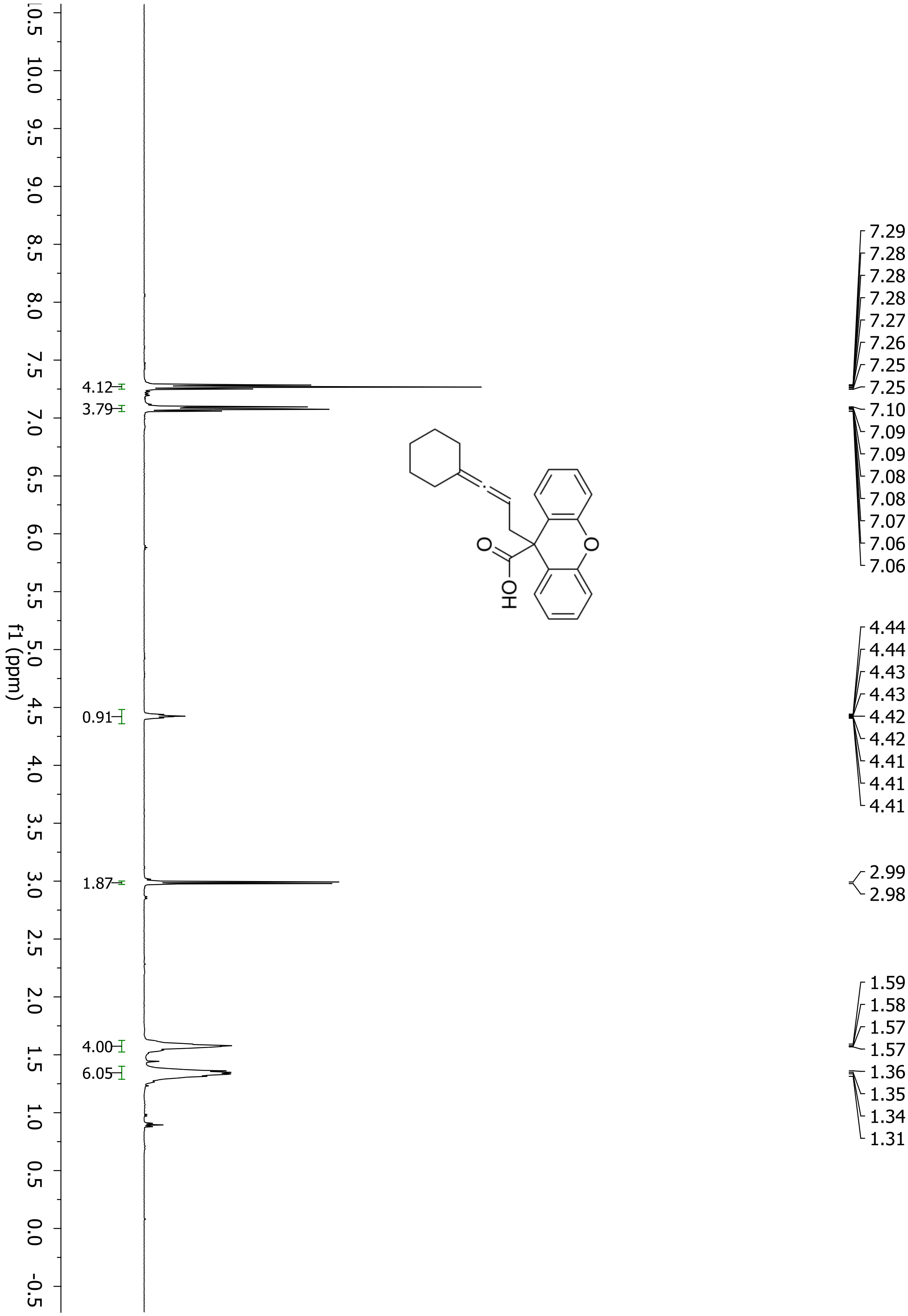
f1 (ppm)
4.18
3.75
0.92
1.95
2.00
2.04
3.92
7.27
7.26
7.25
7.24
7.24
7.23
7.22
7.21
7.07
7.05
7.03
7.03
4.60
4.59
4.59
4.58
4.57
4.56
4.55
3.00
2.99
1.87
1.87
1.86
1.86
1.84
1.83
1.82
1.62
1.62
1.61
1.60
1.57
1.43
1.43
1.42
1.41
178.46
150.89
128.95
127.41
123.34
O
OH

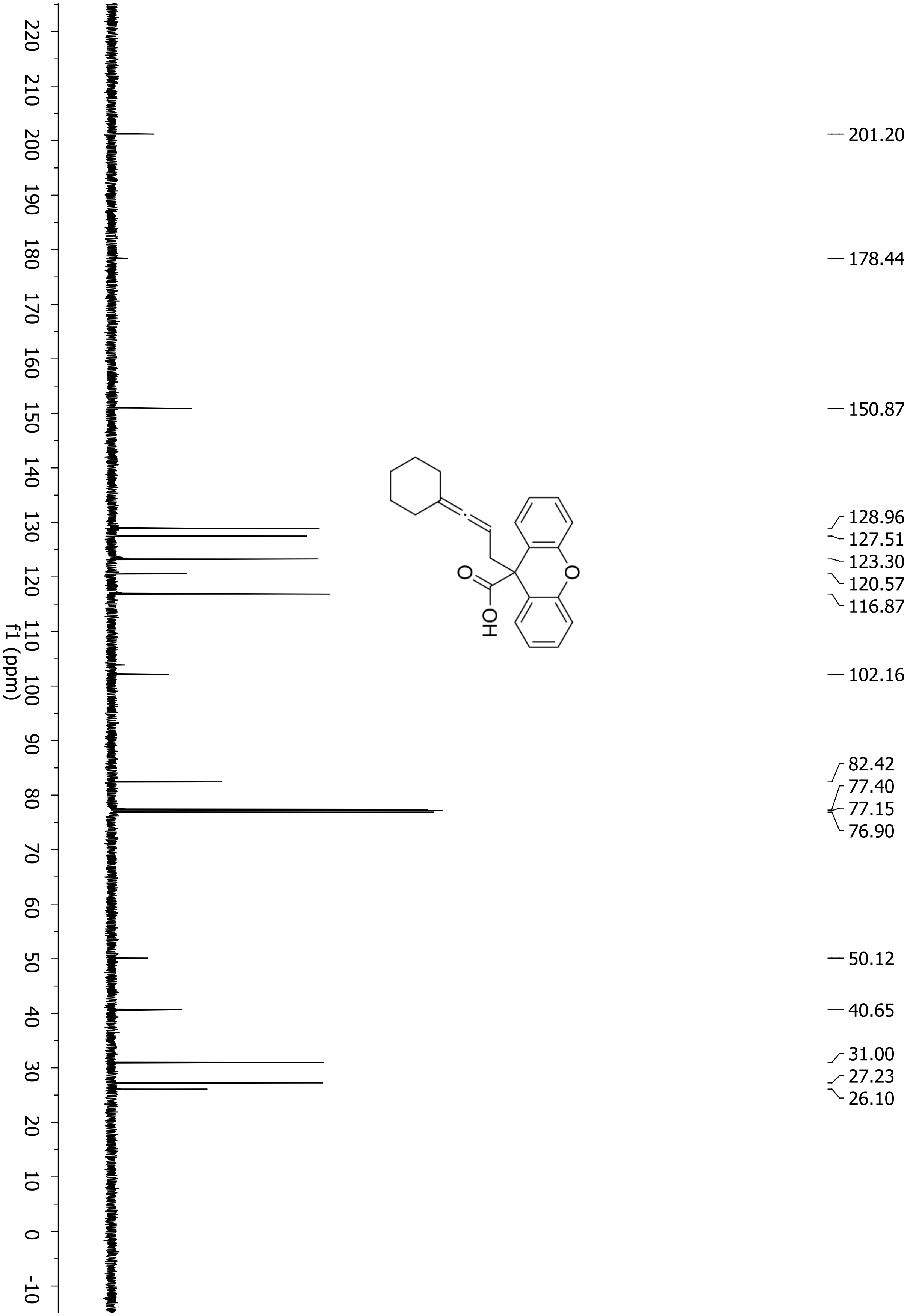


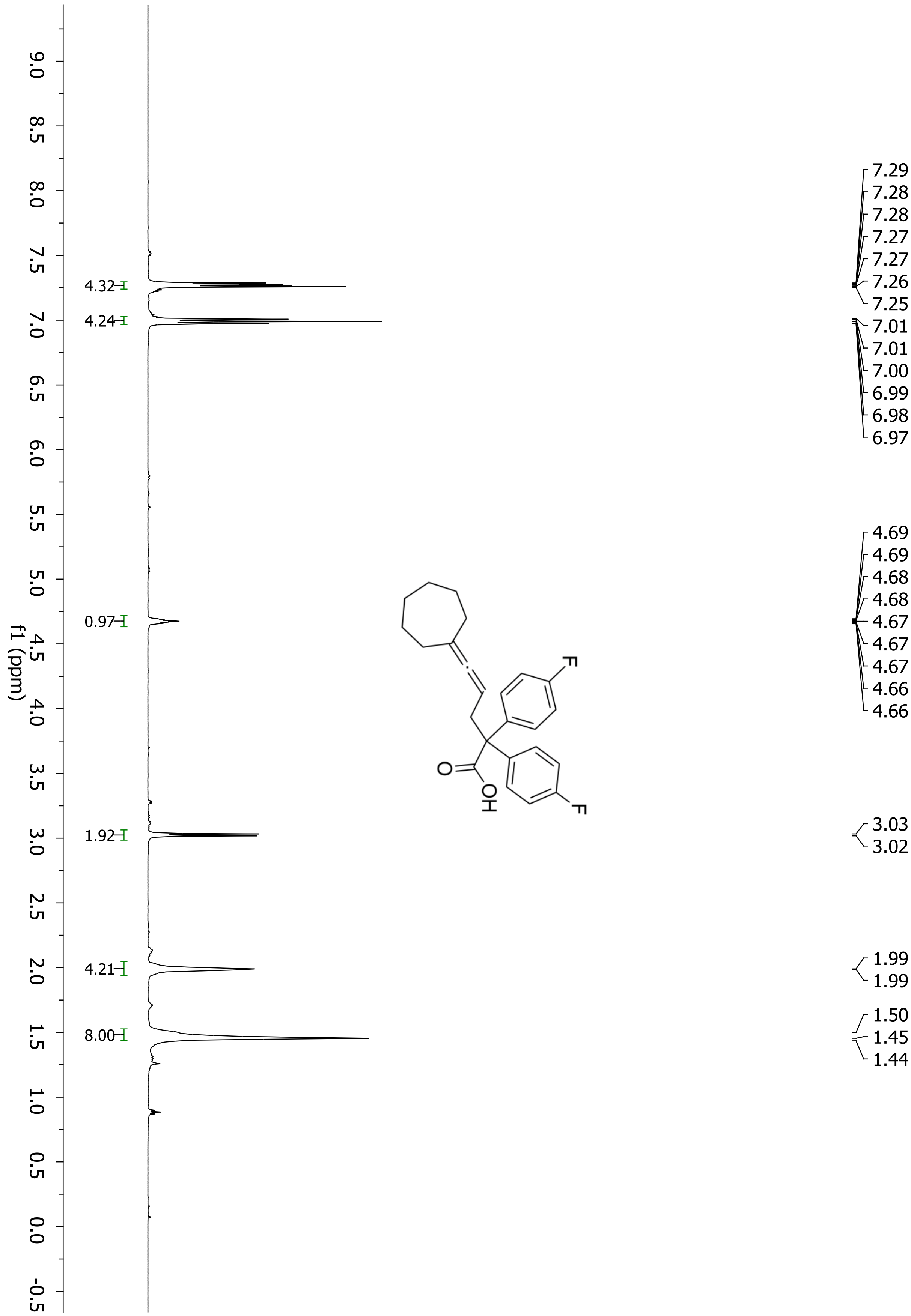
f1 (ppm)
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
10.19
1.00
2.18
4.26
5.93
OH
O
11.24
7.32
7.32
7.31
7.30
7.29
7.29
7.28
7.27
7.27
7.26
7.25
7.25
7.24
7.23
7.23
7.22
7.21
7.21
7.20
4.72
4.71
4.70
4.70
4.69
4.68
4.68
4.67
3.08
3.06
1.85
1.83
1.42

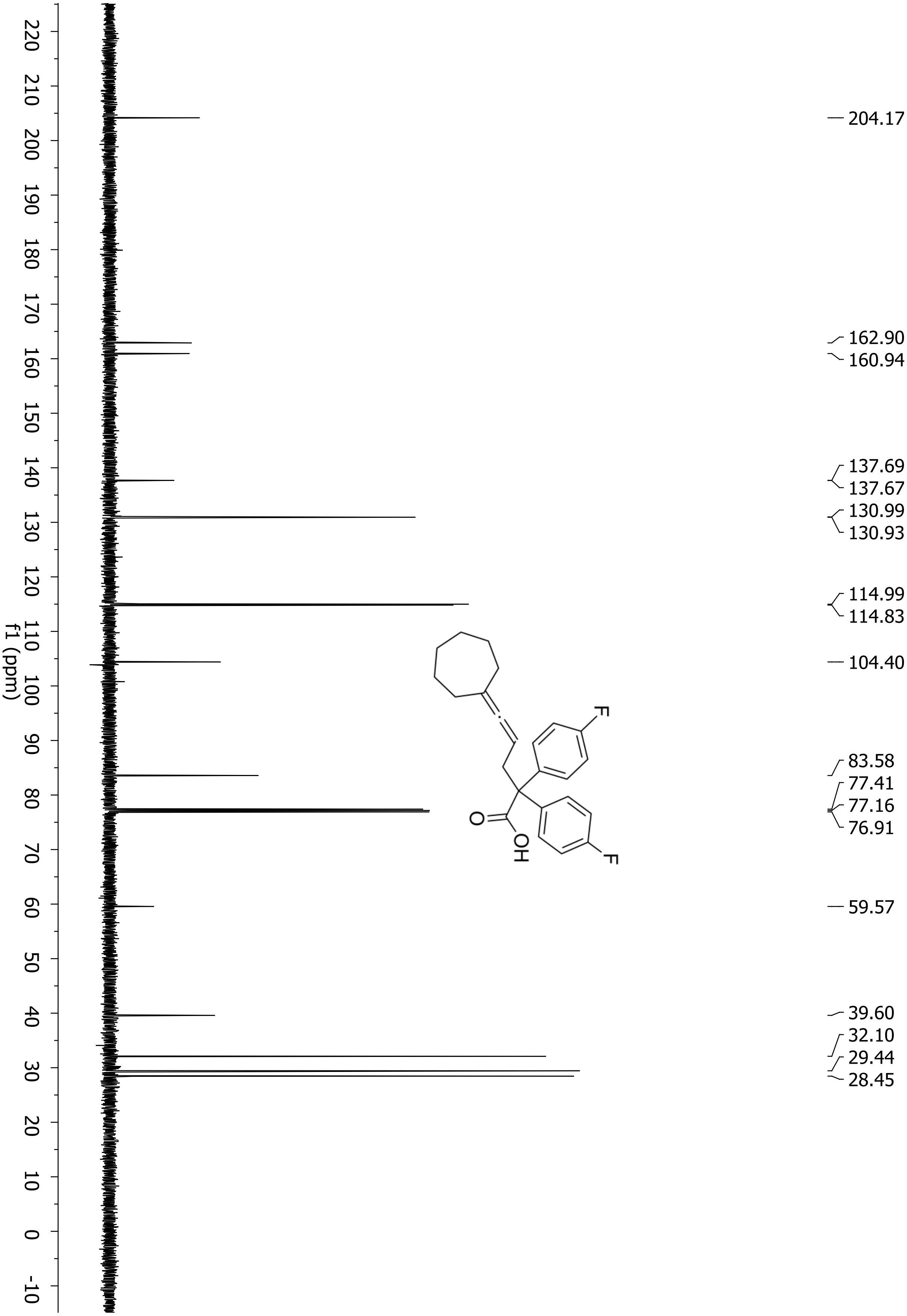

7.83
0.95
1.92
4.00
5.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)
F
F
O
OH

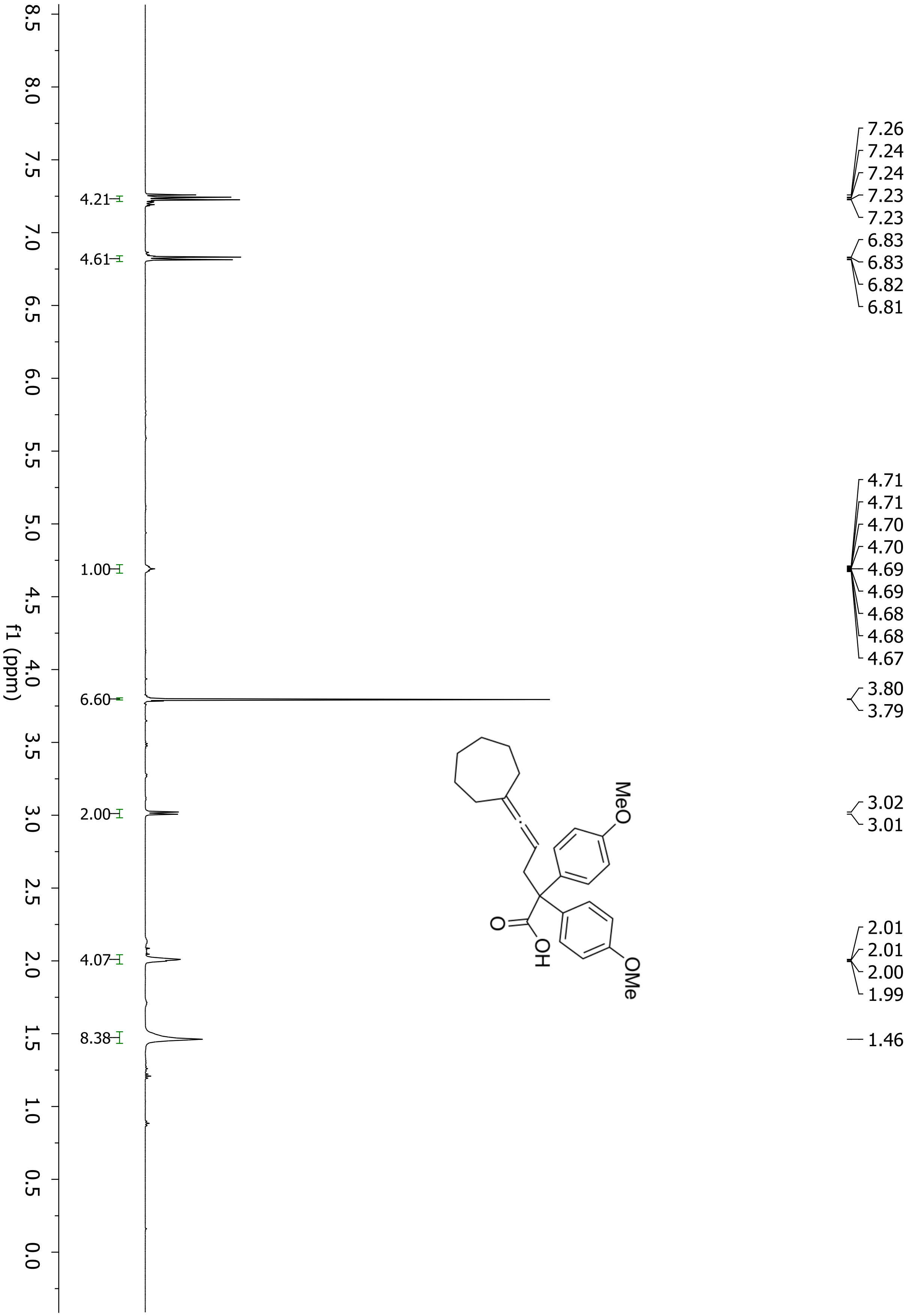

200.77
162.70
160.73
138.04
130.95
130.89
114.81
114.64
102.18
84.20
77.41
77.16
76.91
59.84
39.78
31.10
27.37
26.17
f1 (ppm)
F
F
O
OH

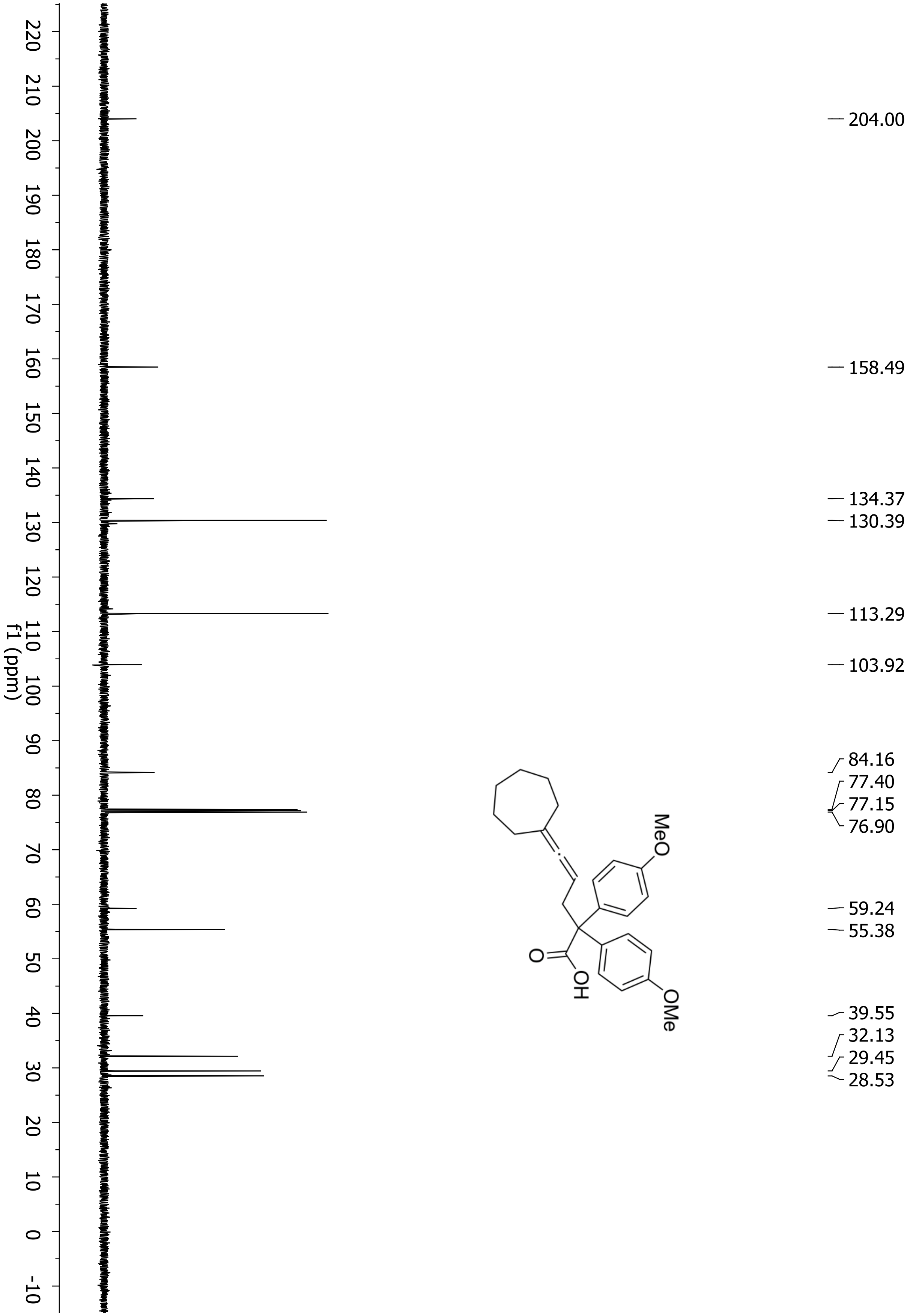

7.29
7.28
7.28
7.28
7.27
7.26
7.25
7.25
7.10
7.09
7.09
7.08
7.08
7.07
7.06
7.06
4.44
4.44
4.43
4.43
4.42
4.42
4.41
4.41
4.41
2.99
2.98
1.59
1.58
1.57
1.57
1.36
1.35
1.34
1.31
4.12
3.79
0.91
1.87
4.00
6.05
OH
O
f1 (ppm)

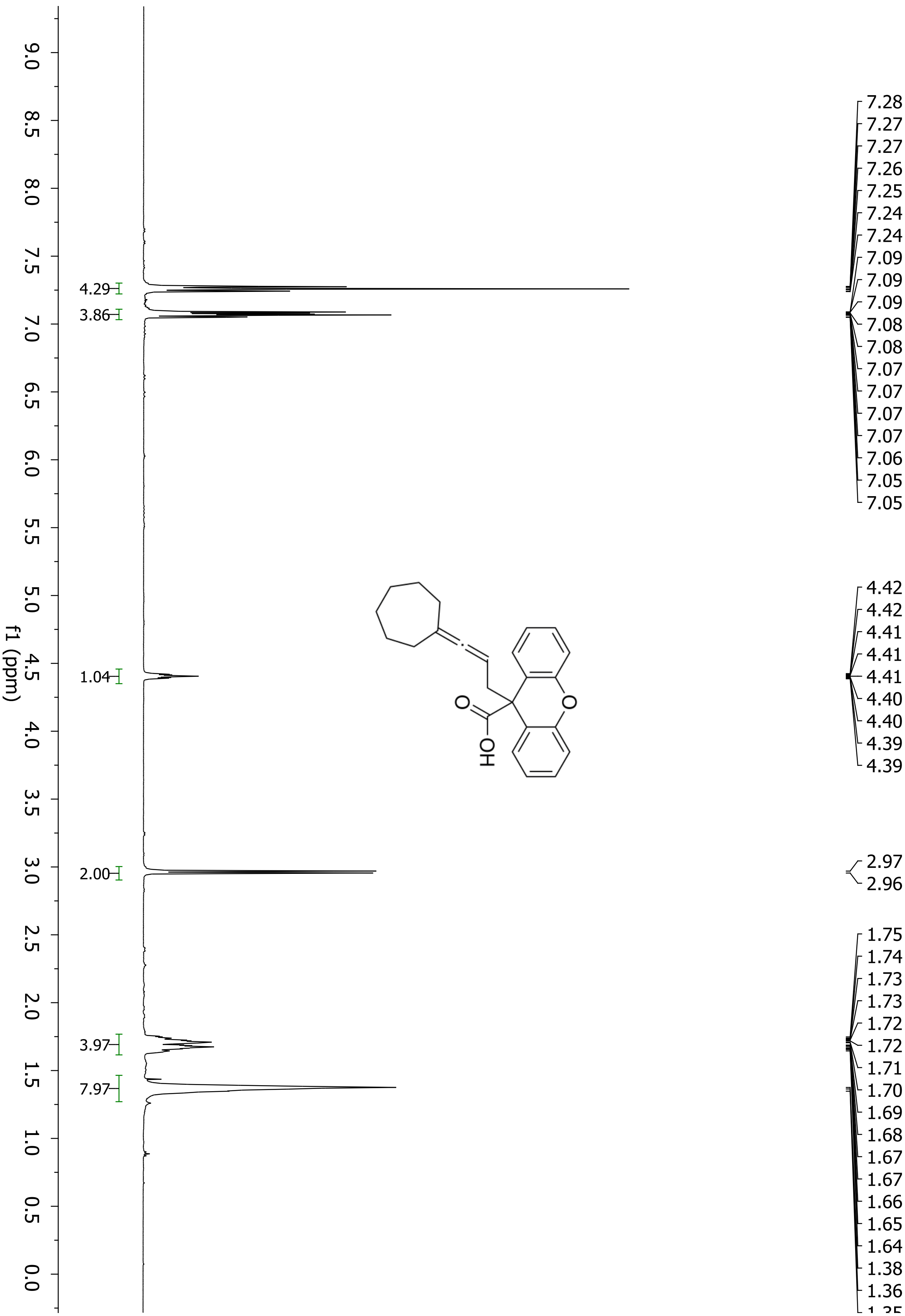

201.20
178.44
150.87
128.96
127.51
123.30
120.57
116.87
102.16
82.42
77.40
77.15
76.90
50.12
40.65
31.00
27.23
26.10
f1 (ppm)

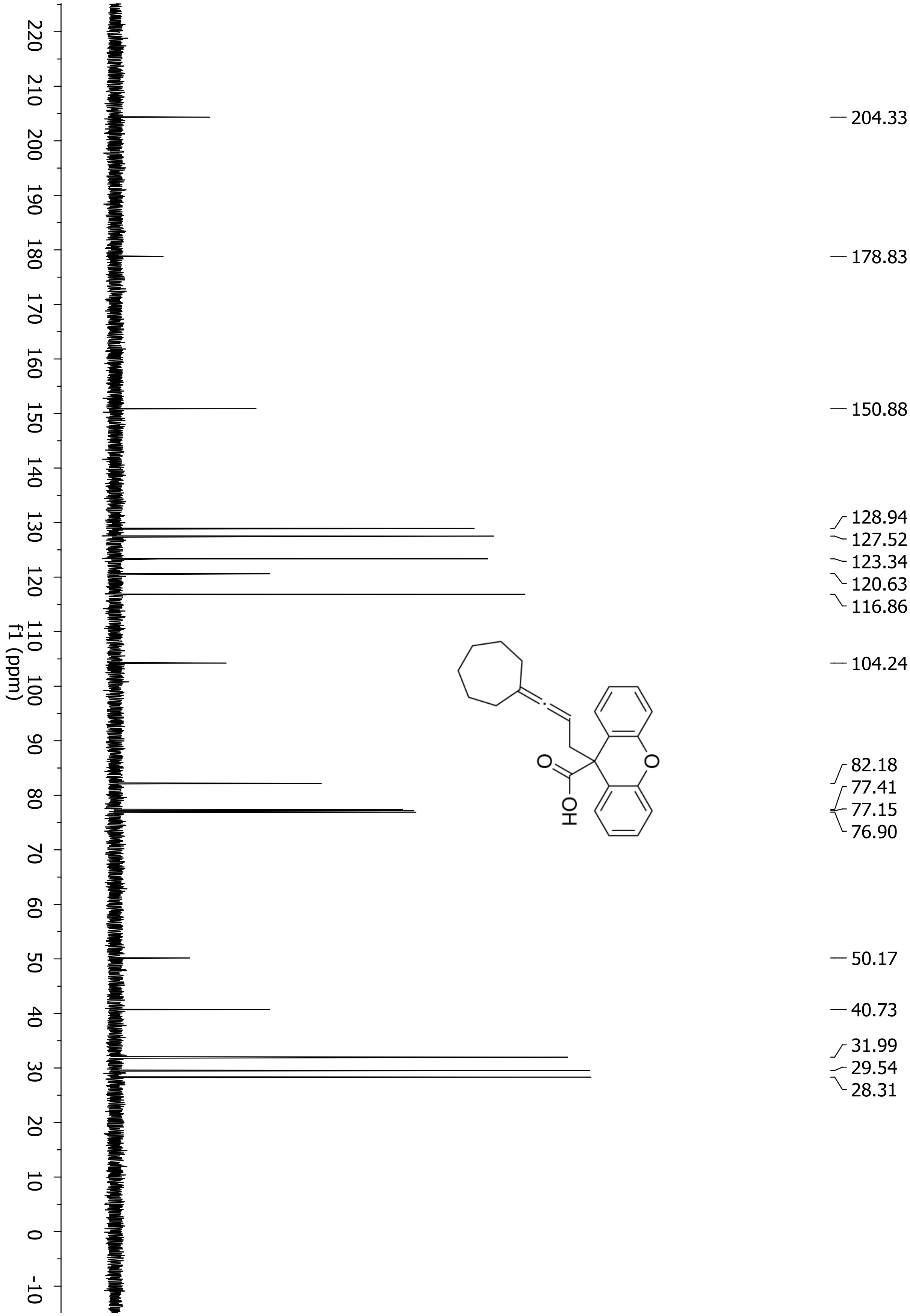

7.29
7.28
7.28
7.27
7.27
7.26
7.25
7.01
7.01
7.00
6.99
6.98
6.97
4.69
4.69
4.68
4.68
4.67
4.67
4.67
4.66
4.66
3.03
3.02
1.99
1.99
1.50
1.45
1.44
4.32
4.24
0.97
1.92
4.21
8.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
F
F
O
OH


204.17
162.90
160.94
137.69
137.67
130.99
130.93
114.99
114.83
104.40
83.58
77.41
77.16
76.91
59.57
39.60
32.10
29.44
28.45
f1 (ppm)
F
F
O
OH

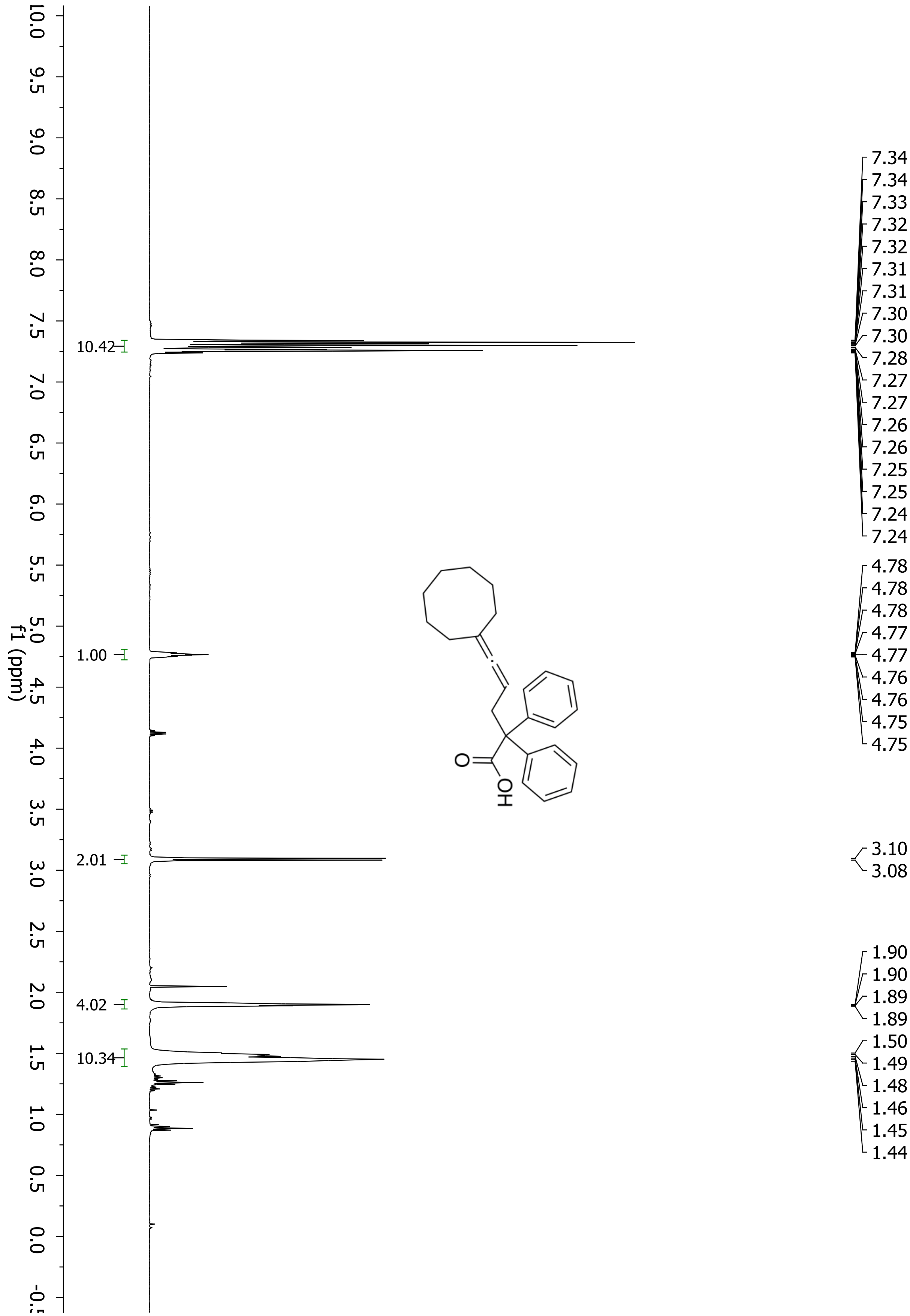



204.00
158.49
134.37
130.39
113.29
103.92
84.16
77.40
77.15
76.90
59.24
55.38
39.55
32.13
29.45
28.53
f1 (ppm)
MeO
OMe
O
OH

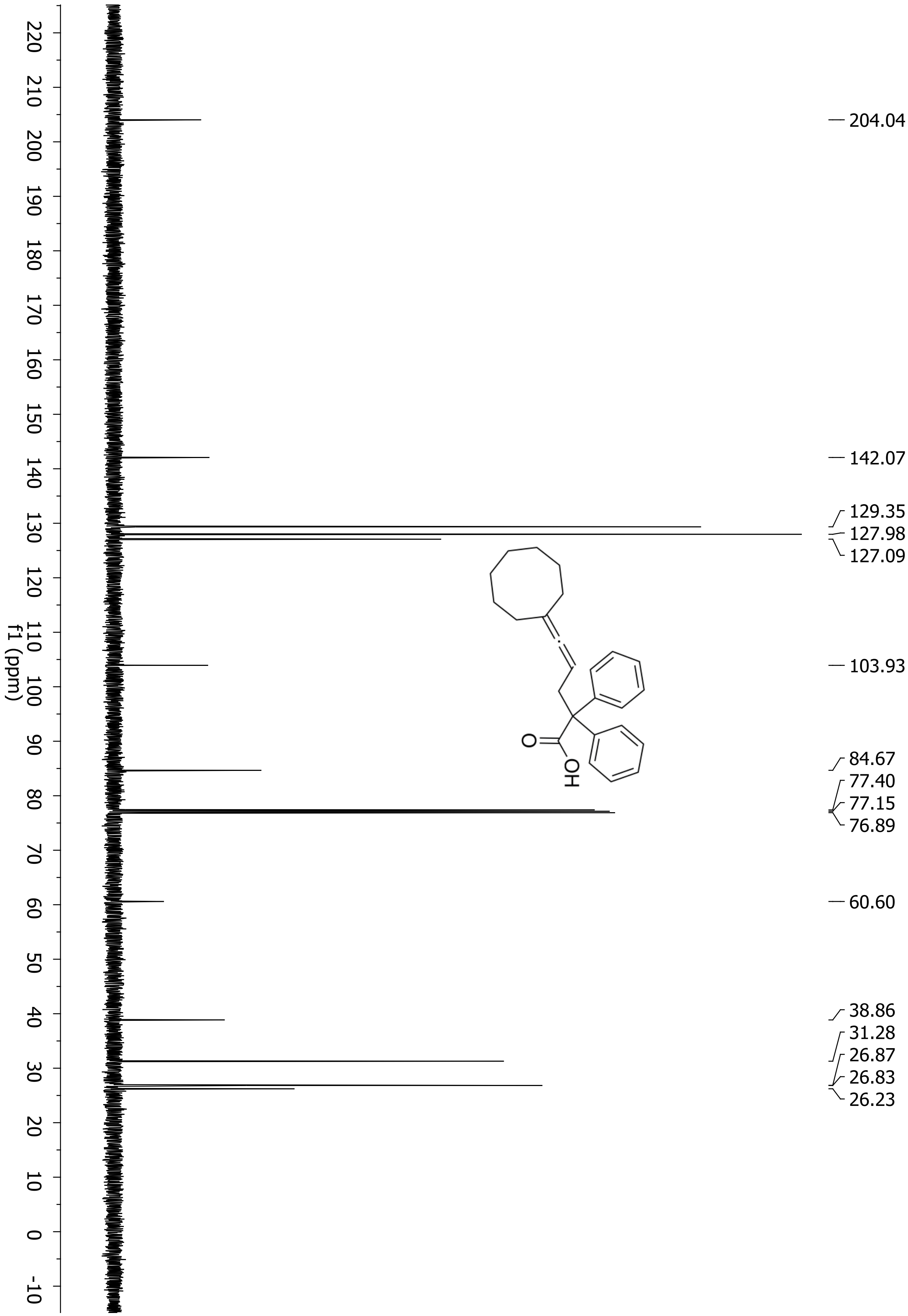

f1 (ppm)
4.29
3.86
1.04
2.00
3.97
7.97
7.28
7.27
7.27
7.26
7.25
7.24
7.24
7.09
7.09
7.09
7.08
7.08
7.07
7.07
7.07
7.07
7.06
7.05
7.05
4.42
4.42
4.41
4.41
4.41
4.40
4.40
4.39
4.39
2.97
2.96
1.75
1.74
1.73
1.73
1.72
1.72
1.71
1.70
1.69
1.68
1.67
1.67
1.66
1.65
1.64
1.38
1.36
O
OH
O



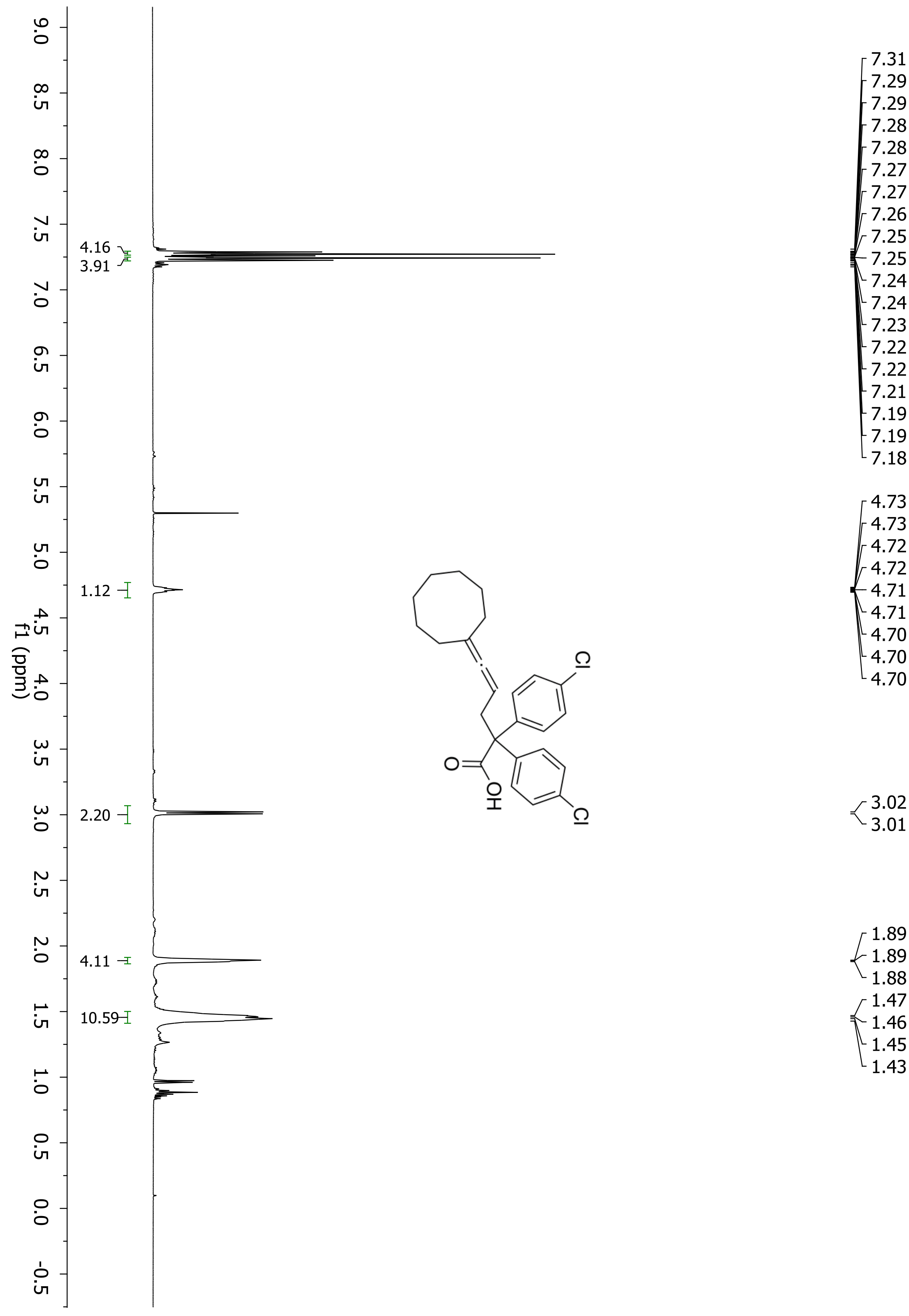
204.33
178.83
150.88
128.94
127.52
123.34
120.63
116.86
104.24
82.18
77.41
77.15
76.90
50.17
40.73
31.99
29.54
28.31
O
OH
O
f1 (ppm)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

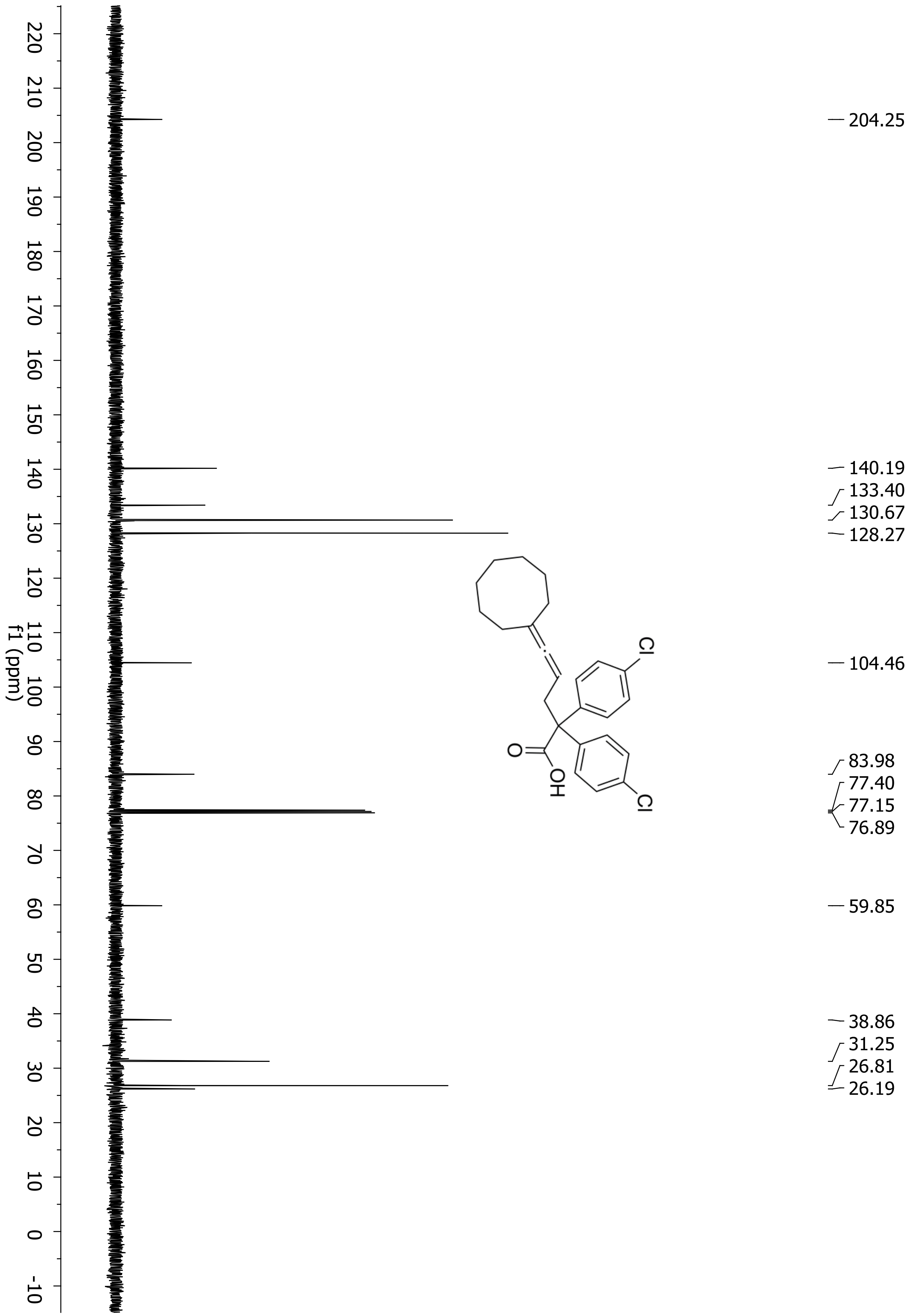


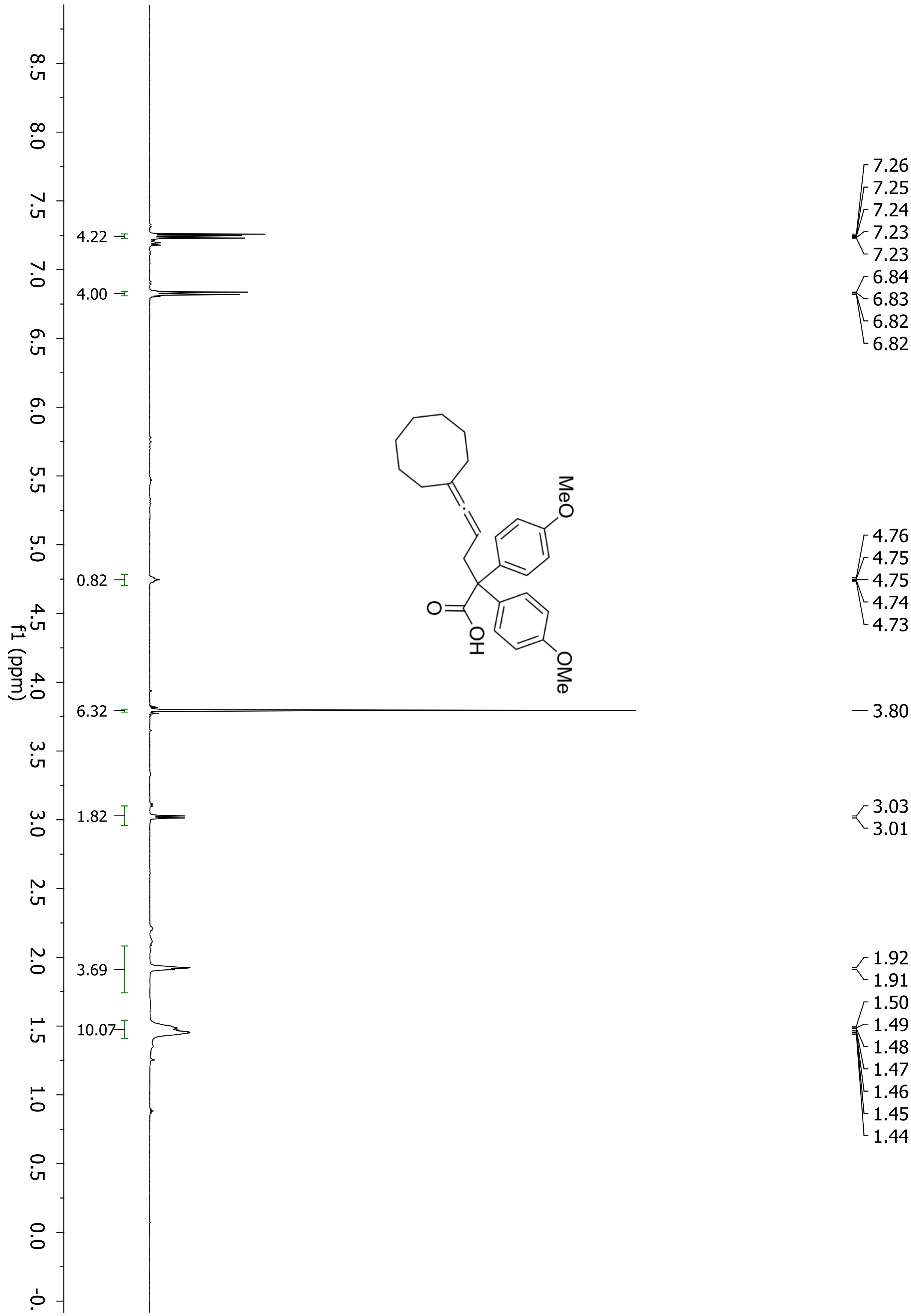
7.34
7.34
7.33
7.32
7.32
7.31
7.31
7.30
7.30
7.28
7.27
7.27
7.26
7.26
7.25
7.25
7.24
7.24
4.78
4.78
4.78
4.77
4.77
4.76
4.76
4.75
4.75
3.10
3.08
1.90
1.90
1.89
1.89
1.50
1.49
1.48
1.46
1.45
1.44
10.42
1.00
2.01
4.02
10.34
OH
O
f1 (ppm)

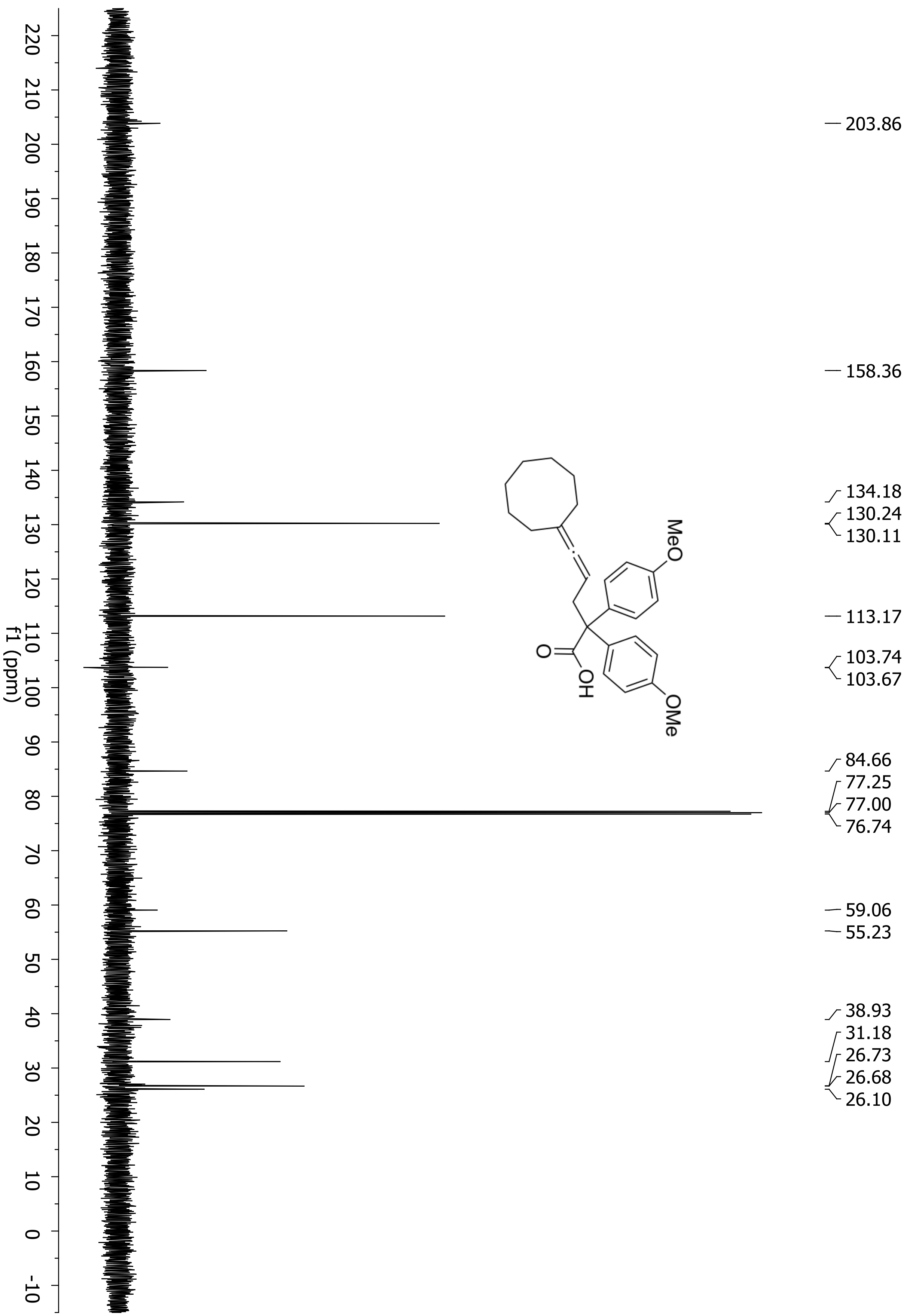


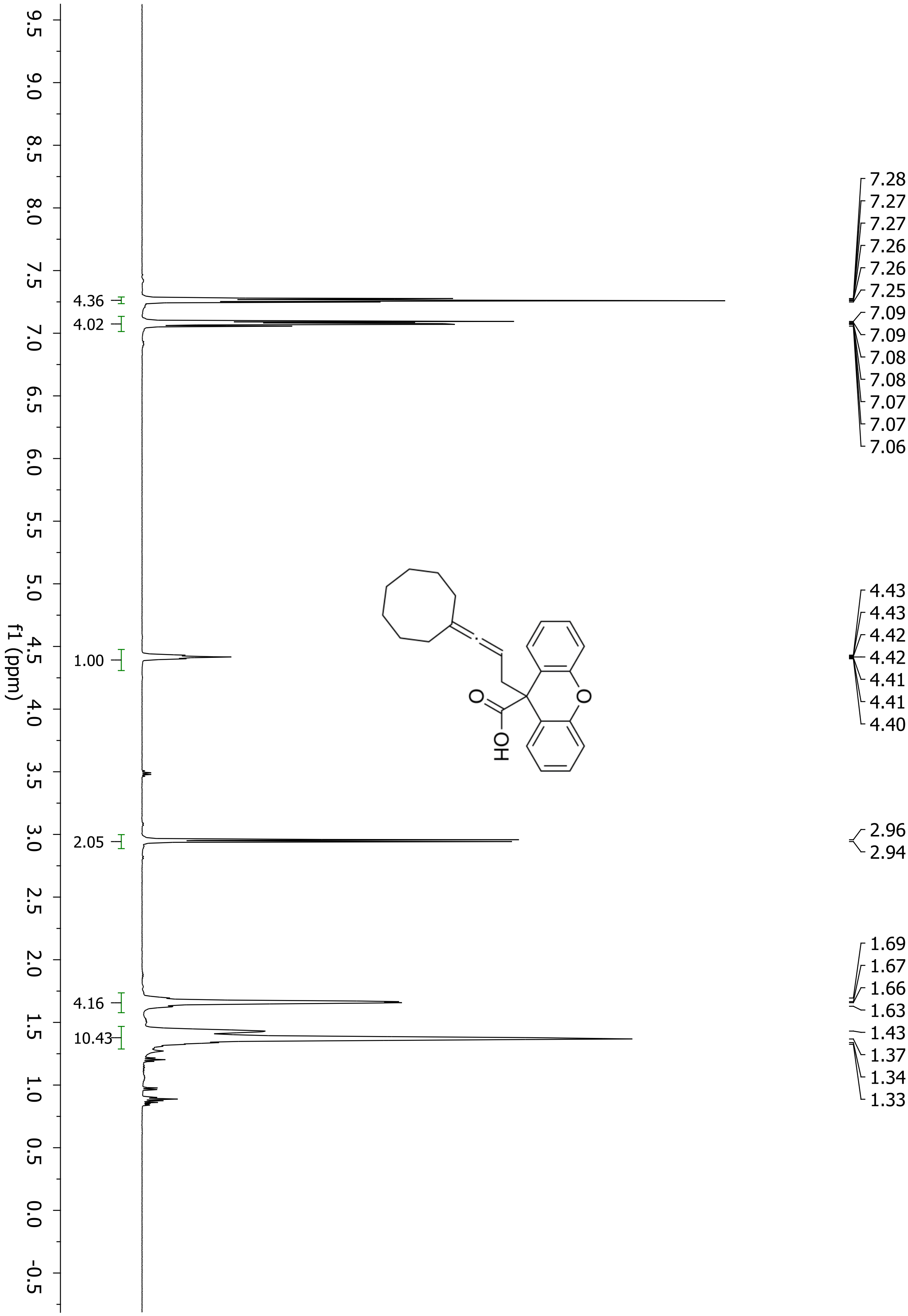
204.04
142.07
129.35
127.98
127.09
103.93
84.67
77.40
77.15
76.89
60.60
38.86
31.28
26.87
26.83
26.23
f1 (ppm)
O
OH


7.31
7.29
7.29
7.28
7.28
7.27
7.27
7.26
7.25
7.25
7.24
7.24
7.23
7.22
7.22
7.21
7.19
7.19
7.18
4.73
4.73
4.72
4.72
4.71
4.71
4.70
4.70
4.70
3.02
3.01
1.89
1.89
1.88
1.47
1.46
1.45
1.43
4.16
3.91
1.12
2.20
4.11
10.59
f1 (ppm)
Cl
Cl
O
OH

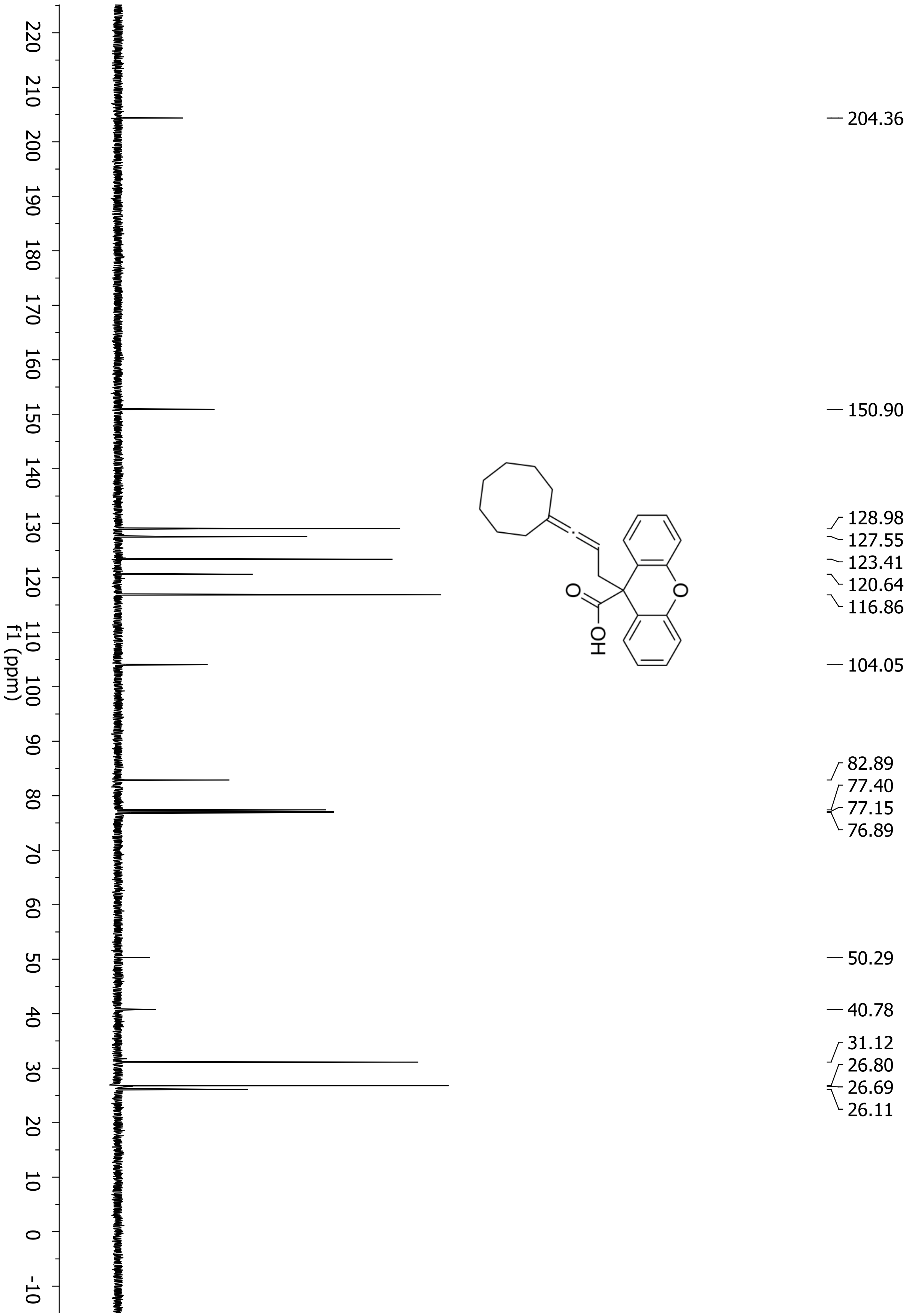

204.25
140.19
133.40
130.67
128.27
104.46
83.98
77.40
77.15
76.89
59.85
38.86
31.25
26.81
26.19
f1 (ppm)
Cl
Cl
O
OH


7.26
7.25
7.24
7.23
7.23
6.84
6.83
6.82
6.82
4.76
4.75
4.75
4.74
4.73
3.80
3.03
3.01
1.92
1.91
1.50
1.49
1.48
1.47
1.46
1.45
1.44
4.22
4.00
0.82
6.32
1.82
3.69
10.07
MeO
OMe
OH
O
f1 (ppm)

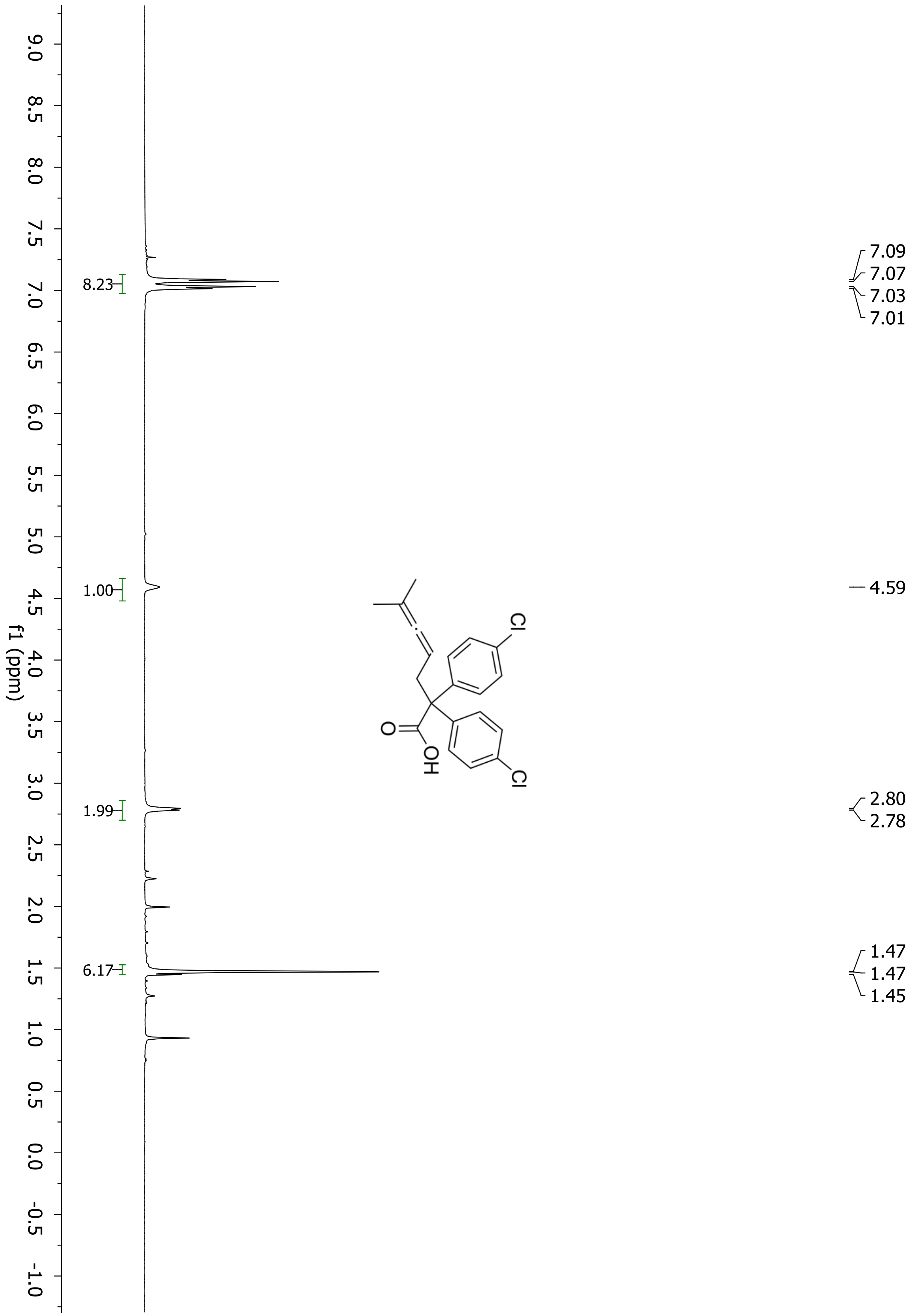

203.86
158.36
134.18
130.24
130.11
113.17
103.74
103.67
84.66
77.25
77.00
76.74
59.06
55.23
38.93
31.18
26.73
26.68
26.10
MeO
OMe
O
OH
f1 (ppm)



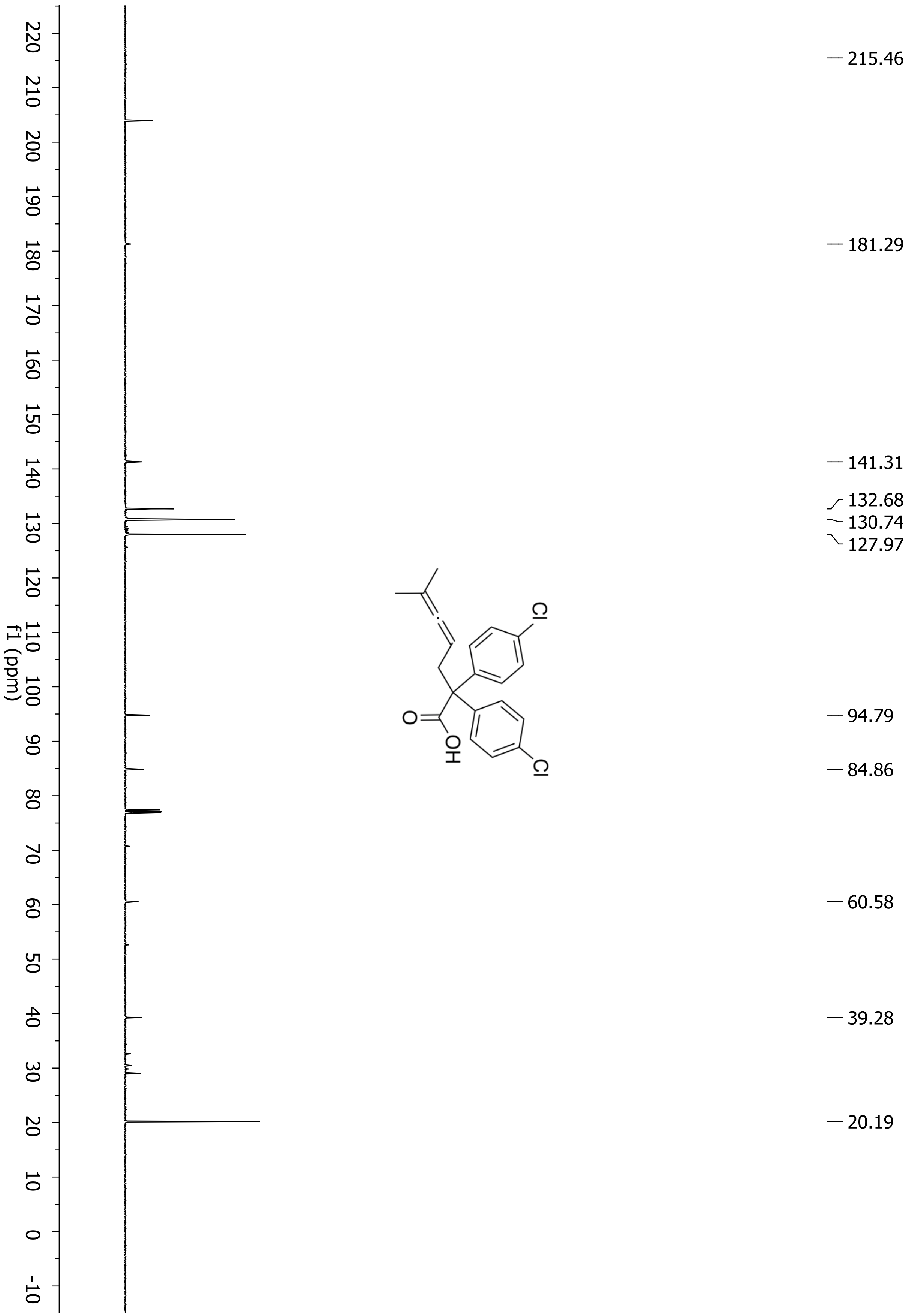
7.28
7.27
7.27
7.26
7.26
7.25
7.09
7.09
7.08
7.08
7.07
7.07
7.06
4.43
4.43
4.42
4.42
4.41
4.41
4.40
2.96
2.94
1.69
1.67
1.66
1.63
1.43
1.37
1.34
1.33
4.36
4.02
1.00
2.05
4.16
10.43
OH
O
O
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

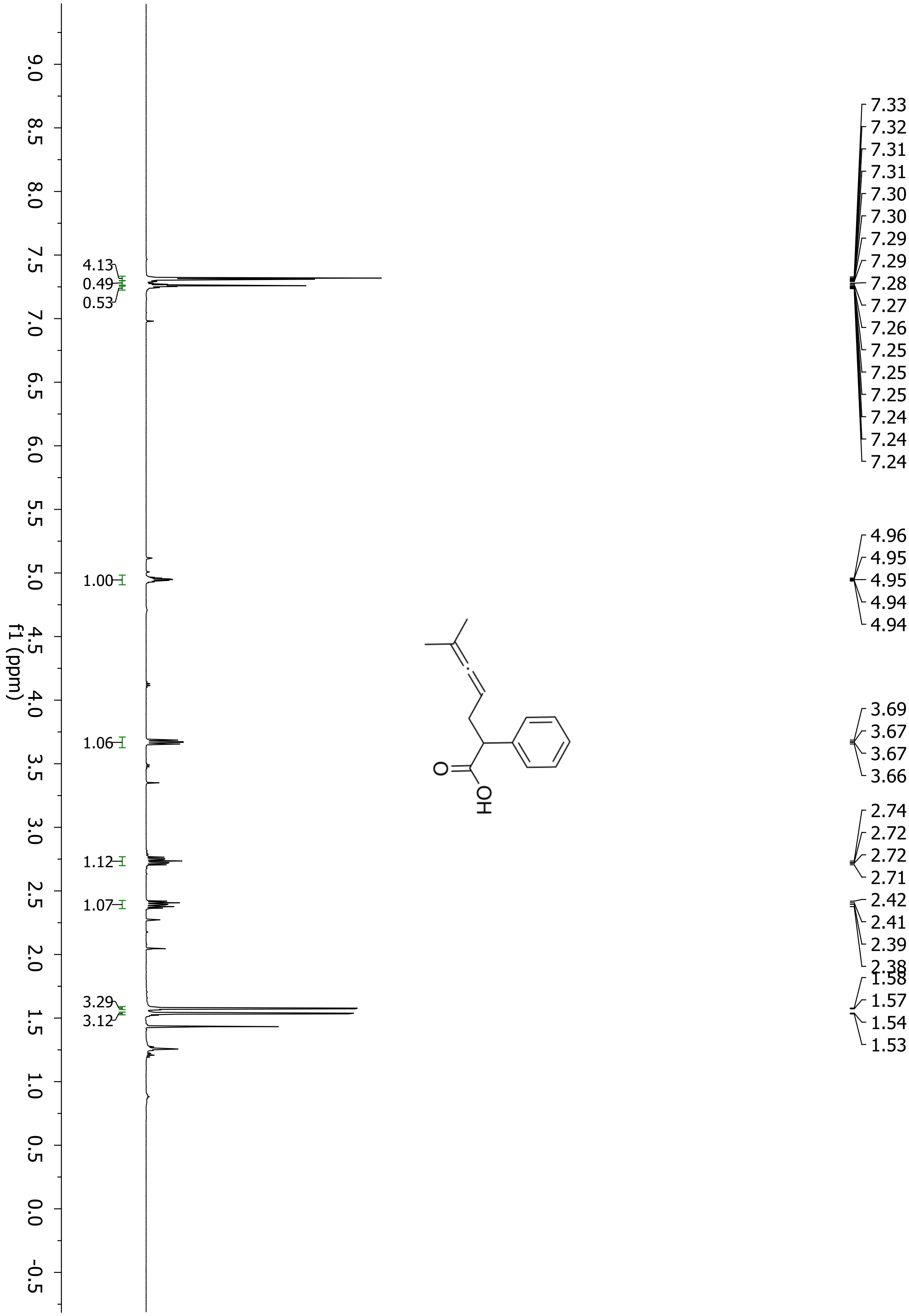


204.36
150.90
128.98
127.55
123.41
120.64
116.86
104.05
82.89
77.40
77.15
76.89
50.29
40.78
31.12
26.80
26.69
26.11
f1 (ppm)
O
OH
O

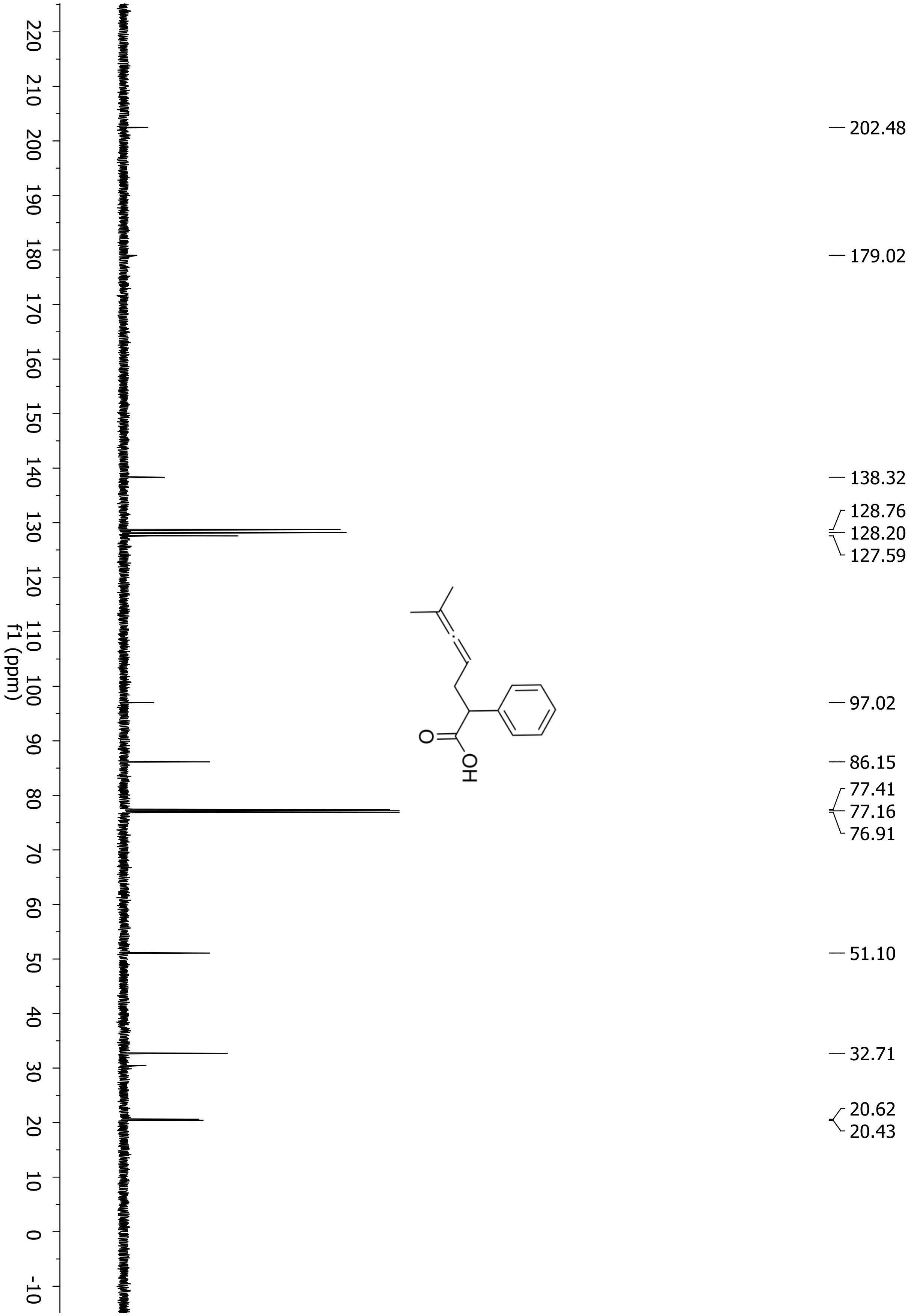


7.09
7.07
7.03
7.01
4.59
2.80
2.78
1.47
1.47
1.45
8.23
1.00
1.99
6.17
f1 (ppm)
Cl
Cl
OH
O

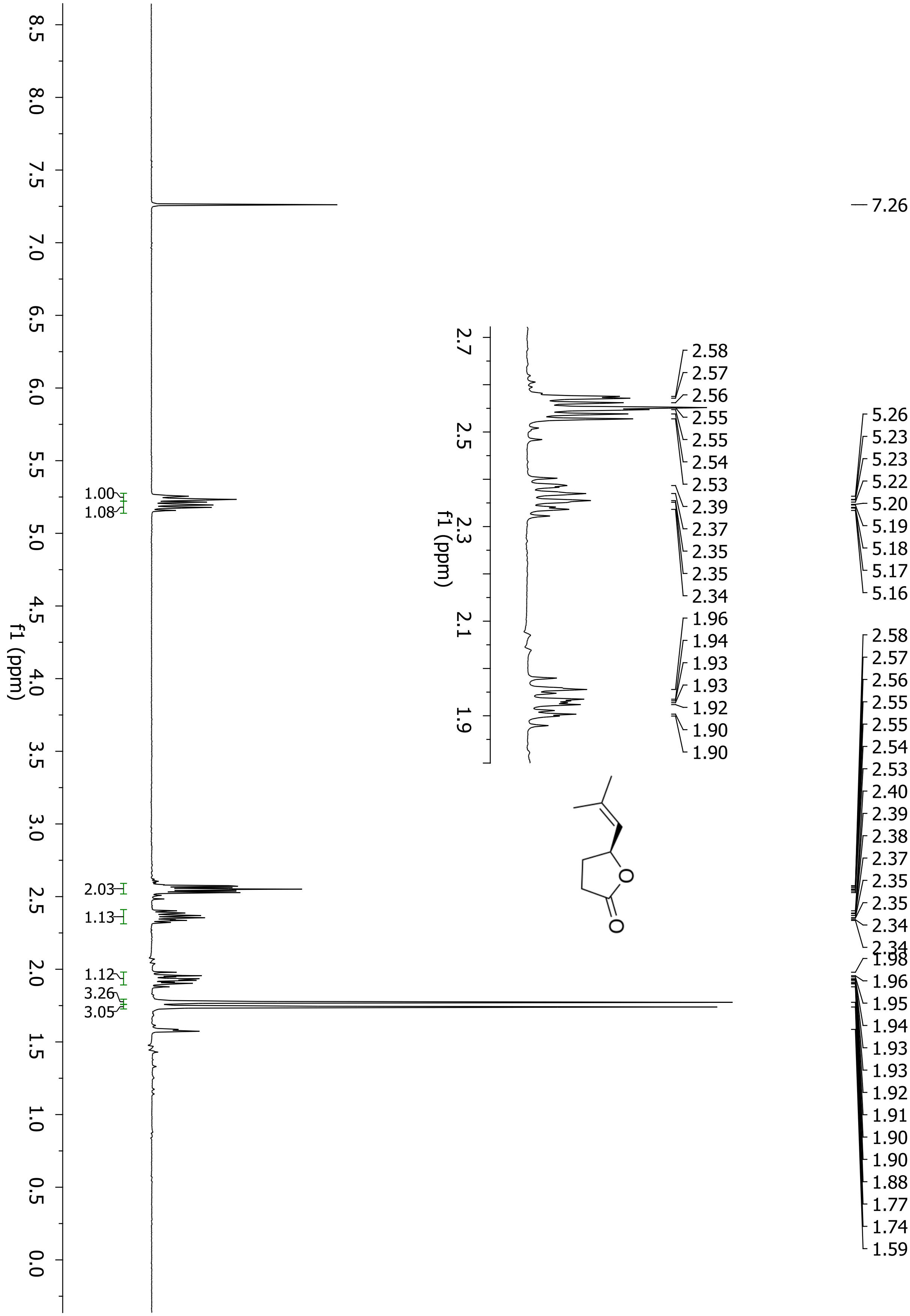

215.46
181.29
141.31
132.68
130.74
127.97
94.79
84.86
60.58
39.28
20.19
f1 (ppm)
Cl
Cl
O
OH

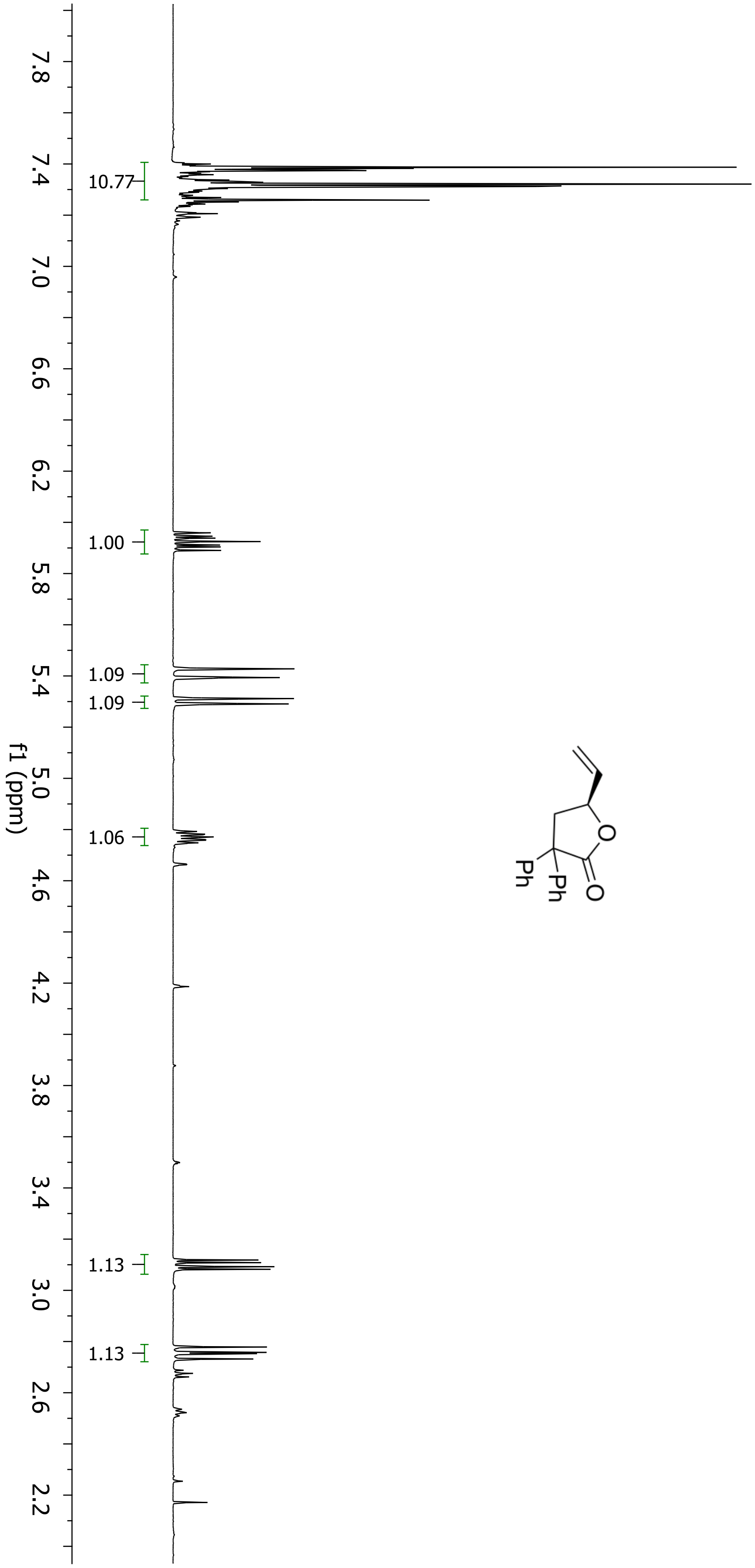


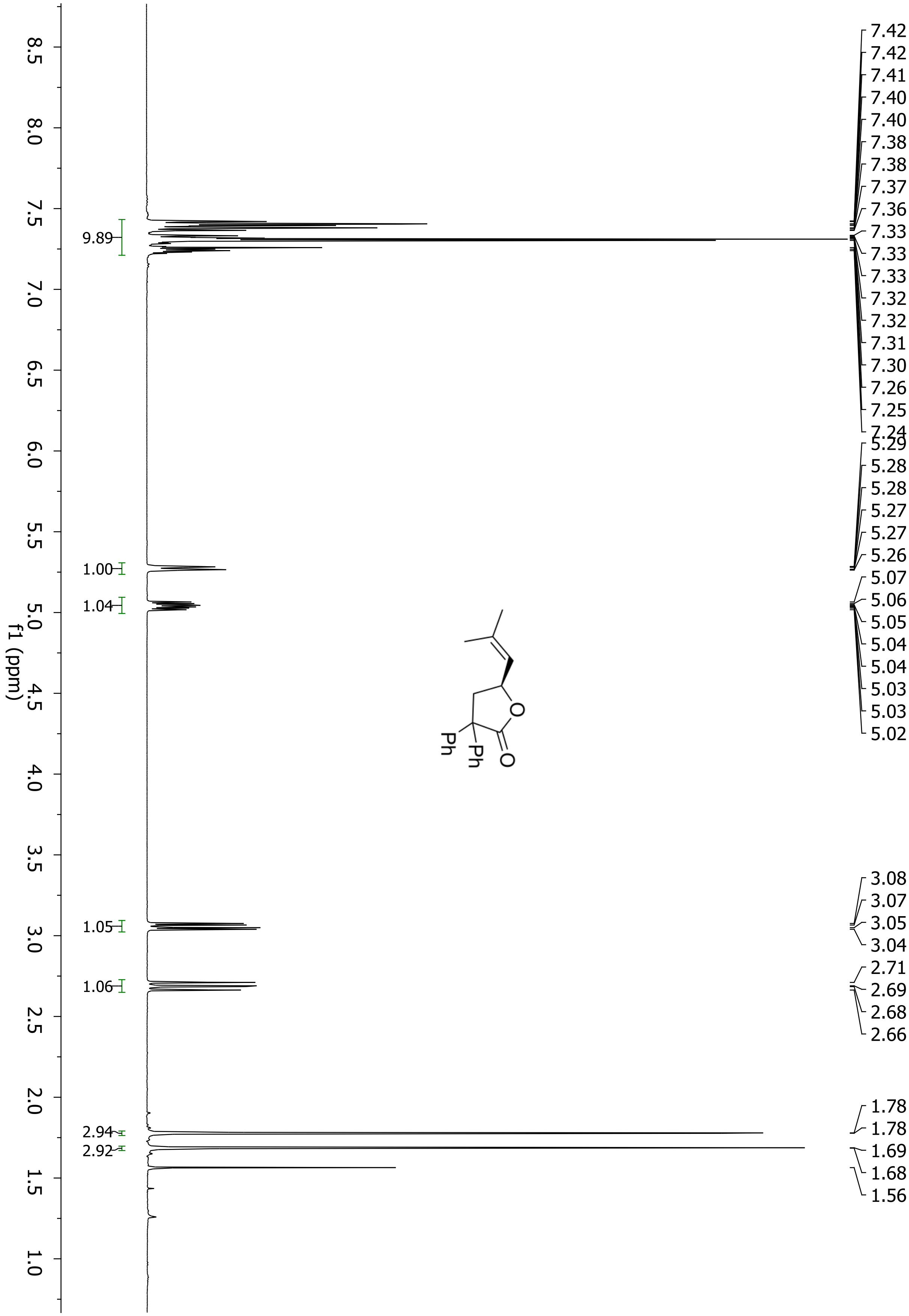
7.33
7.32
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.27
7.26
7.25
7.25
7.25
7.24
7.24
7.24
4.96
4.95
4.95
4.94
4.94
3.69
3.67
3.67
3.66
2.74
2.72
2.72
2.71
2.42
2.41
2.39
2.38
1.58
1.57
1.54
1.53
4.13
0.49
0.53
1.00
1.06
1.12
1.07
3.29
3.12
OH
O
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

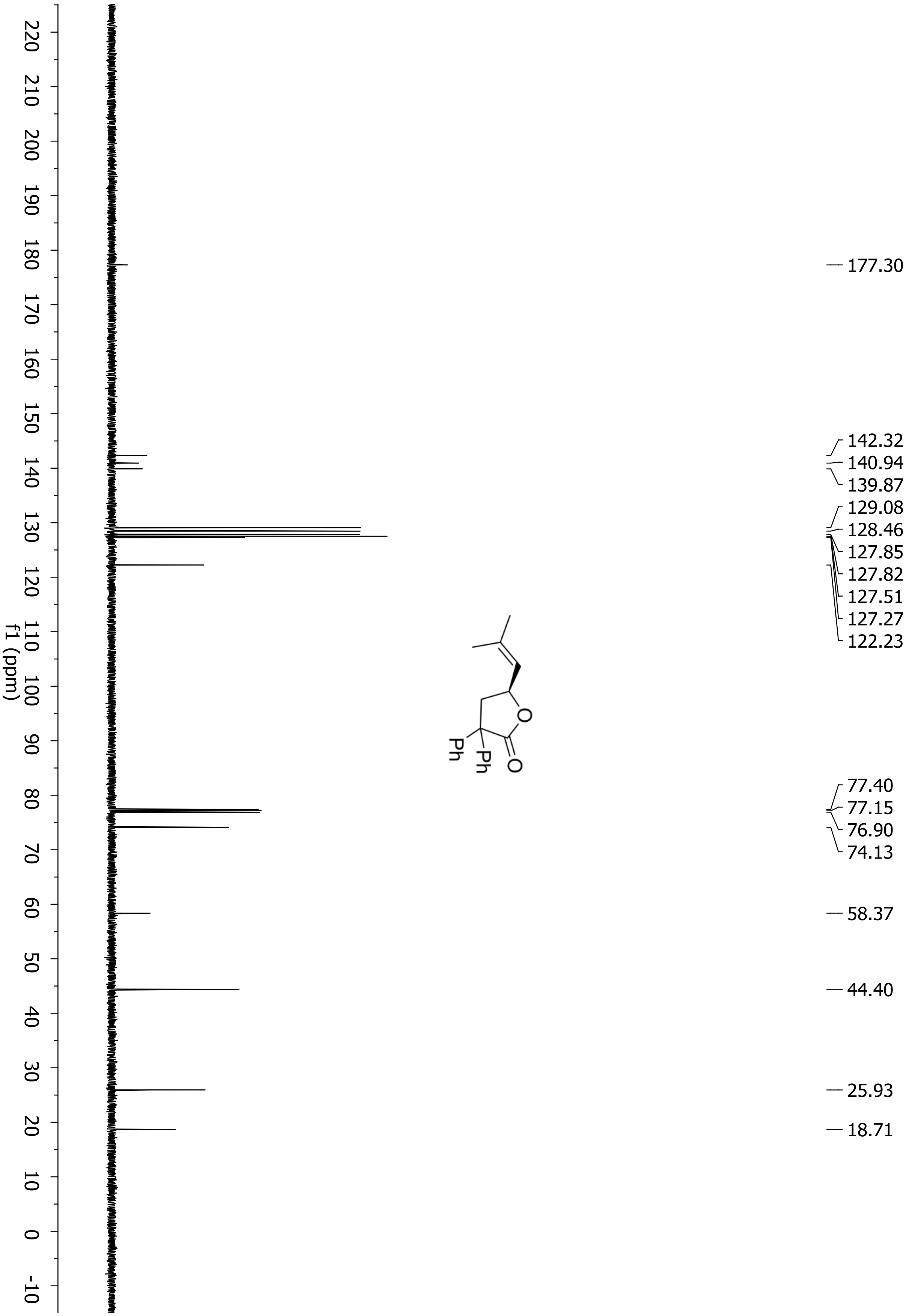


202.48
179.02
138.32
128.76
128.20
127.59
97.02
86.15
77.41
77.16
76.91
51.10
32.71
20.62
20.43
O
OH
f1 (ppm)

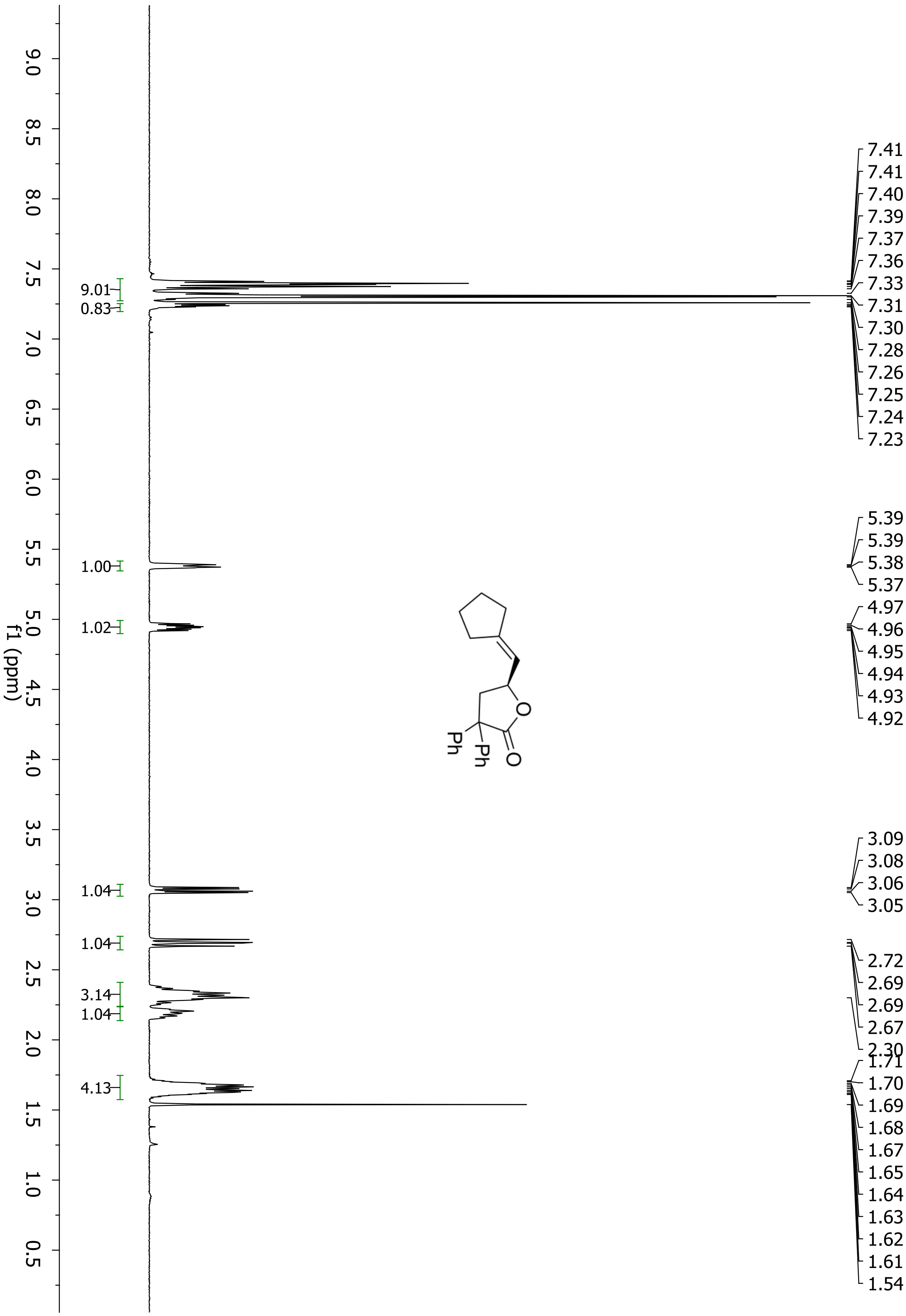

f1 (ppm)
7.26
5.26
5.23
5.23
5.22
5.20
5.19
5.18
5.17
5.16
2.58
2.57
2.56
2.55
2.55
2.54
2.53
2.40
2.39
2.38
2.37
2.35
2.35
2.34
2.34
1.98
1.96
1.95
1.94
1.93
1.93
1.92
1.91
1.90
1.90
1.88
1.77
1.74
1.59
1.00
1.08
2.03
1.13
1.12
3.26
3.05
O
O


7.8
7.4
7.0
6.6
6.2
5.8
5.4
5.0
4.6
4.2
3.8
3.4
3.0
2.6
2.2
f1 (ppm)
10.77
1.00
1.09
1.09
1.06
1.13
1.13
O
O
Ph
Ph

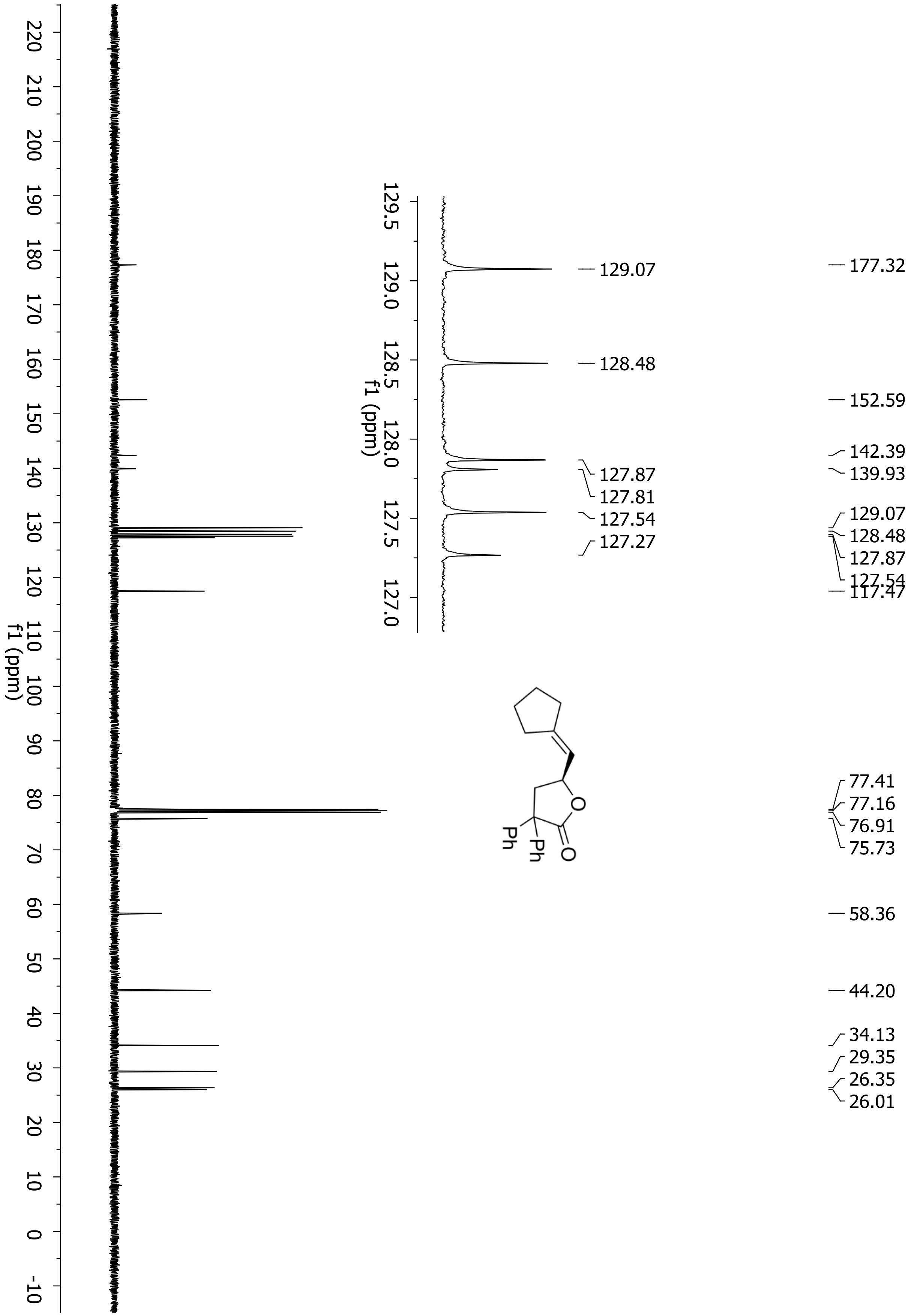

7.42
7.42
7.41
7.40
7.40
7.38
7.38
7.37
7.36
7.33
7.33
7.33
7.32
7.32
7.31
7.30
7.26
7.25
7.24
5.29
5.28
5.28
5.27
5.27
5.26
5.07
5.06
5.05
5.04
5.04
5.03
5.03
5.02
3.08
3.07
3.05
3.04
2.71
2.69
2.68
2.66
1.78
1.78
1.69
1.68
1.56
9.89
1.00
1.04
1.05
1.06
2.94
2.92
Ph
Ph
O
O
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

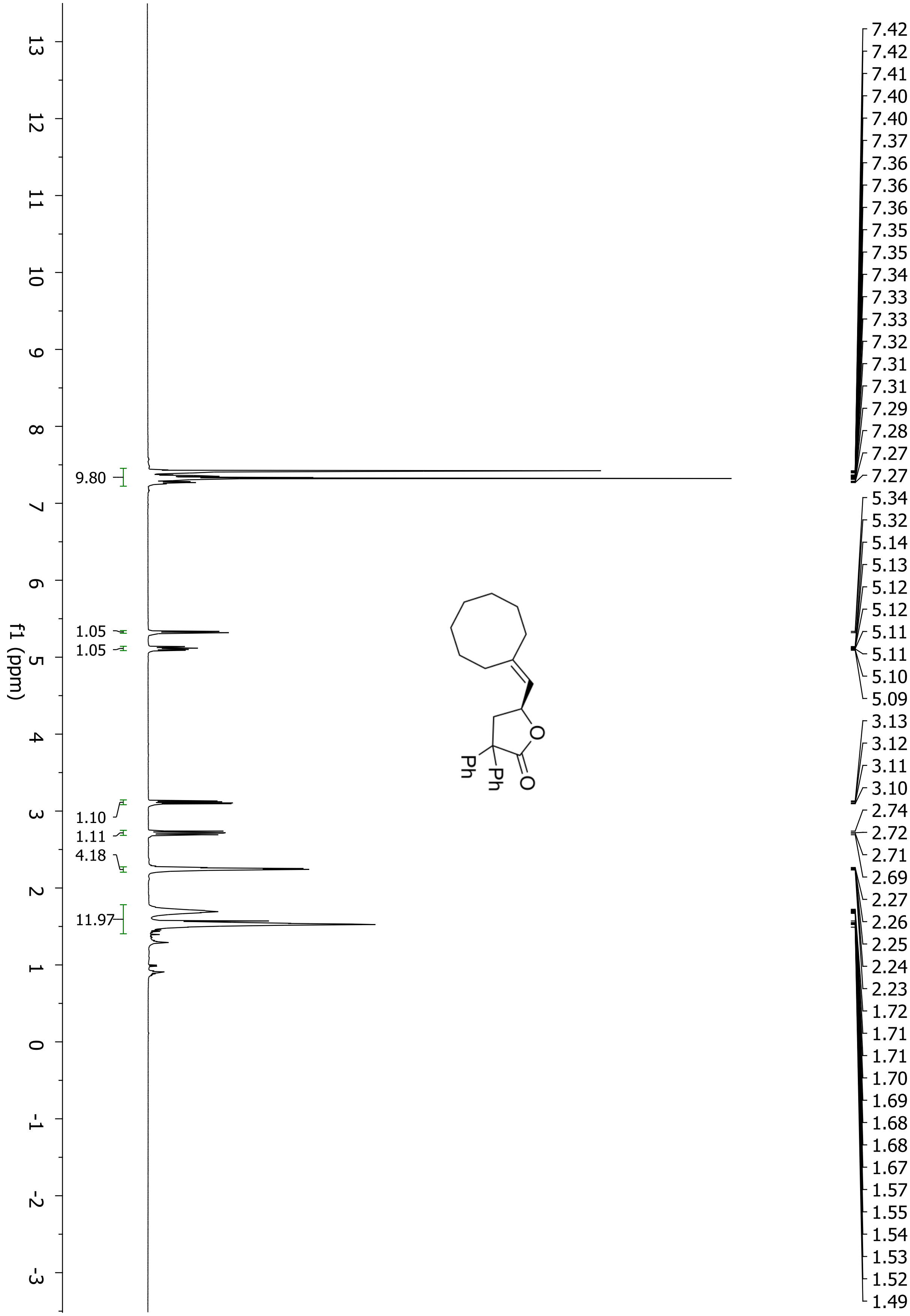


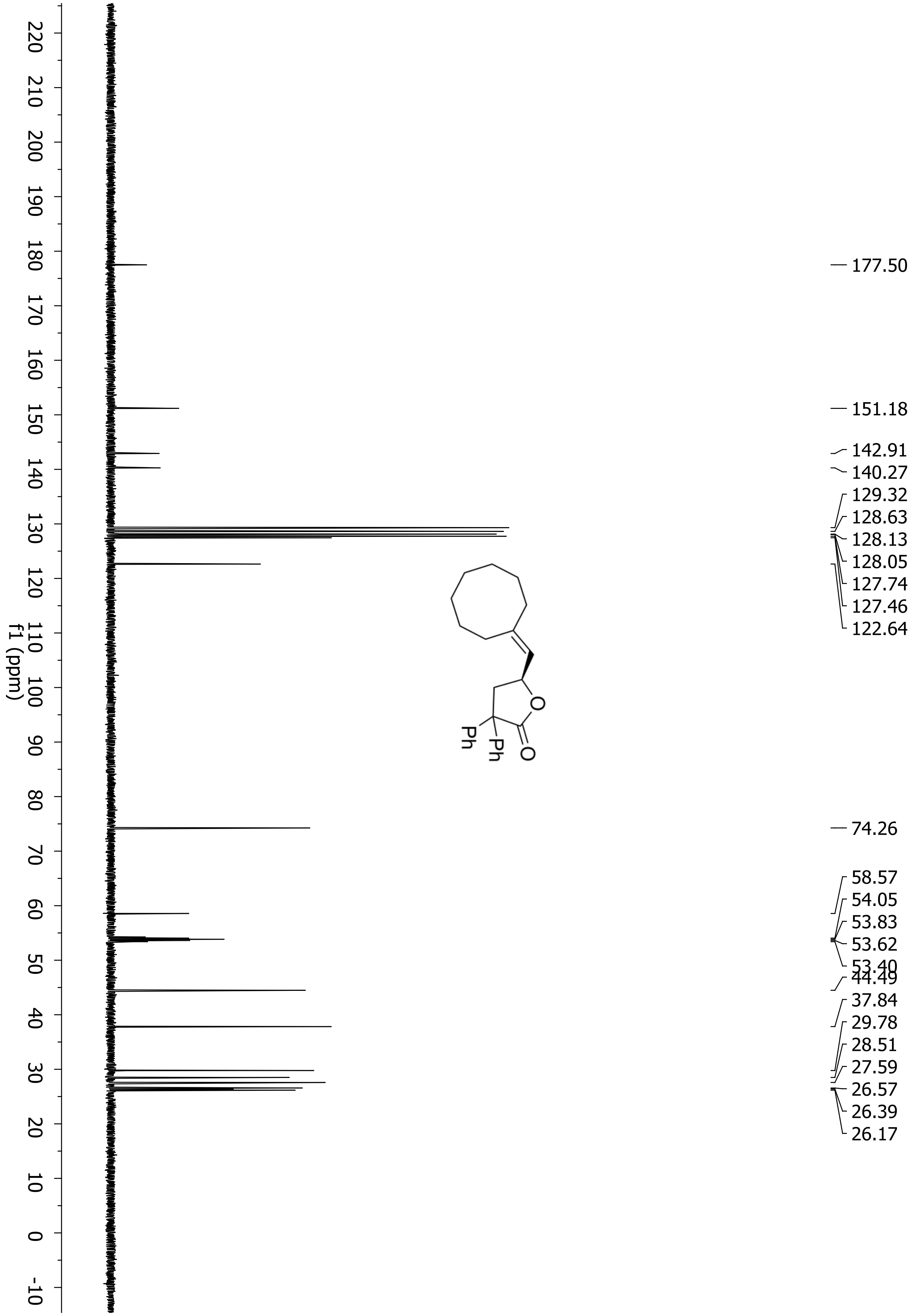
177.30
142.32
140.94
139.87
129.08
128.46
127.85
127.82
127.51
127.27
122.23
77.40
77.15
76.90
74.13
58.37
44.40
25.93
18.71
f1 (ppm)
O
O
Ph
Ph

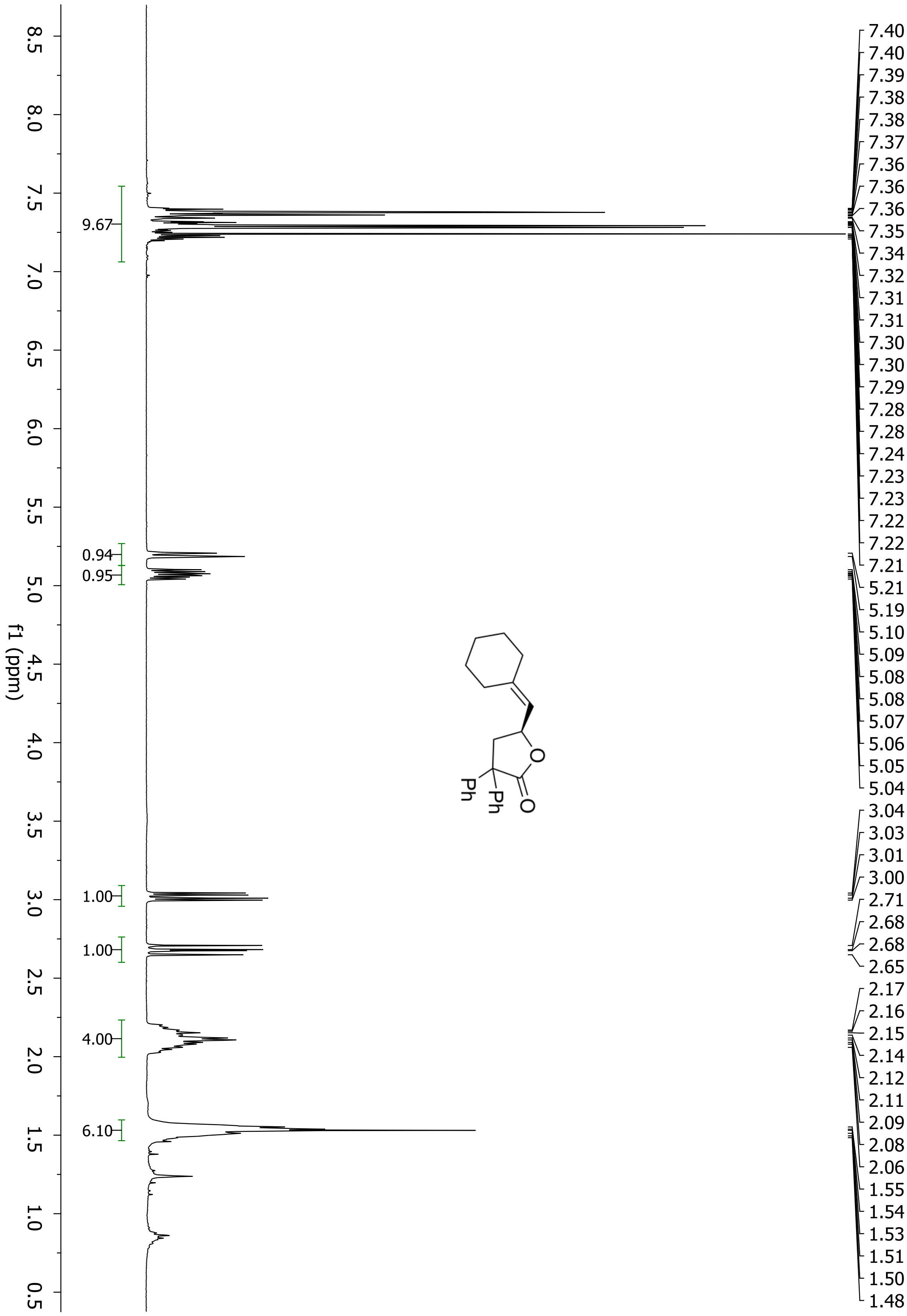


7.41
7.41
7.40
7.39
7.37
7.36
7.33
7.31
7.30
7.28
7.26
7.25
7.24
7.23
5.39
5.39
5.38
5.37
4.97
4.96
4.95
4.94
4.93
4.92
3.09
3.08
3.06
3.05
2.72
2.69
2.69
2.67
2.30
1.71
1.70
1.69
1.68
1.67
1.65
1.64
1.63
1.62
1.61
1.54
9.01
0.83
1.00
1.02
1.04
1.04
3.14
1.04
4.13
O
O
Ph
Ph
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

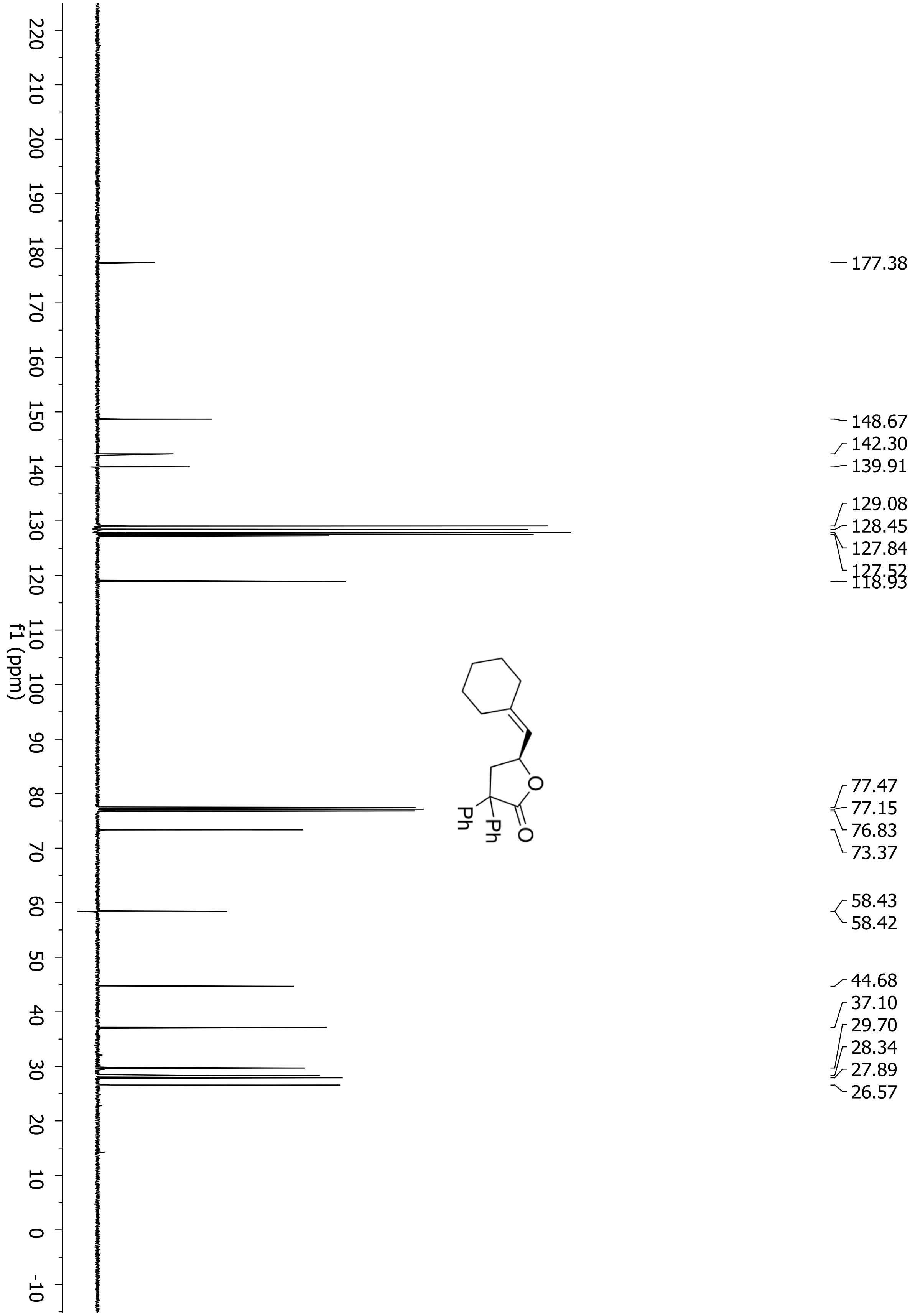

177.32
152.59
142.39
139.93
129.07
128.48
127.87
127.54
117.47
77.41
77.16
76.91
75.73
58.36
44.20
34.13
29.35
26.35
26.01
129.07
128.48
127.87
127.81
127.54
127.27
f1 (ppm)
f1 (ppm)
Ph
Ph
O
O

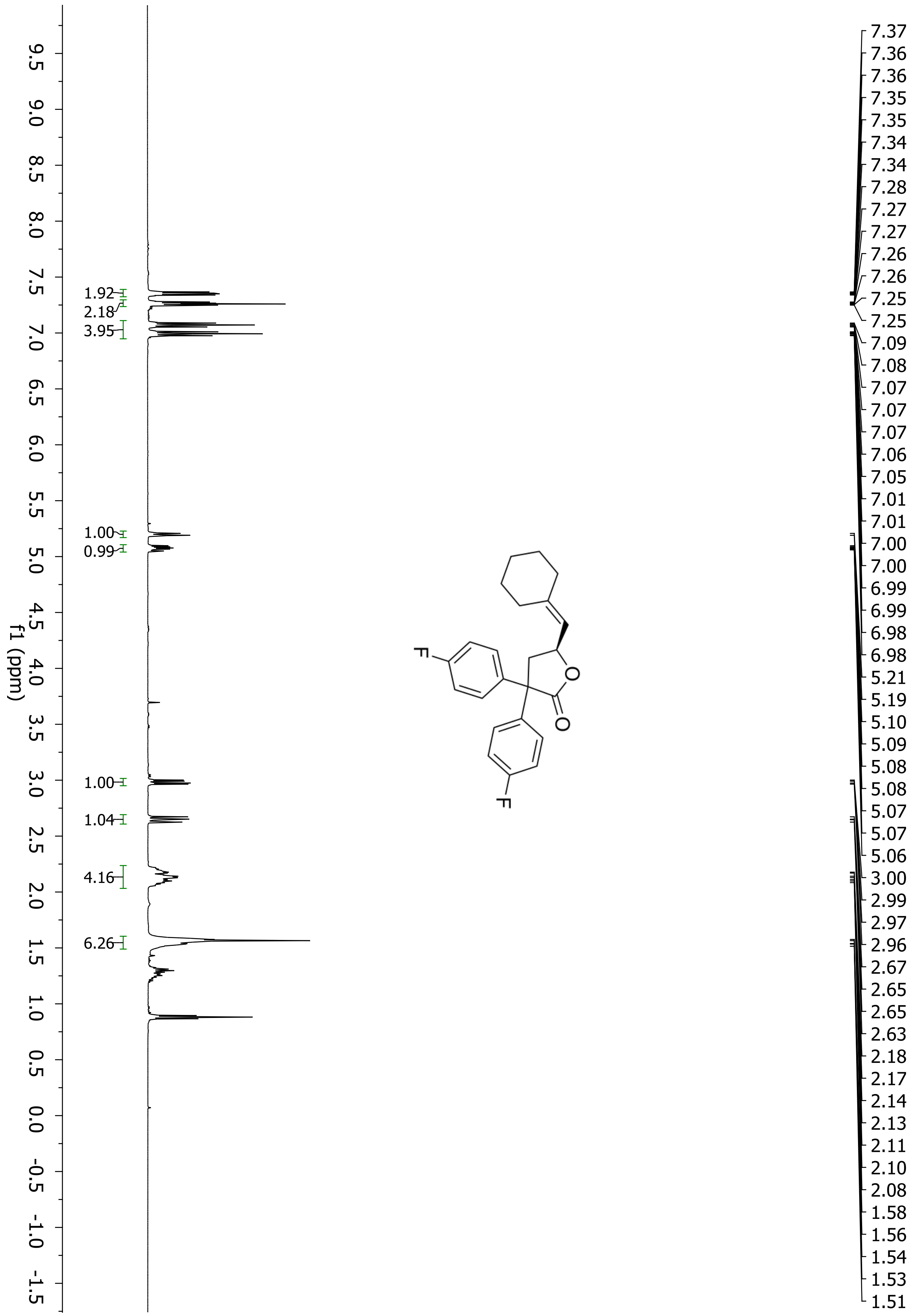

7.42
7.42
7.41
7.40
7.40
7.37
7.36
7.36
7.36
7.35
7.35
7.34
7.33
7.33
7.32
7.31
7.31
7.29
7.28
7.27
7.27
5.34
5.32
5.14
5.13
5.12
5.12
5.11
5.11
5.10
5.09
3.13
3.12
3.11
3.10
2.74
2.72
2.71
2.69
2.27
2.26
2.25
2.24
2.23
1.72
1.71
1.71
1.70
1.69
1.68
1.68
1.67
1.57
1.55
1.54
1.53
1.52
1.49
9.80
1.05
1.05
1.10
1.11
4.18
11.97
f1 (ppm)
O
O
Ph
Ph

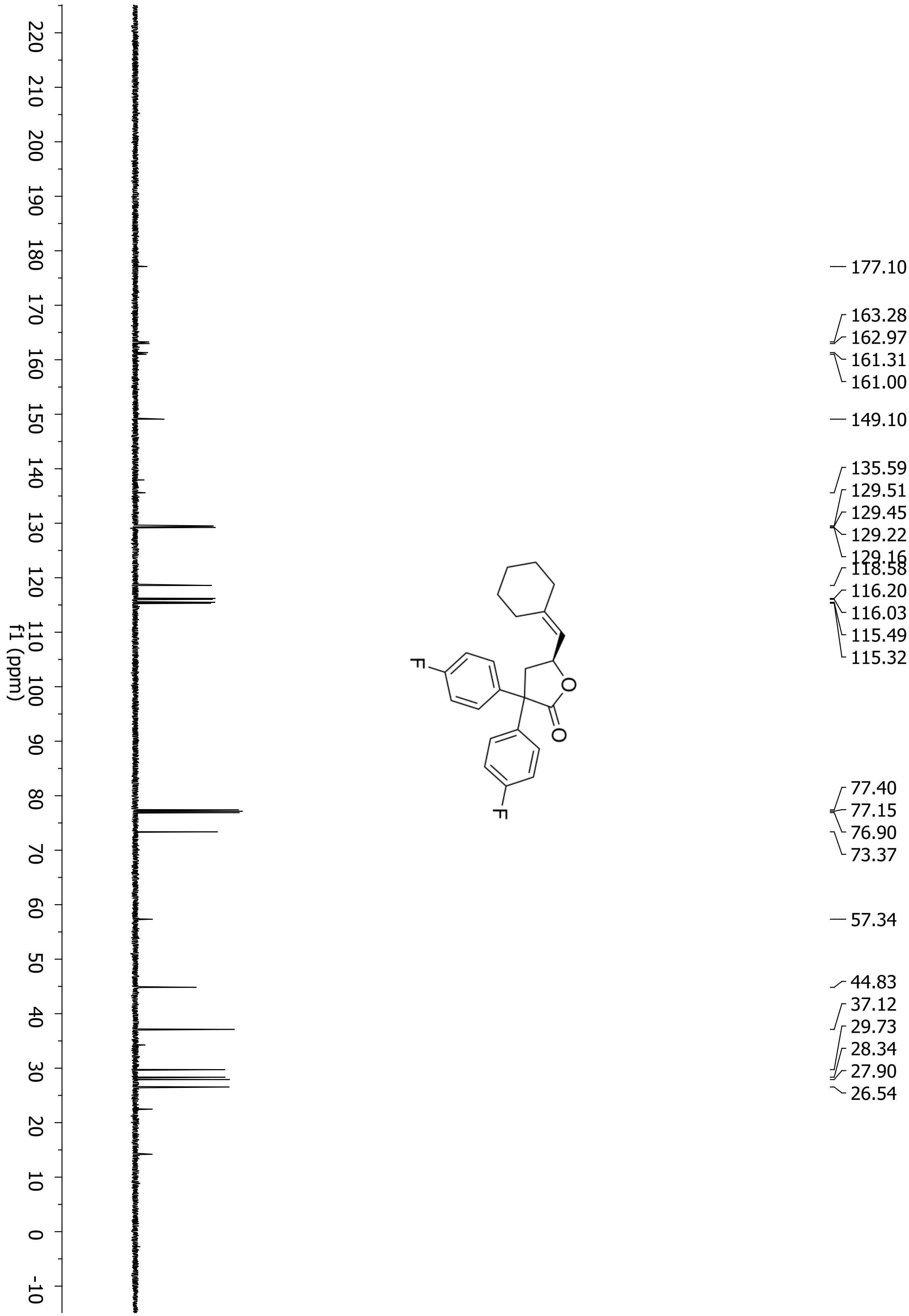

177.50
151.18
142.91
140.27
129.32
128.63
128.13
128.05
127.74
127.46
122.64
74.26
58.57
54.05
53.83
53.62
53.40
44.49
37.84
29.78
28.51
27.59
26.57
26.39
26.17
f1 (ppm)
Ph
Ph
O
O

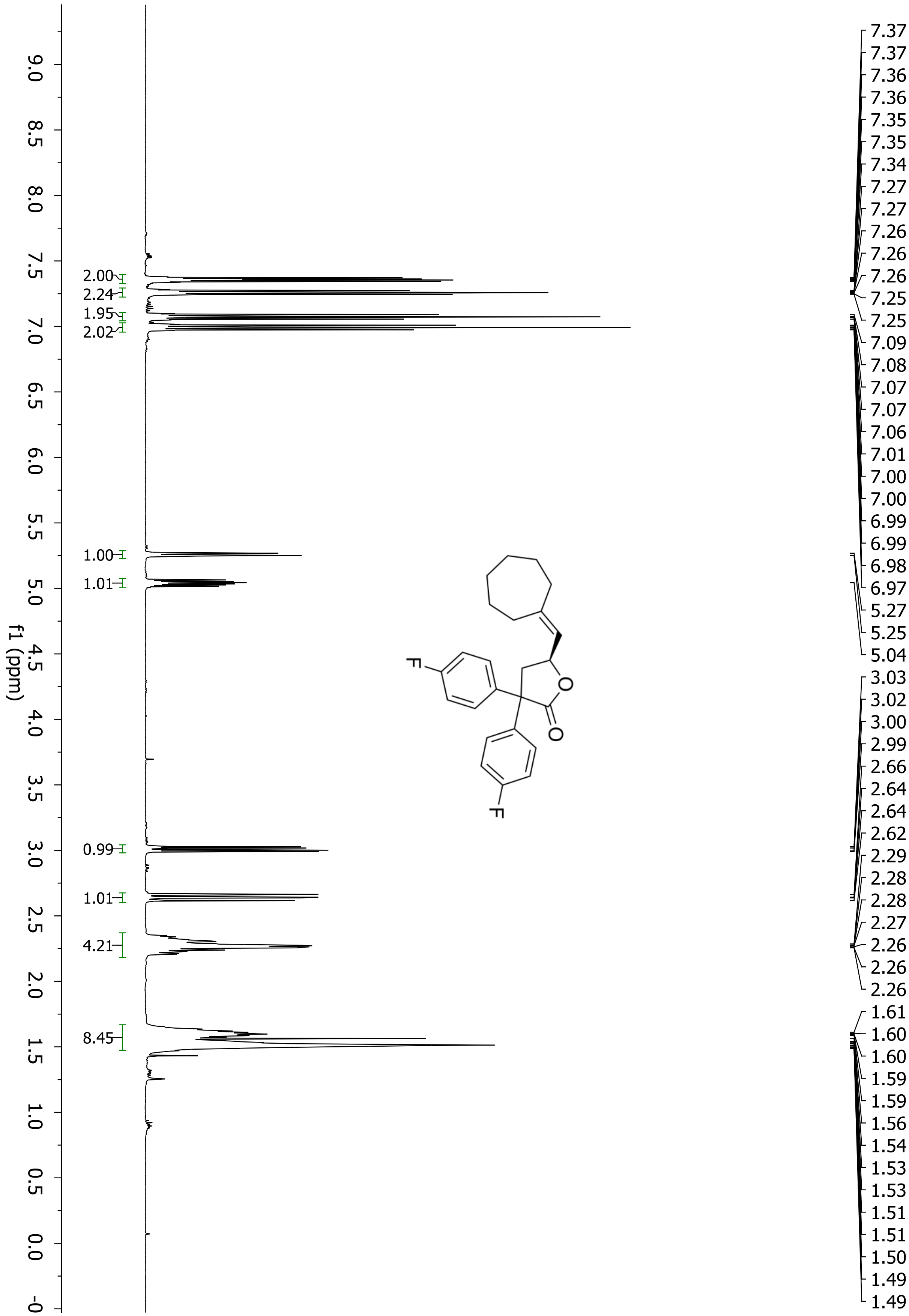


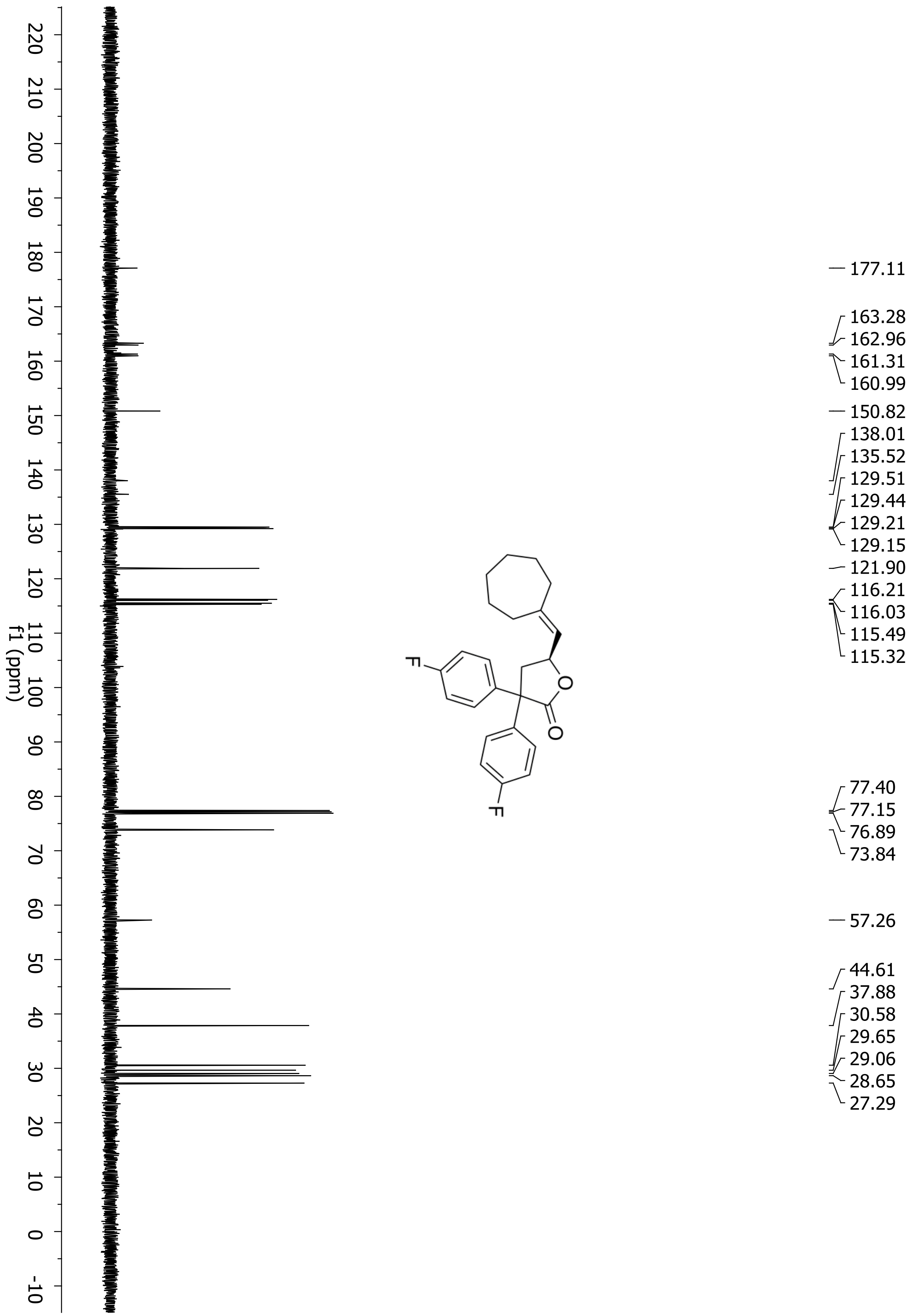
7.40
7.40
7.39
7.38
7.38
7.37
7.36
7.36
7.36
7.35
7.34
7.32
7.31
7.31
7.30
7.30
7.29
7.28
7.28
7.24
7.23
7.23
7.23
7.22
7.22
7.21
5.21
5.19
5.10
5.09
5.08
5.08
5.08
5.07
5.06
5.05
5.04
3.04
3.03
3.01
3.00
2.71
2.68
2.68
2.65
2.17
2.16
2.15
2.14
2.12
2.11
2.09
2.08
2.06
1.55
1.54
1.53
1.51
1.50
1.48
9.67
0.94
0.95
1.00
1.00
4.00
6.10
f1 (ppm)
Ph
Ph
O
O

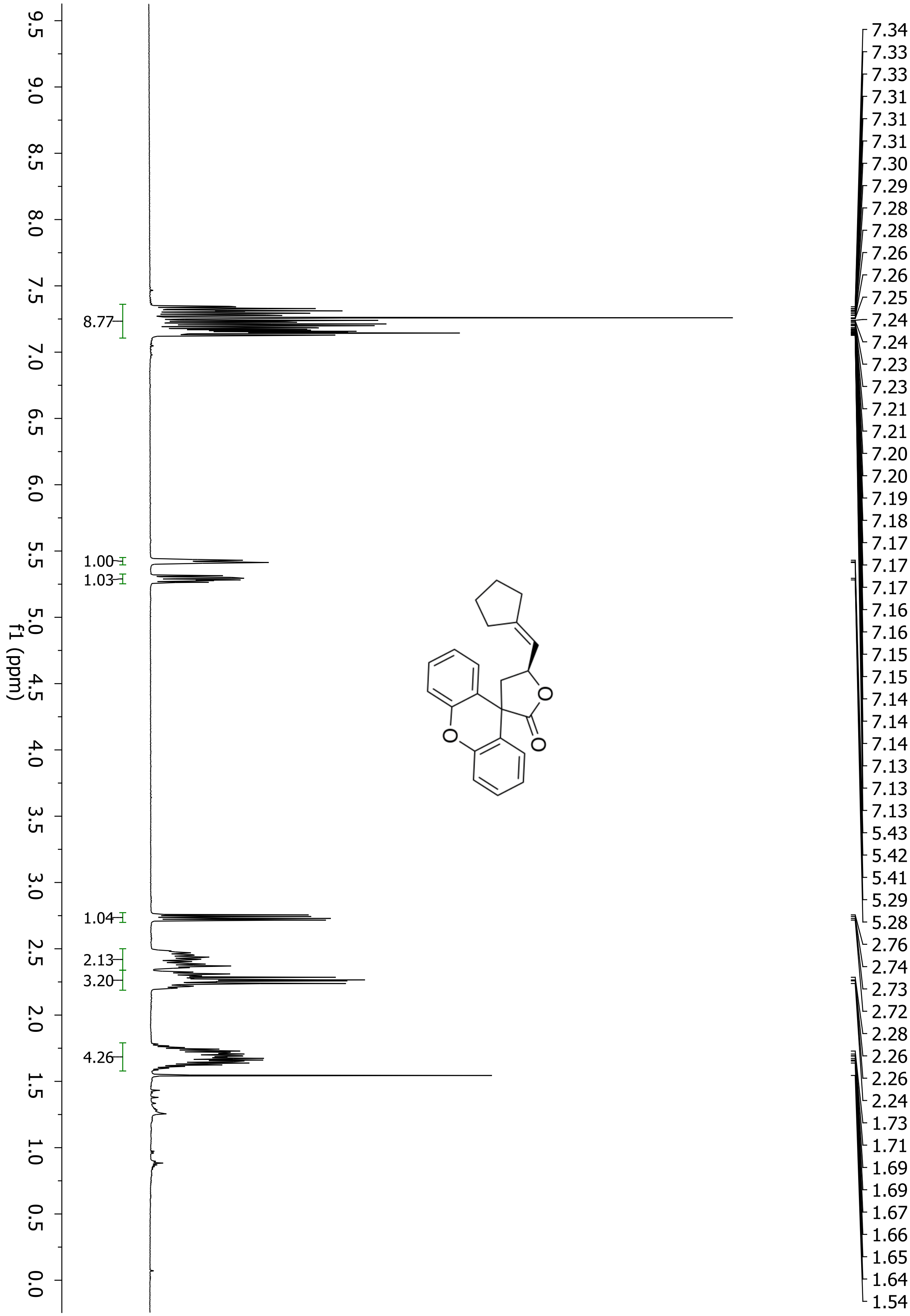

177.38
148.67
142.30
139.91
129.08
128.45
127.84
127.52
118.93
77.47
77.15
76.83
73.37
58.43
58.42
44.68
37.10
29.70
28.34
27.89
26.57
f1 (ppm)
Ph
Ph
O
O

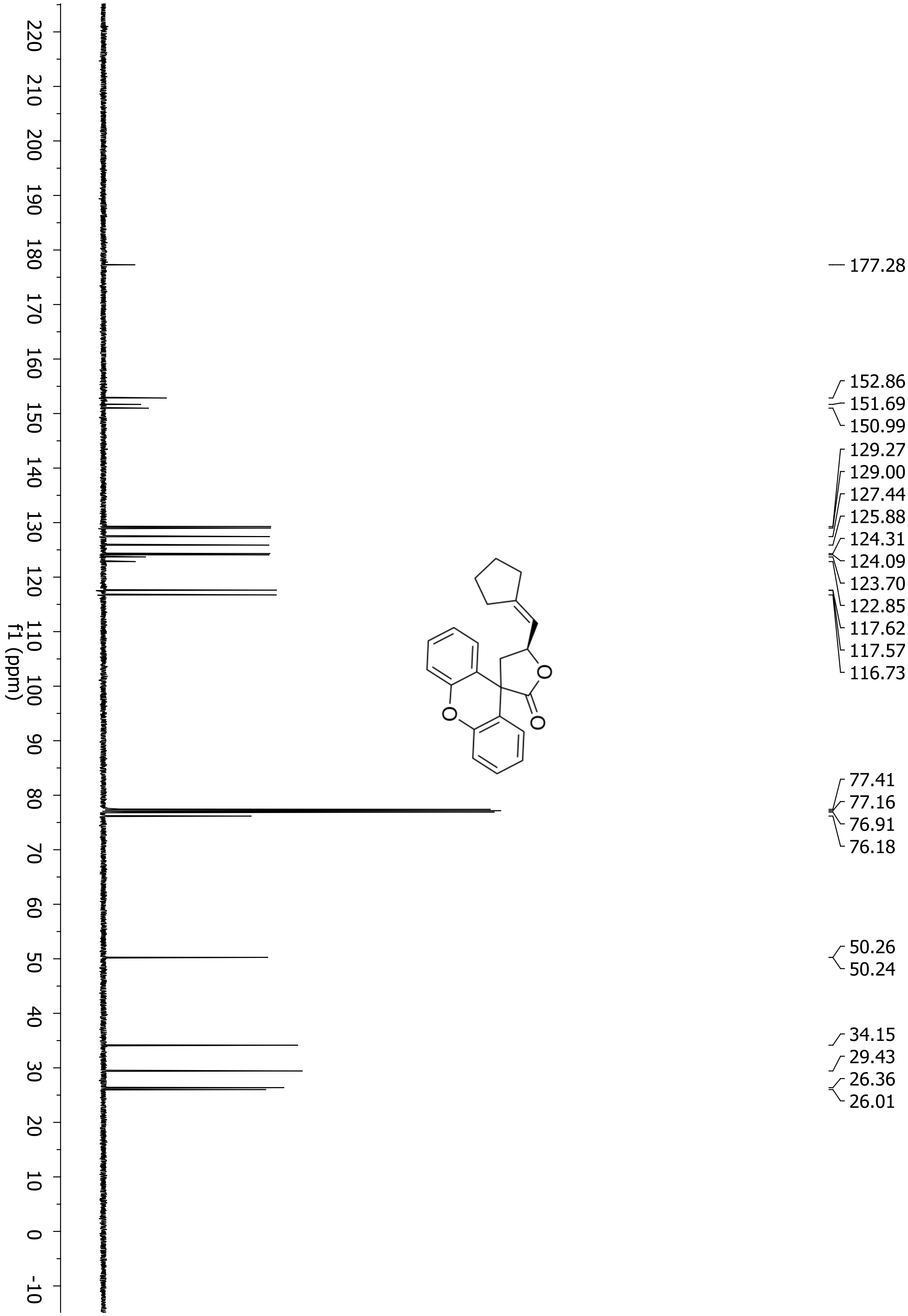

7.37
7.36
7.36
7.35
7.35
7.34
7.34
7.28
7.27
7.27
7.26
7.26
7.25
7.25
7.09
7.08
7.07
7.07
7.07
7.06
7.05
7.01
7.01
7.00
7.00
6.99
6.99
6.98
6.98
5.21
5.19
5.10
5.09
5.08
5.08
5.07
5.07
5.06
3.00
2.99
2.97
2.96
2.67
2.65
2.65
2.63
2.18
2.17
2.14
2.13
2.11
2.10
2.08
1.58
1.56
1.54
1.53
1.51
1.92
2.18
3.95
1.00
0.99
1.00
1.04
4.16
6.26
f1 (ppm)
F
F
O
O

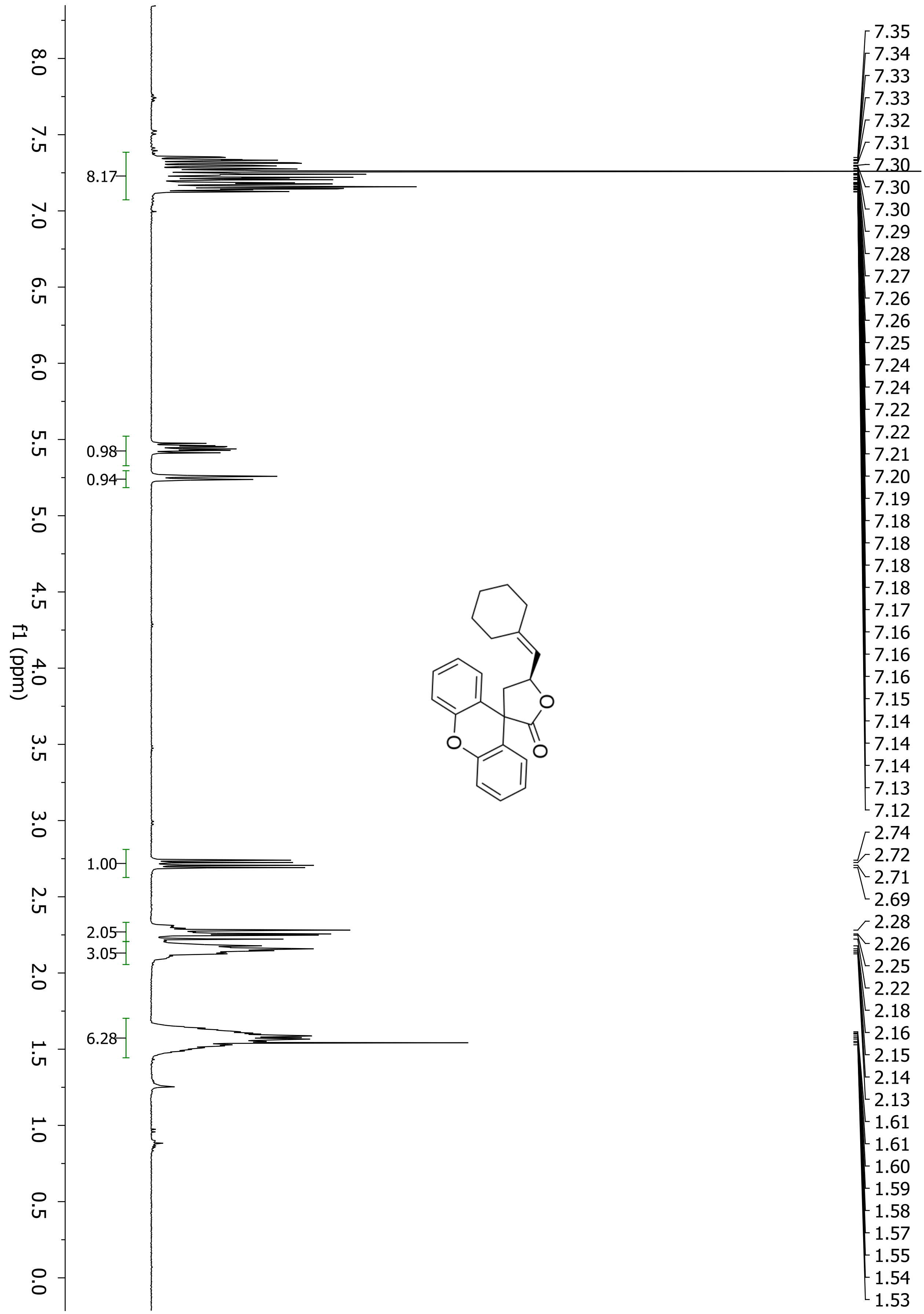

177.10
163.28
162.97
161.31
161.00
149.10
135.59
129.51
129.45
129.22
129.16
118.58
116.20
116.03
115.49
115.32
77.40
77.15
76.90
73.37
57.34
44.83
37.12
29.73
28.34
27.90
26.54
f1 (ppm)


7.37
7.37
7.36
7.36
7.35
7.35
7.34
7.27
7.27
7.26
7.26
7.26
7.25
7.25
7.09
7.08
7.07
7.07
7.06
7.01
7.00
7.00
6.99
6.99
6.98
6.97
5.27
5.25
5.04
3.03
3.02
3.00
2.99
2.66
2.64
2.64
2.62
2.29
2.28
2.28
2.27
2.26
2.26
2.26
1.61
1.60
1.60
1.59
1.59
1.56
1.54
1.53
1.53
1.51
1.51
1.50
1.49
1.49
2.00
2.24
1.95
2.02
1.00
1.01
0.99
1.01
4.21
8.45
f1 (ppm)
O
O
F
F

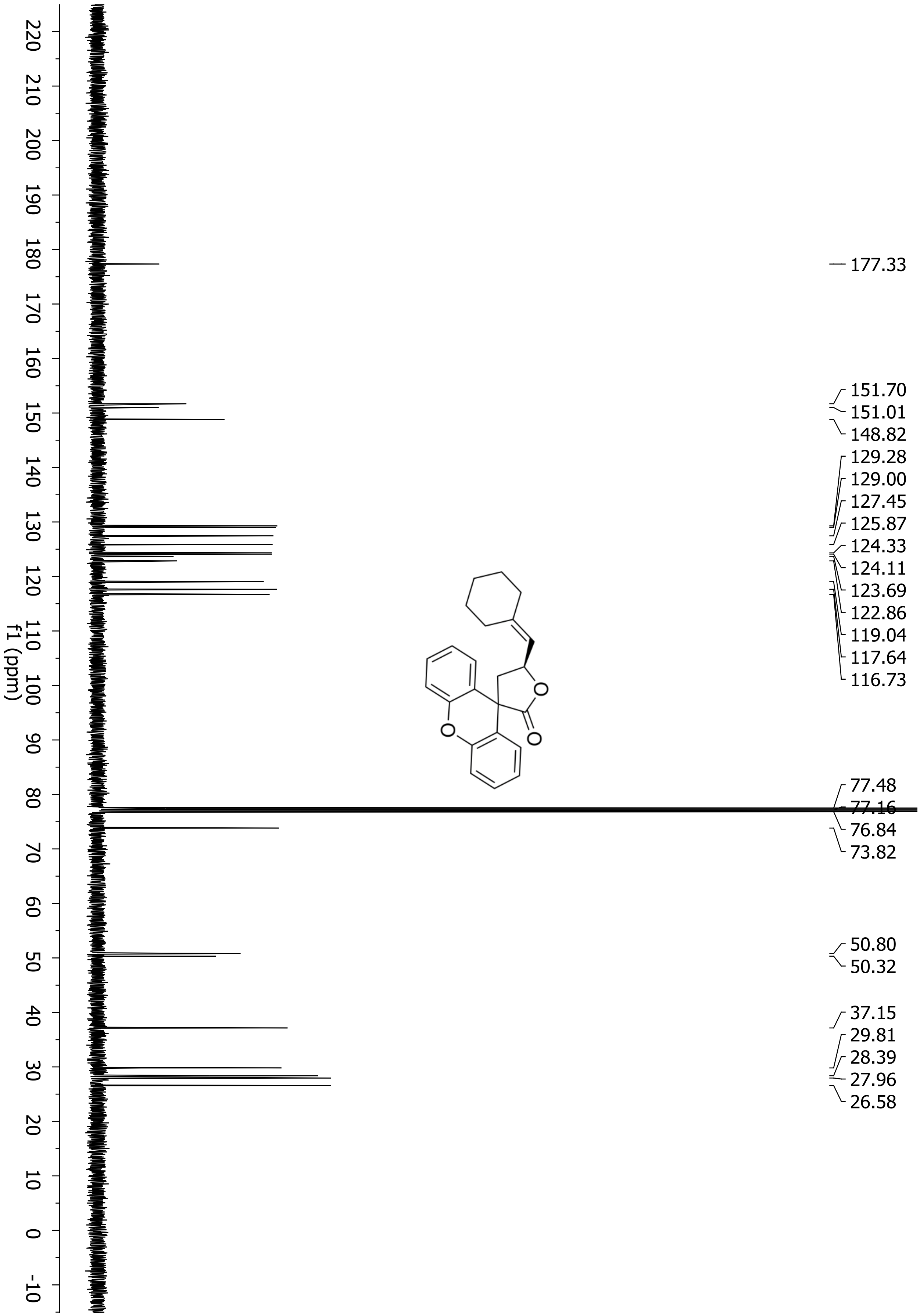

177.11
163.28
162.96
161.31
160.99
150.82
138.01
135.52
129.51
129.44
129.21
129.15
121.90
116.21
116.03
115.49
115.32
77.40
77.15
76.89
73.84
57.26
44.61
37.88
30.58
29.65
29.06
28.65
27.29
F
O
O
F
f1 (ppm)

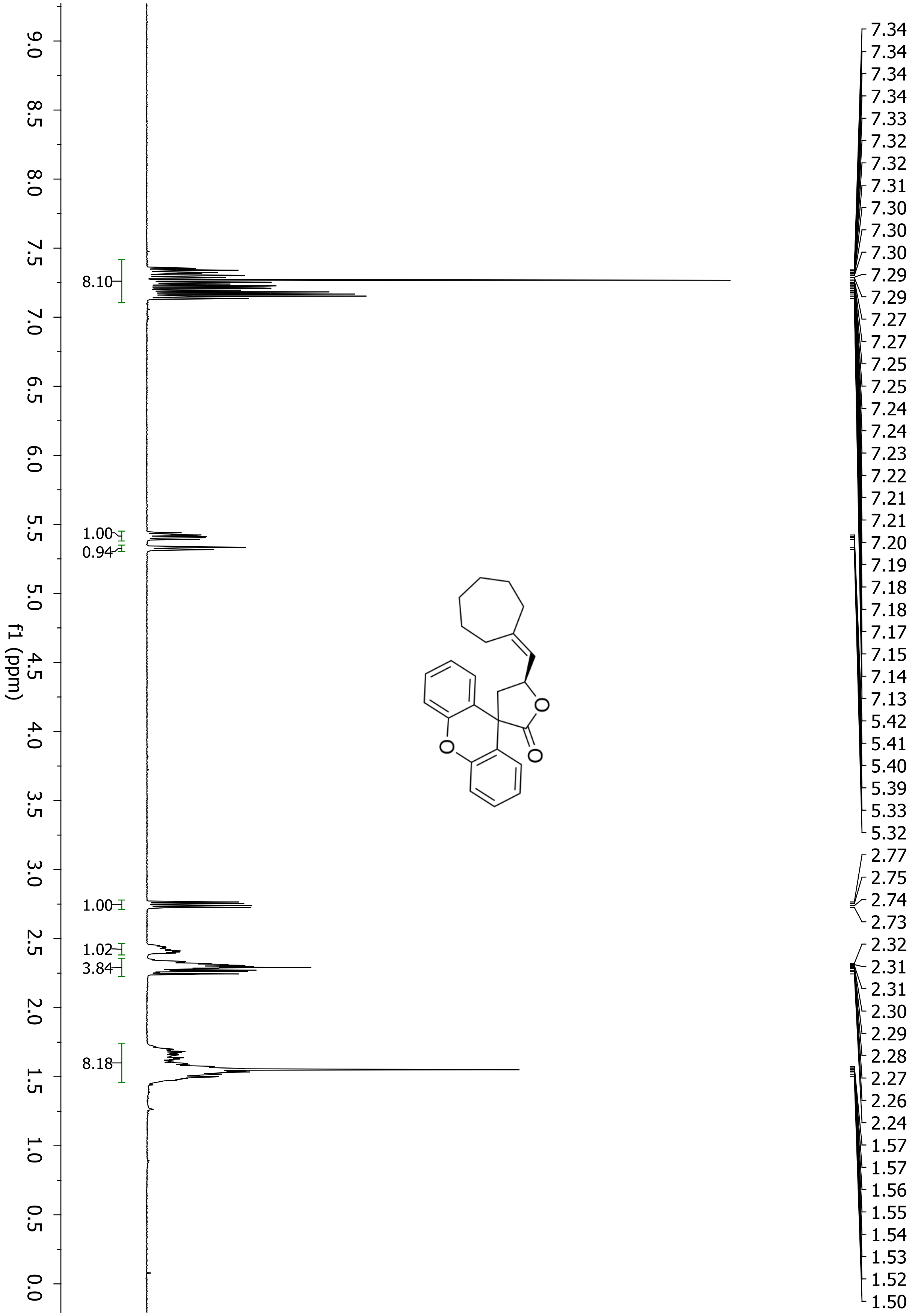

7.34
7.33
7.33
7.31
7.31
7.31
7.30
7.29
7.28
7.28
7.26
7.26
7.25
7.24
7.24
7.23
7.23
7.21
7.21
7.20
7.20
7.19
7.18
7.17
7.17
7.17
7.16
7.16
7.15
7.15
7.14
7.14
7.14
7.13
7.13
7.13
5.43
5.42
5.41
5.29
5.28
2.76
2.74
2.73
2.72
2.28
2.26
2.26
2.24
1.73
1.71
1.69
1.69
1.67
1.66
1.65
1.64
1.54
8.77
1.00
1.03
1.04
2.13
3.20
4.26
f1 (ppm)


177.28
152.86
151.69
150.99
129.27
129.00
127.44
125.88
124.31
124.09
123.70
122.85
117.62
117.57
116.73
77.41
77.16
76.91
76.18
50.26
50.24
34.15
29.43
26.36
26.01
f1 (ppm)

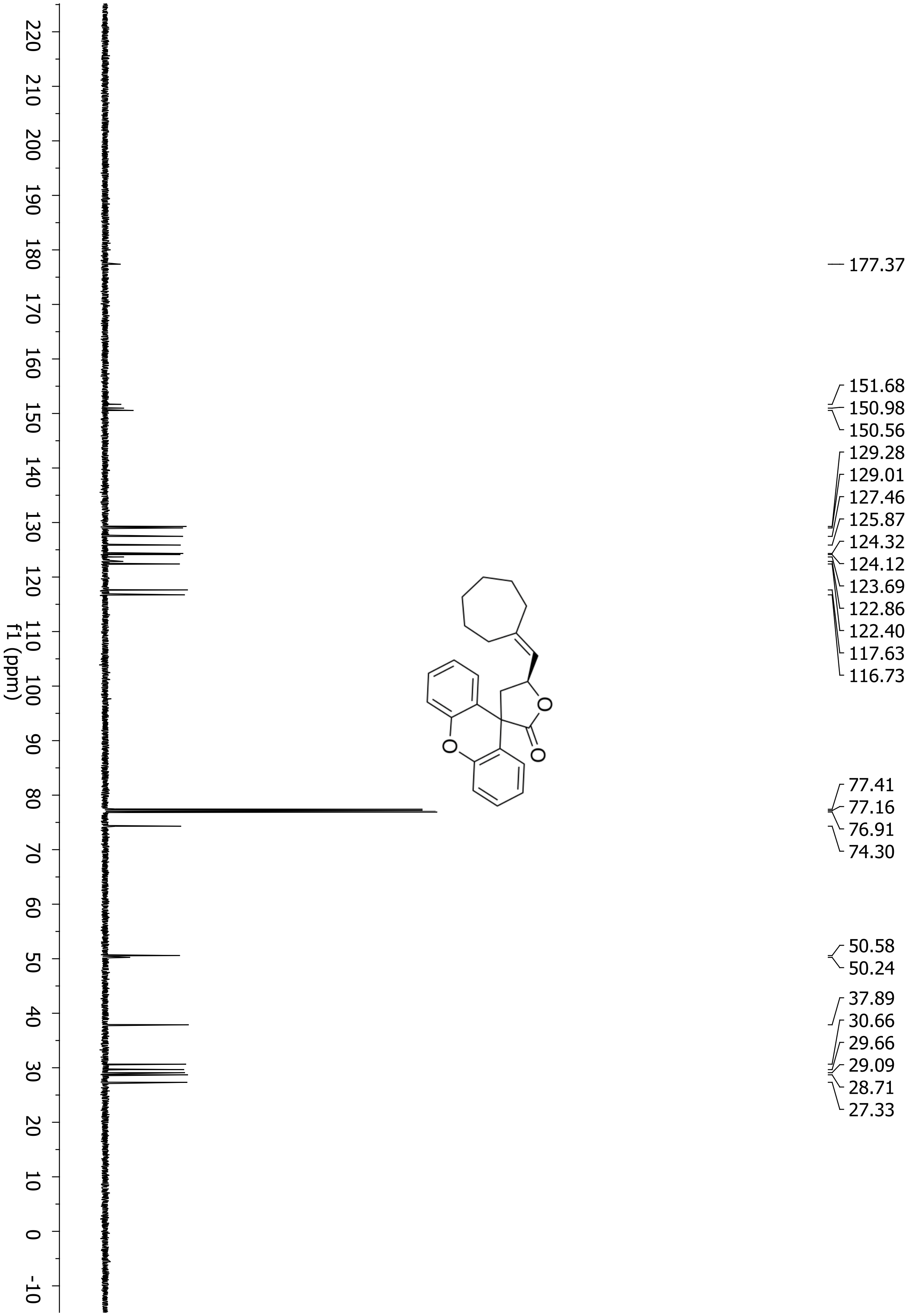


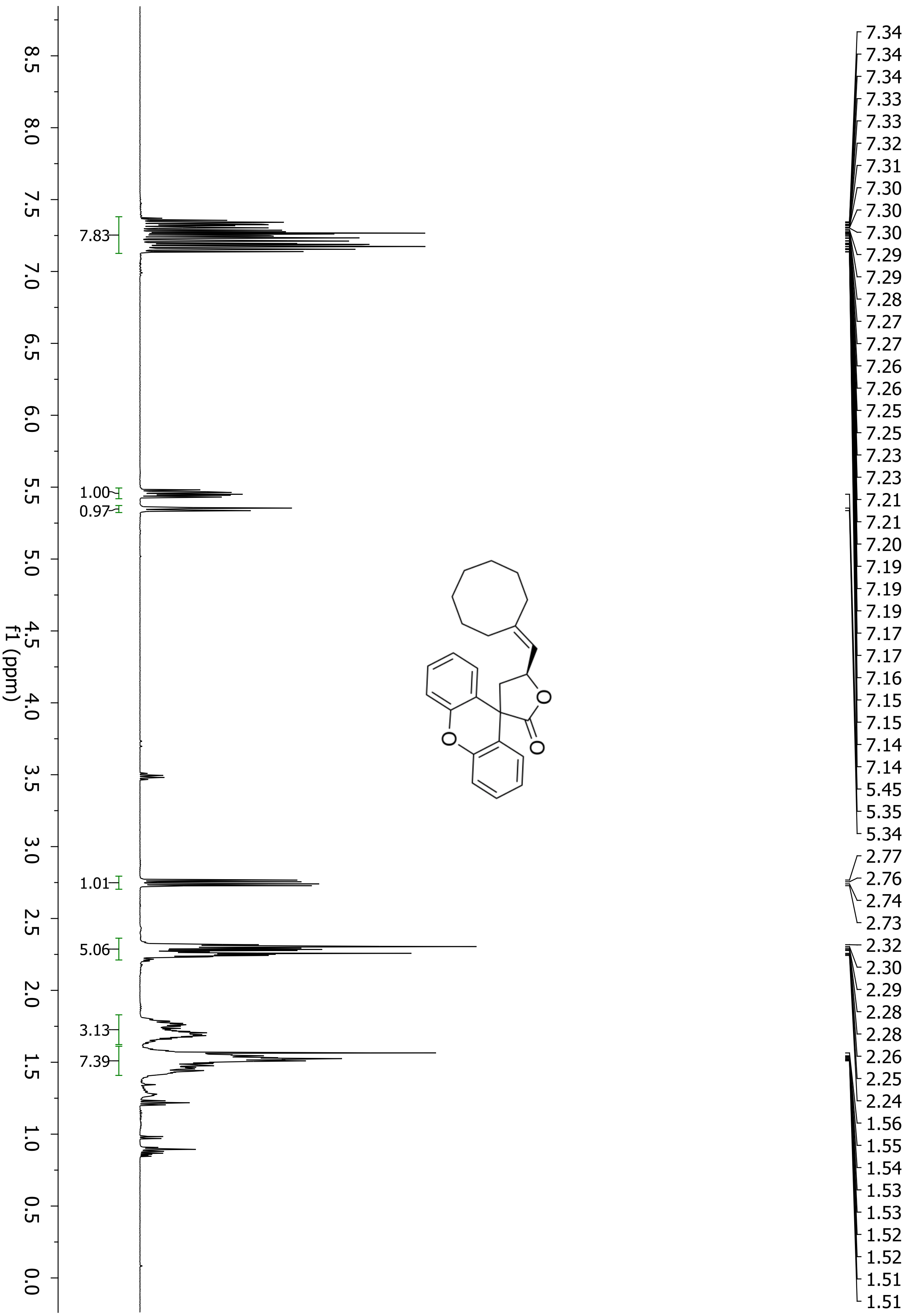
7.35
7.34
7.33
7.33
7.32
7.31
7.30
7.30
7.30
7.29
7.28
7.27
7.26
7.26
7.25
7.24
7.24
7.22
7.22
7.21
7.20
7.19
7.18
7.18
7.18
7.18
7.17
7.16
7.16
7.16
7.15
7.14
7.14
7.14
7.13
7.12
2.74
2.72
2.71
2.69
2.28
2.26
2.25
2.22
2.18
2.16
2.15
2.14
2.13
1.61
1.61
1.60
1.59
1.58
1.57
1.55
1.54
1.53
8.17
0.98
0.94
1.00
2.05
3.05
6.28
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


177.33
151.70
151.01
148.82
129.28
129.00
127.45
125.87
124.33
124.11
123.69
122.86
119.04
117.64
116.73
77.48
77.16
76.84
73.82
50.80
50.32
37.15
29.81
28.39
27.96
26.58
f1 (ppm)

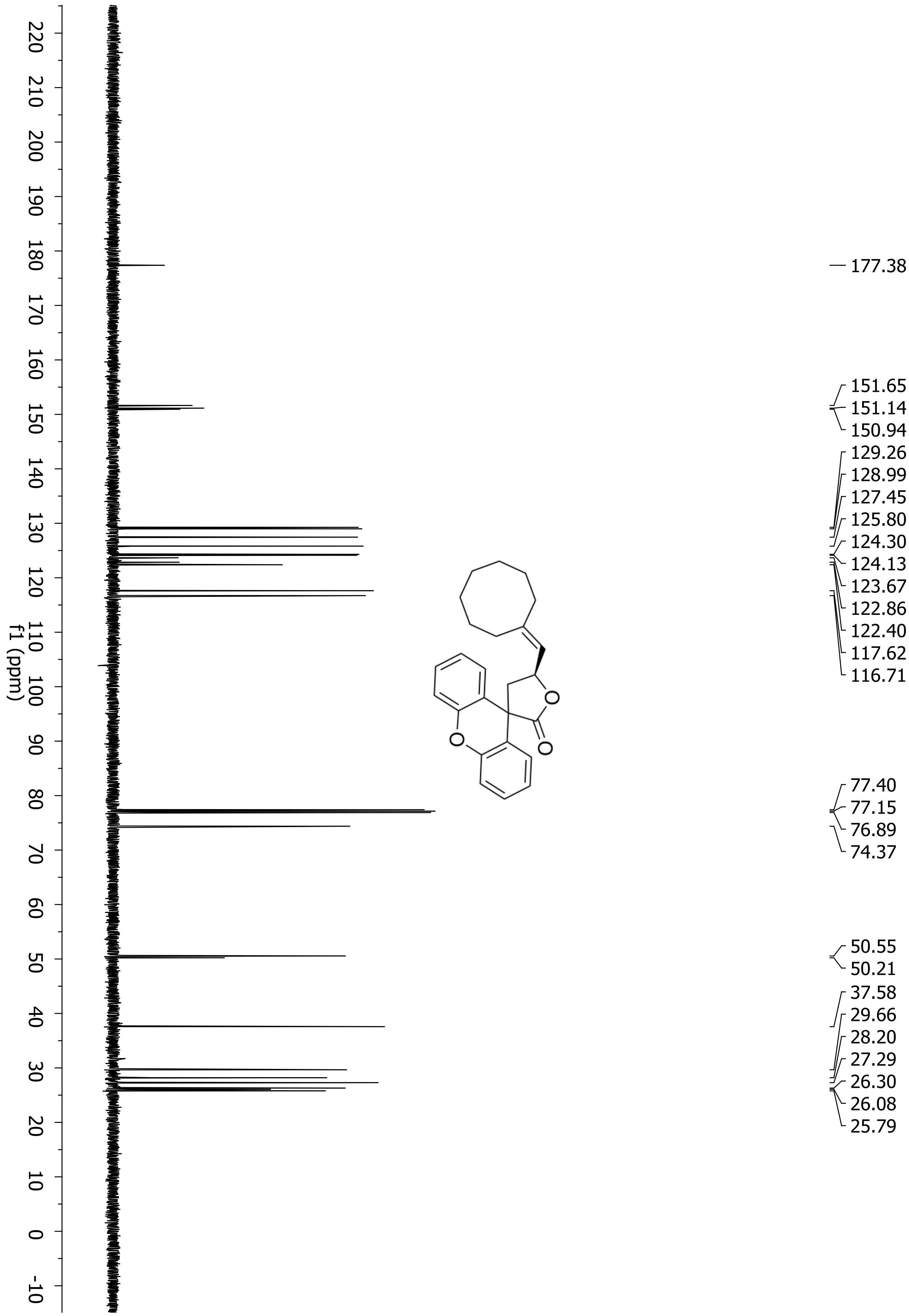


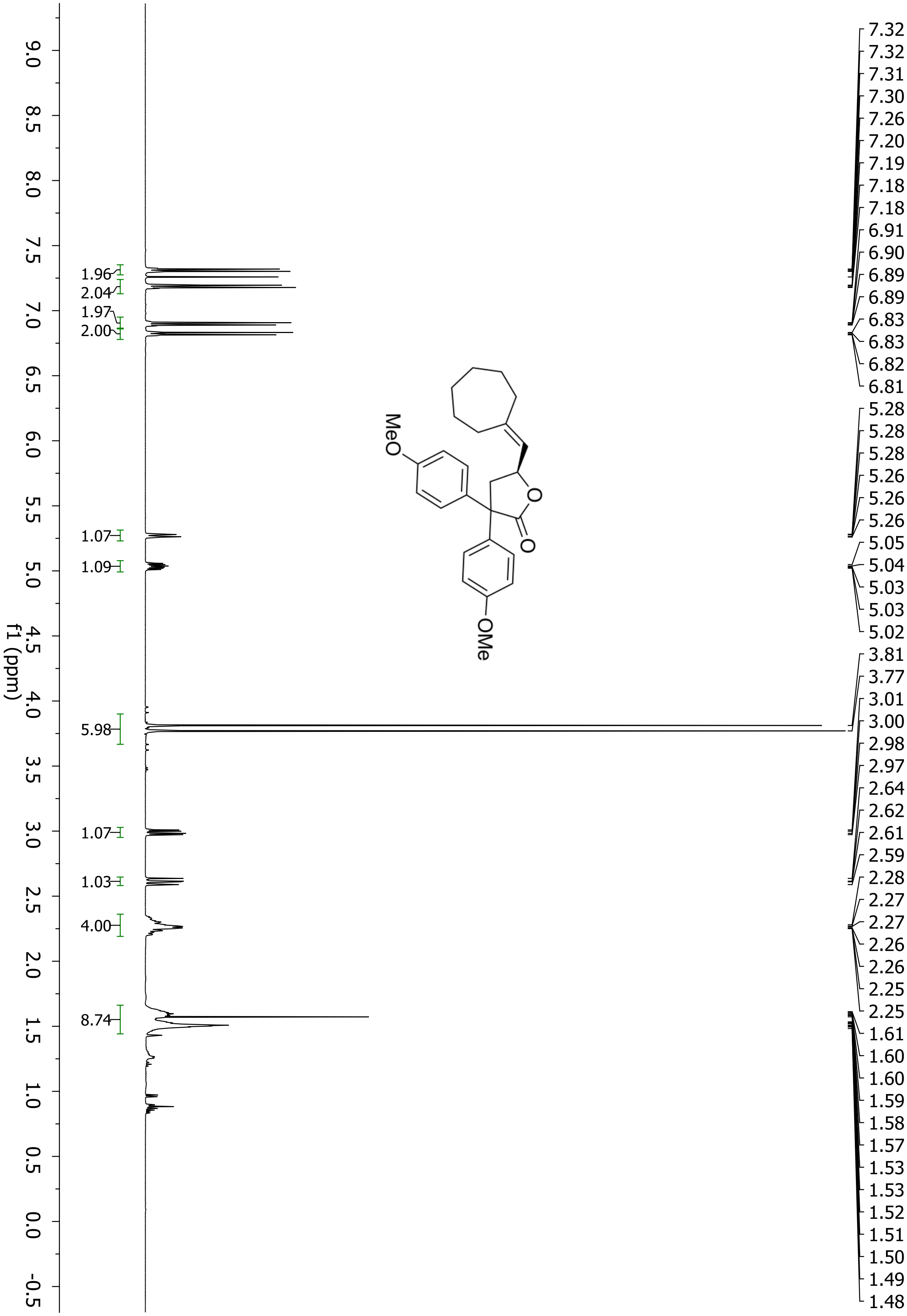
7.34
7.34
7.34
7.34
7.33
7.32
7.32
7.31
7.30
7.30
7.30
7.29
7.29
7.27
7.27
7.25
7.25
7.24
7.24
7.23
7.22
7.21
7.21
7.20
7.19
7.18
7.18
7.17
7.15
7.14
7.13
5.42
5.41
5.40
5.39
5.33
5.32
2.77
2.75
2.74
2.73
2.32
2.31
2.31
2.30
2.29
2.28
2.27
2.26
2.24
1.57
1.57
1.56
1.55
1.54
1.53
1.52
1.50
8.10
1.00
0.94
1.00
1.02
3.84
8.18
f1 (ppm)

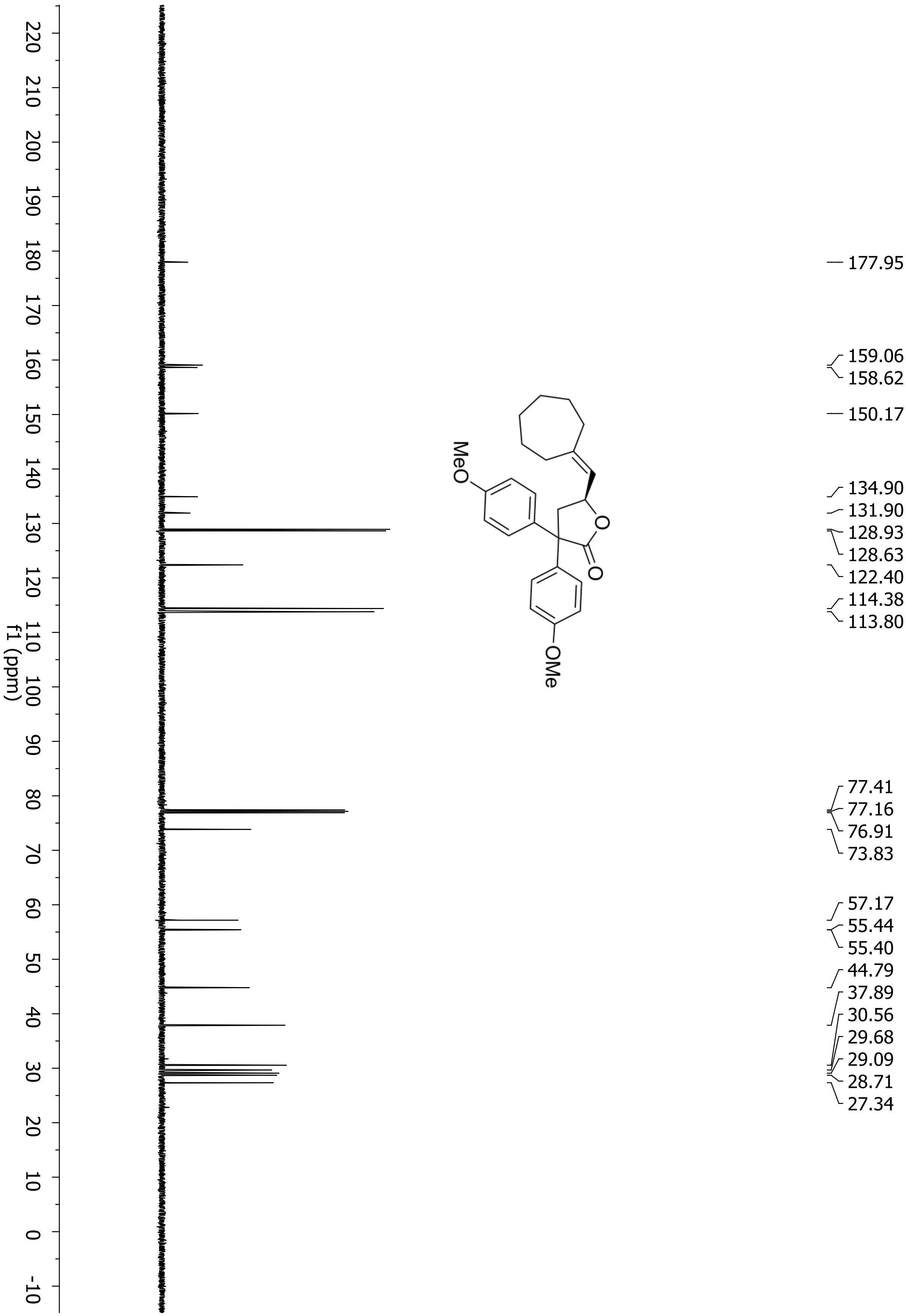

177.37
151.68
150.98
150.56
129.28
129.01
127.46
125.87
124.32
124.12
123.69
122.86
122.40
117.63
116.73
77.41
77.16
76.91
74.30
50.58
50.24
37.89
30.66
29.66
29.09
28.71
27.33
f1 (ppm)
O
O
O

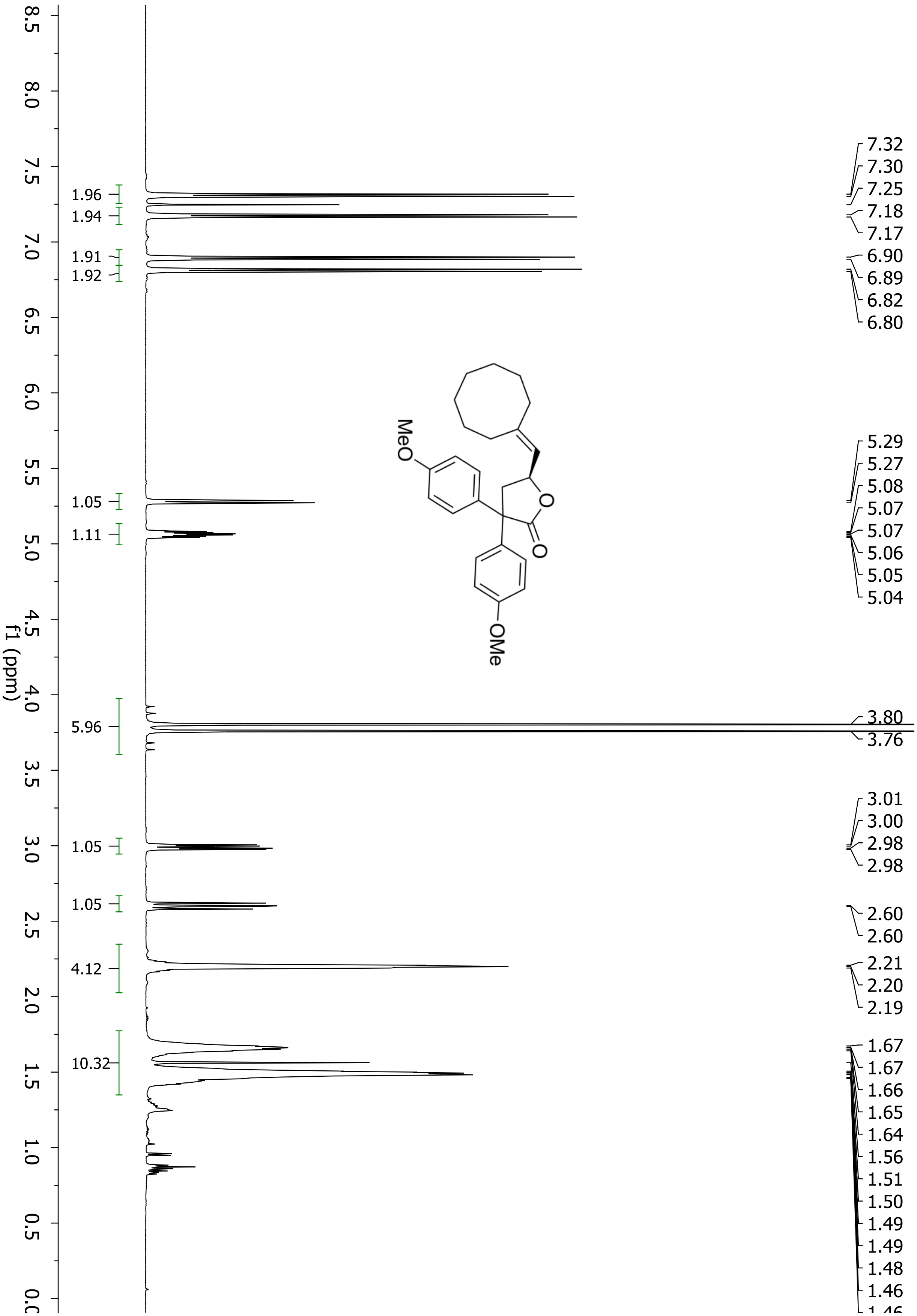


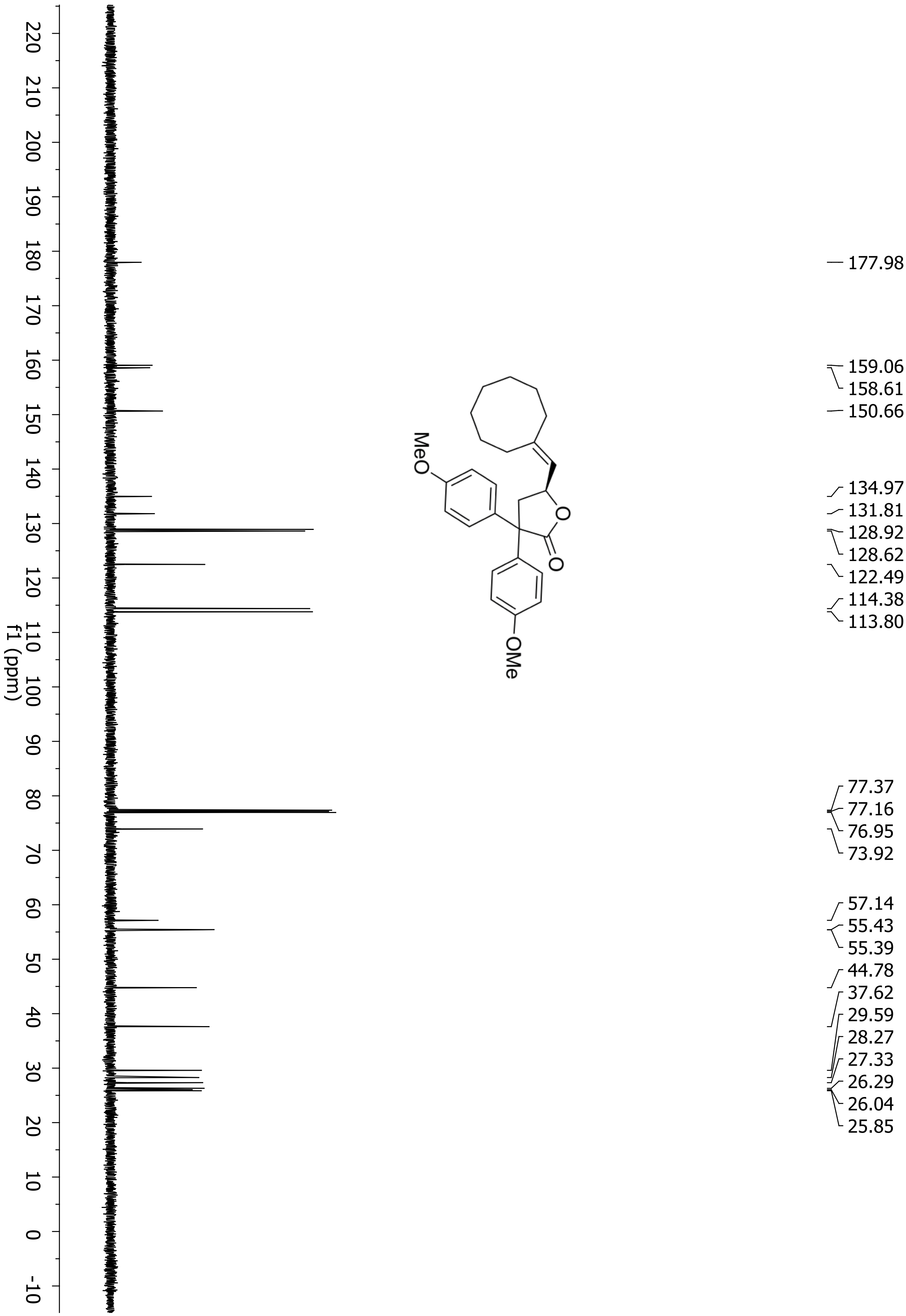
7.34
7.34
7.34
7.33
7.33
7.32
7.31
7.30
7.30
7.30
7.29
7.29
7.28
7.27
7.27
7.26
7.26
7.25
7.25
7.23
7.23
7.21
7.21
7.20
7.19
7.19
7.19
7.17
7.17
7.16
7.15
7.15
7.14
7.14
5.45
5.35
5.34
2.77
2.76
2.74
2.73
2.32
2.30
2.29
2.28
2.28
2.26
2.25
2.24
1.56
1.55
1.54
1.53
1.53
1.52
1.52
1.51
1.51
7.83
1.00
0.97
1.01
5.06
3.13
7.39
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
O
O
O

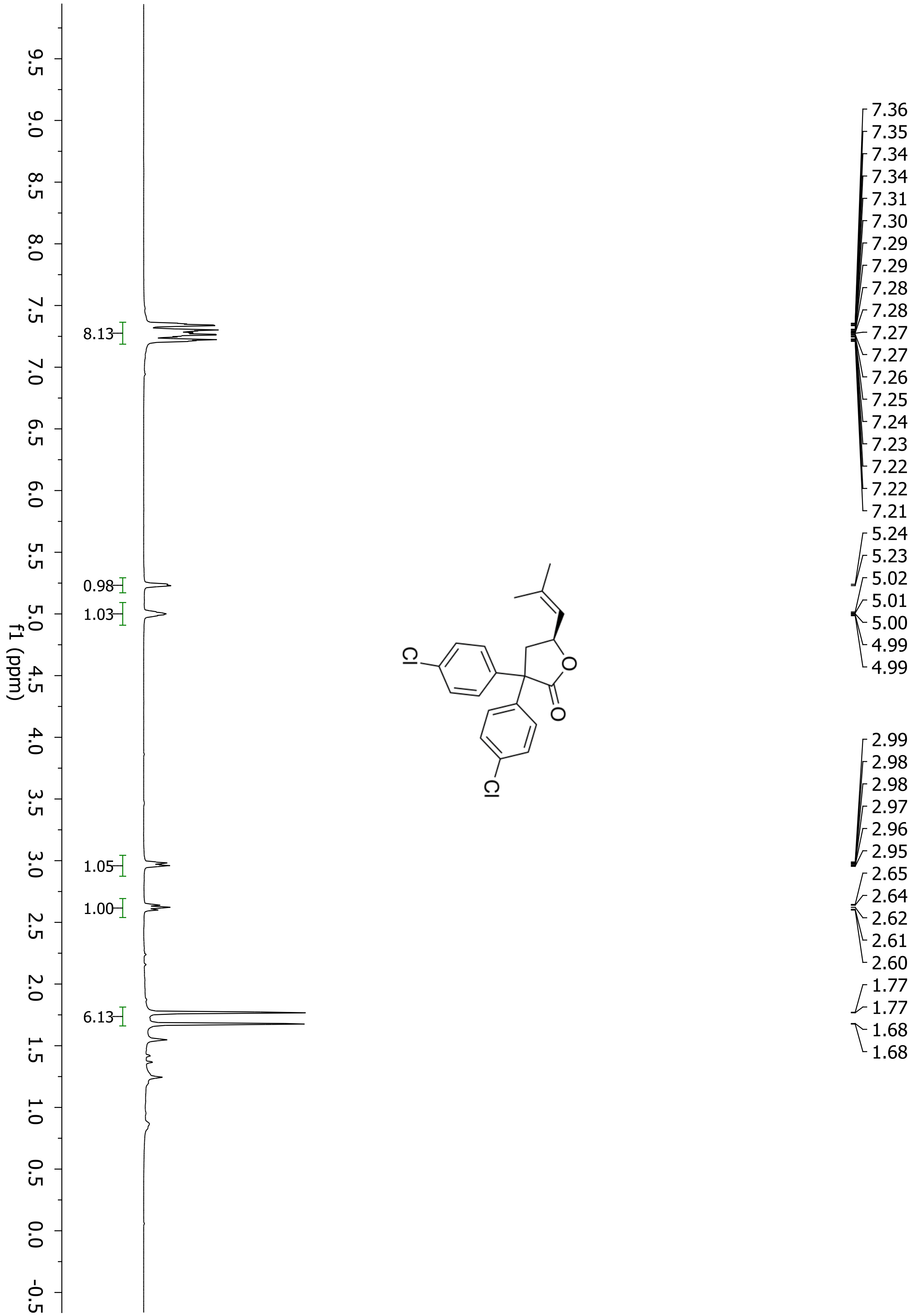

177.38
151.65
151.14
150.94
129.26
128.99
127.45
125.80
124.30
124.13
123.67
122.86
122.40
117.62
116.71
77.40
77.15
76.89
74.37
50.55
50.21
37.58
29.66
28.20
27.29
26.30
26.08
25.79
f1 (ppm)
O
O
O


7.32
7.32
7.31
7.30
7.26
7.20
7.19
7.18
7.18
6.91
6.90
6.89
6.89
6.83
6.83
6.82
6.81
5.28
5.28
5.28
5.26
5.26
5.26
5.05
5.04
5.03
5.03
5.02
3.81
3.77
3.01
3.00
2.98
2.97
2.64
2.62
2.61
2.59
2.28
2.27
2.27
2.26
2.26
2.25
2.25
1.61
1.60
1.60
1.59
1.58
1.57
1.53
1.53
1.52
1.51
1.50
1.49
1.48
1.96
2.04
1.97
2.00
1.07
1.09
5.98
1.07
1.03
4.00
8.74
MeO
OMe
O
O
f1 (ppm)

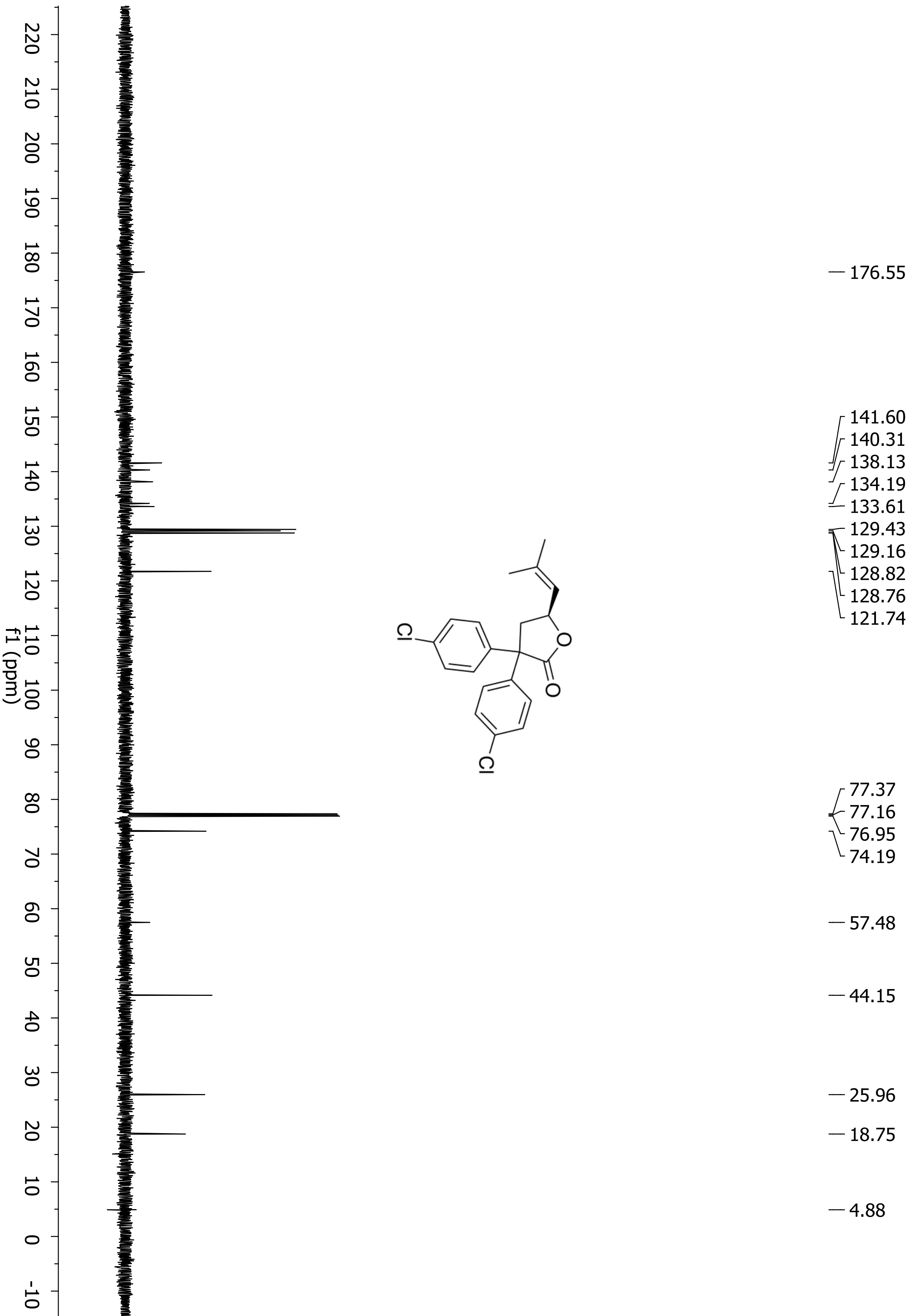

177.95
159.06
158.62
150.17
134.90
131.90
128.93
128.63
122.40
114.38
113.80
77.41
77.16
76.91
73.83
57.17
55.44
55.40
44.79
37.89
30.56
29.68
29.09
28.71
27.34
MeO
OMe
O
f1 (ppm)

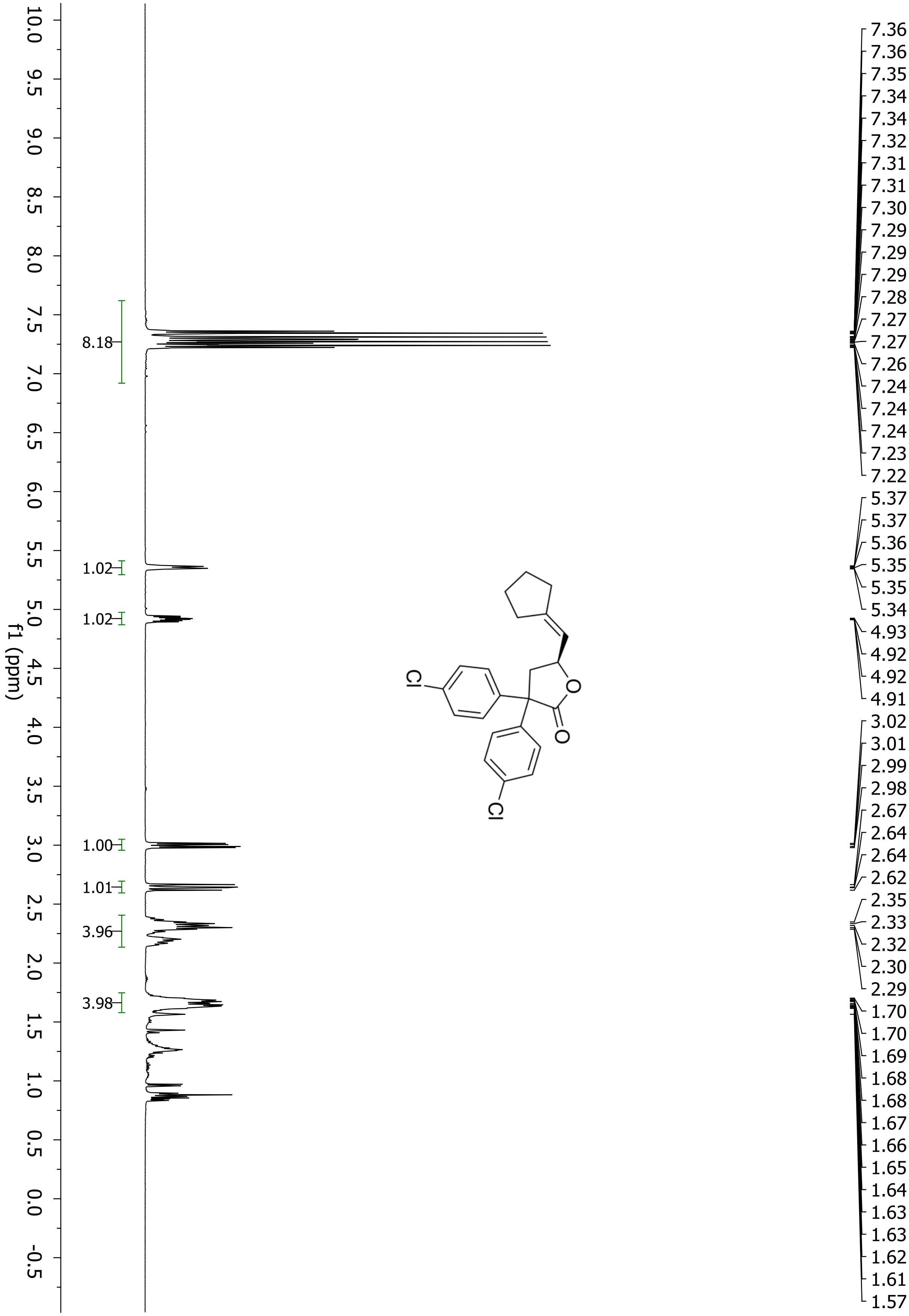

7.32
7.30
7.25
7.18
7.17
6.90
6.89
6.82
6.80
5.29
5.27
5.08
5.07
5.07
5.06
5.05
5.04
3.80
3.76
3.01
3.00
2.98
2.98
2.60
2.60
2.21
2.20
2.19
1.67
1.67
1.66
1.65
1.64
1.56
1.51
1.50
1.49
1.49
1.48
1.46
1.96
1.94
1.91
1.92
1.05
1.11
5.96
1.05
1.05
4.12
10.32
MeO
OMe
O
O
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

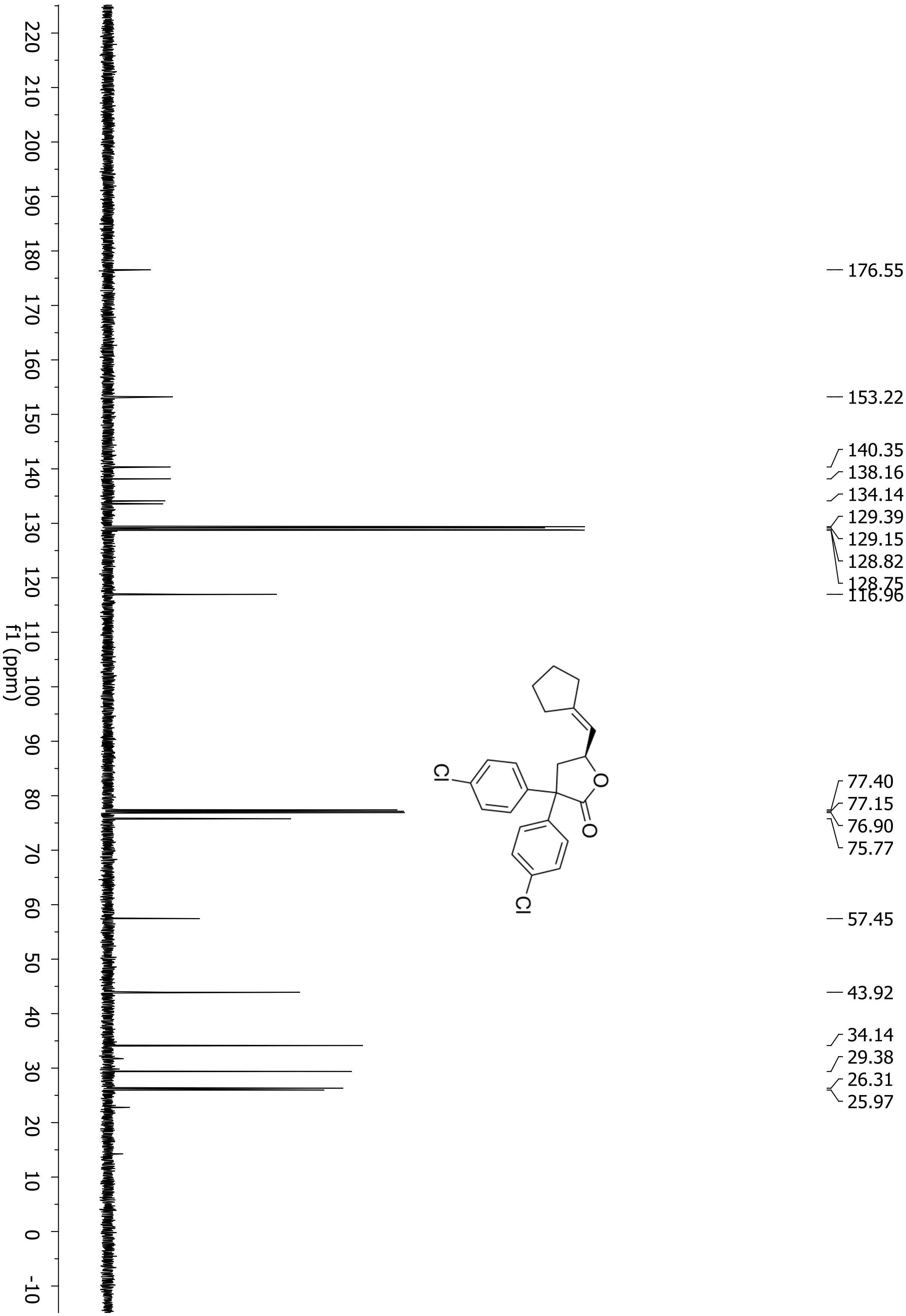

177.98
159.06
158.61
150.66
134.97
131.81
128.92
128.62
122.49
114.38
113.80
77.37
77.16
76.95
73.92
57.14
55.43
55.39
44.78
37.62
29.59
28.27
27.33
26.29
26.04
25.85
MeO
OMe
O
O
f1 (ppm)

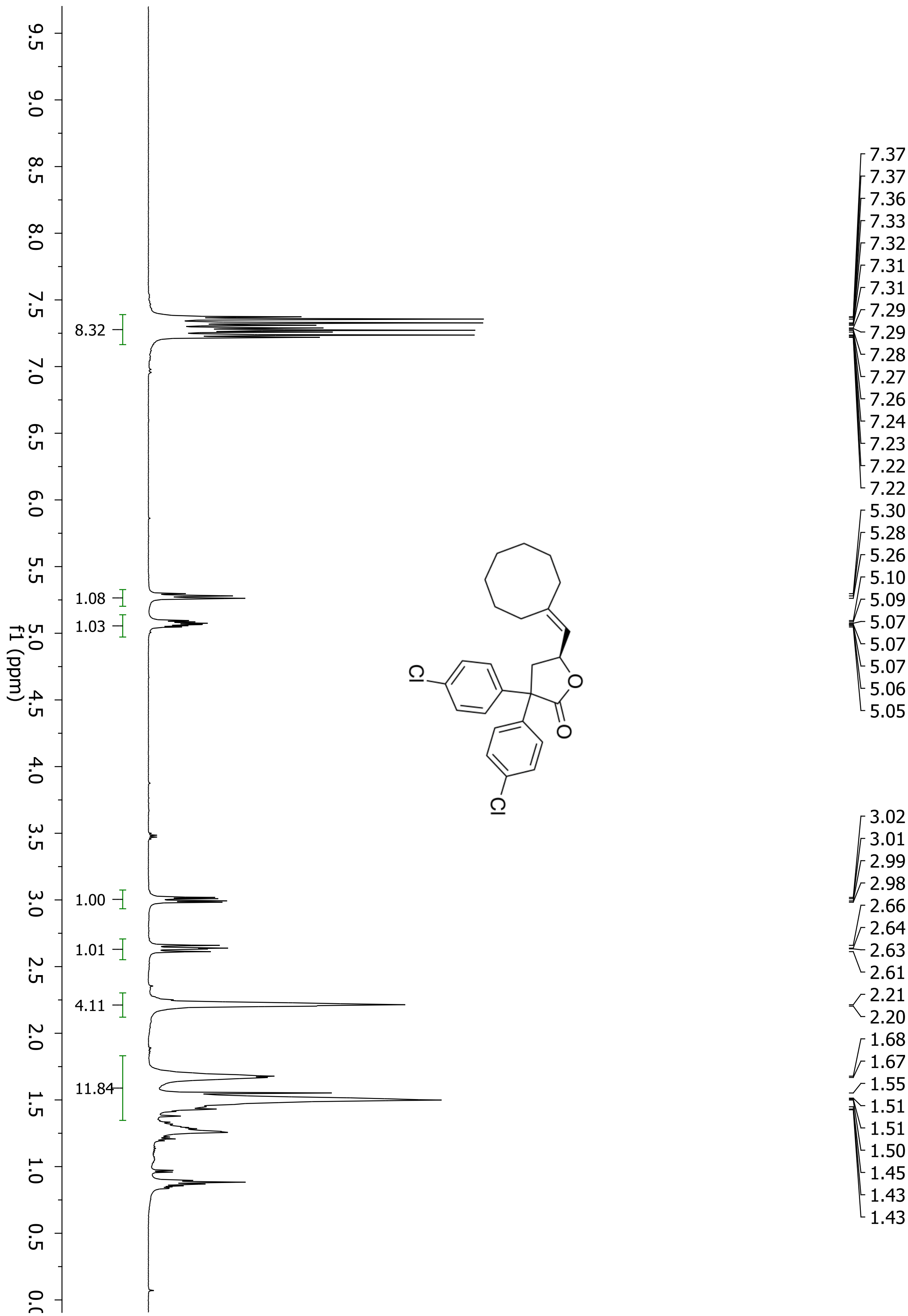


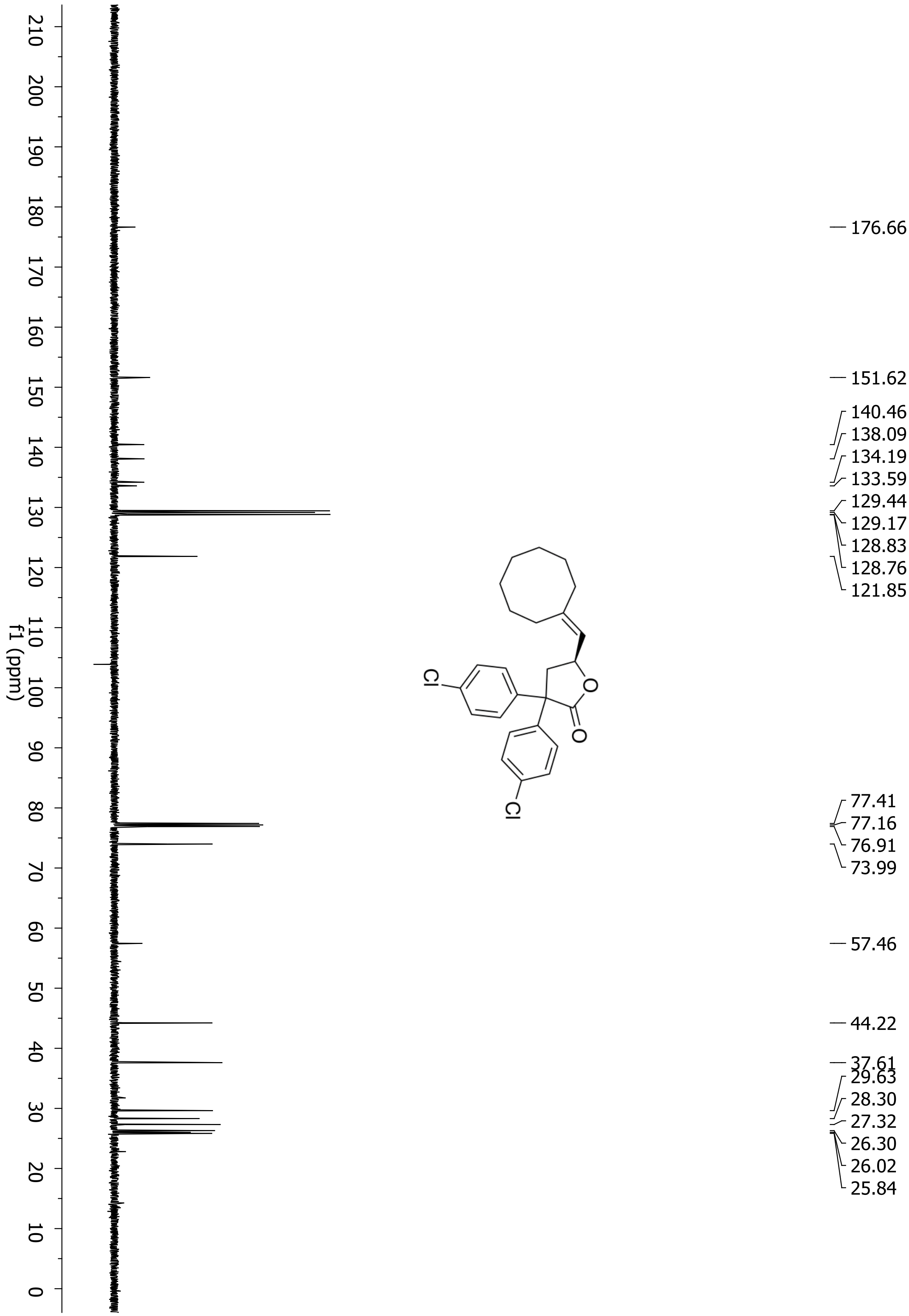
7.36
7.35
7.34
7.34
7.31
7.30
7.29
7.29
7.28
7.28
7.27
7.27
7.26
7.25
7.24
7.23
7.22
7.22
7.21
5.24
5.23
5.02
5.01
5.00
4.99
4.99
2.99
2.98
2.98
2.97
2.96
2.95
2.65
2.64
2.62
2.61
2.60
1.77
1.77
1.68
1.68
8.13
0.98
1.03
1.05
1.00
6.13
Cl
Cl
O
O
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

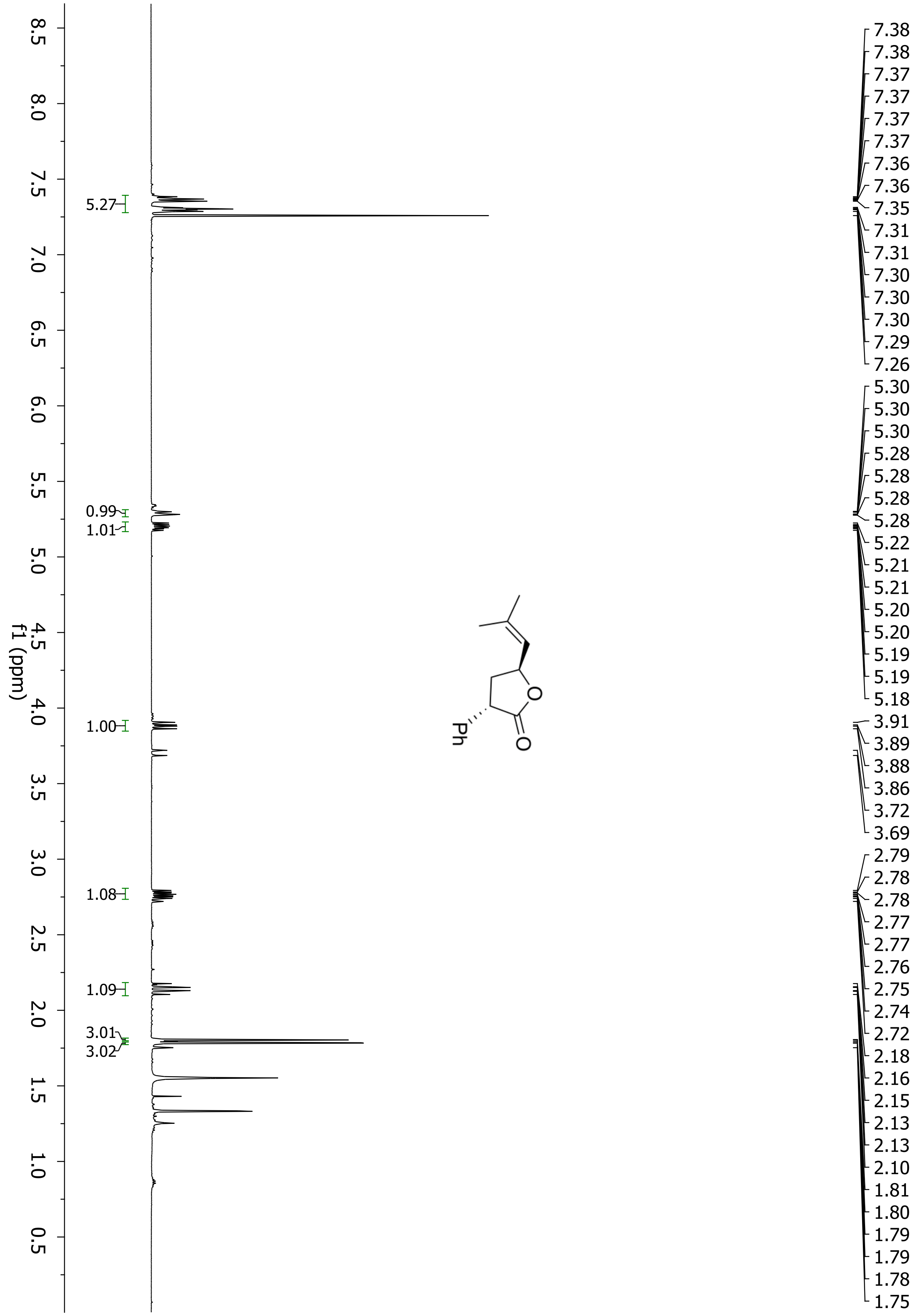

176.55
141.60
140.31
138.13
134.19
133.61
129.43
129.16
128.82
128.76
121.74
77.37
77.16
76.95
74.19
57.48
44.15
25.96
18.75
4.88
f1 (ppm)
Cl
Cl
O
O

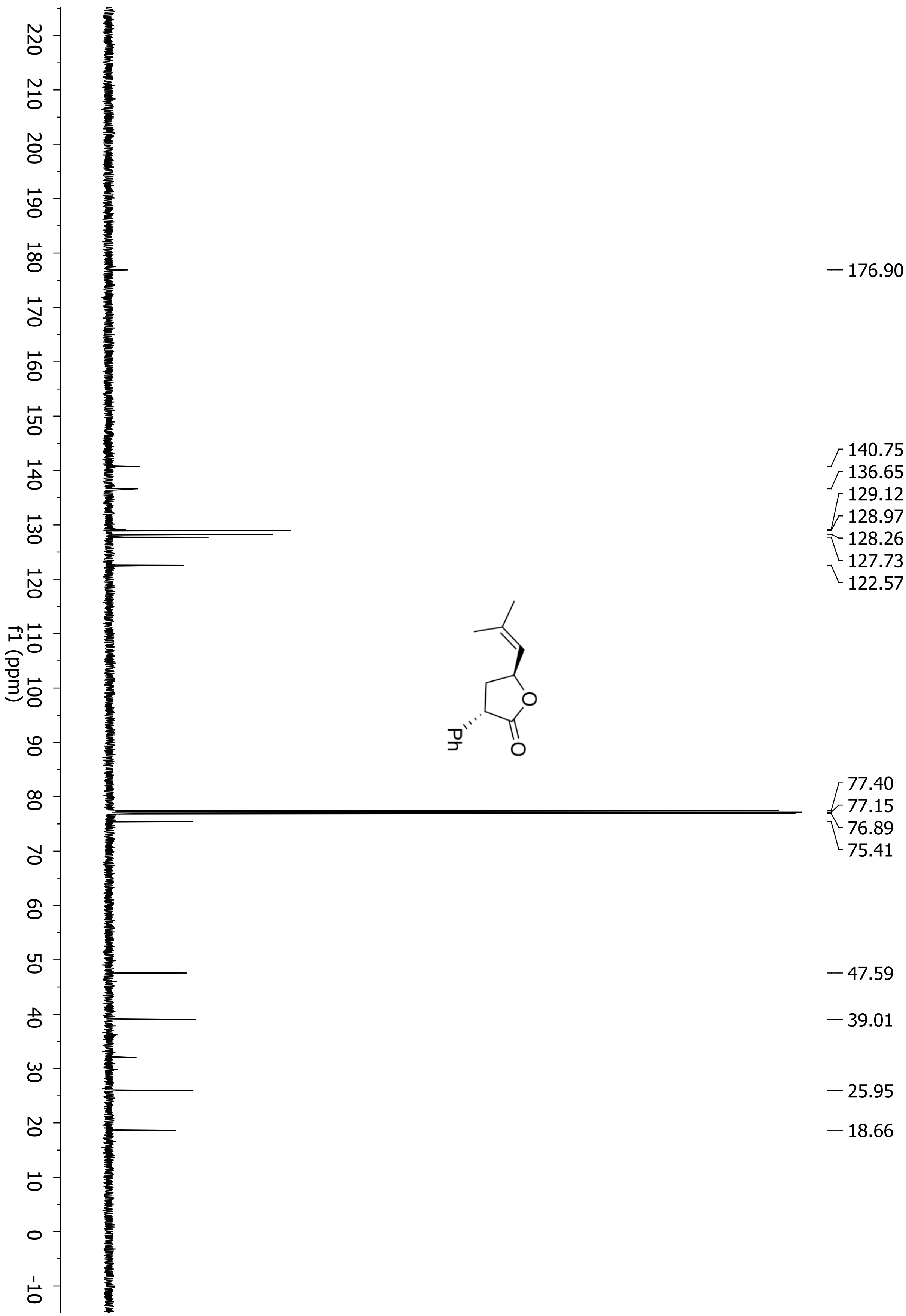

7.36
7.36
7.35
7.34
7.34
7.32
7.31
7.31
7.30
7.29
7.29
7.29
7.28
7.27
7.27
7.26
7.24
7.24
7.24
7.23
7.22
5.37
5.37
5.36
5.35
5.35
5.34
4.93
4.92
4.92
4.91
3.02
3.01
2.99
2.98
2.67
2.64
2.64
2.62
2.35
2.33
2.32
2.30
2.29
1.70
1.70
1.69
1.68
1.68
1.67
1.66
1.65
1.64
1.63
1.63
1.62
1.61
1.57
8.18
1.02
1.02
1.00
1.01
3.96
3.98
Cl
Cl
O
O
f1 (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

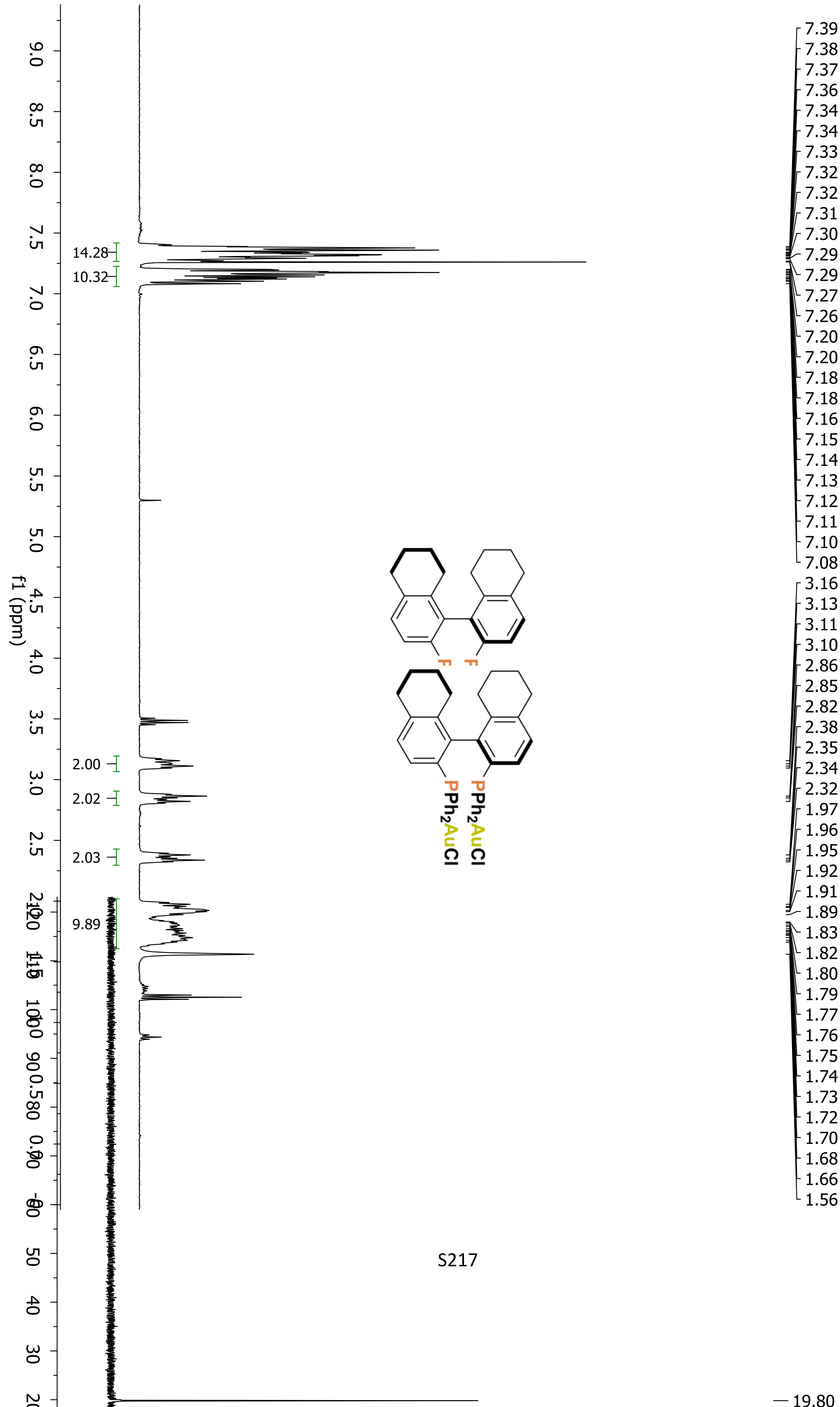

176.55
153.22
140.35
138.16
134.14
129.39
129.15
128.82
128.75
116.96
77.40
77.15
76.90
75.77
57.45
43.92
34.14
29.38
26.31
25.97
f1 (ppm)
Cl
Cl
O
O


7.37
7.37
7.36
7.33
7.32
7.31
7.31
7.29
7.29
7.28
7.27
7.26
7.24
7.23
7.22
7.22
5.30
5.28
5.26
5.10
5.09
5.07
5.07
5.07
5.06
5.05
3.02
3.01
2.99
2.98
2.66
2.64
2.63
2.61
2.21
2.20
1.68
1.67
1.55
1.51
1.51
1.50
1.45
1.43
1.43
8.32
1.08
1.03
1.00
1.01
4.11
11.84
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
Cl
Cl
O
O

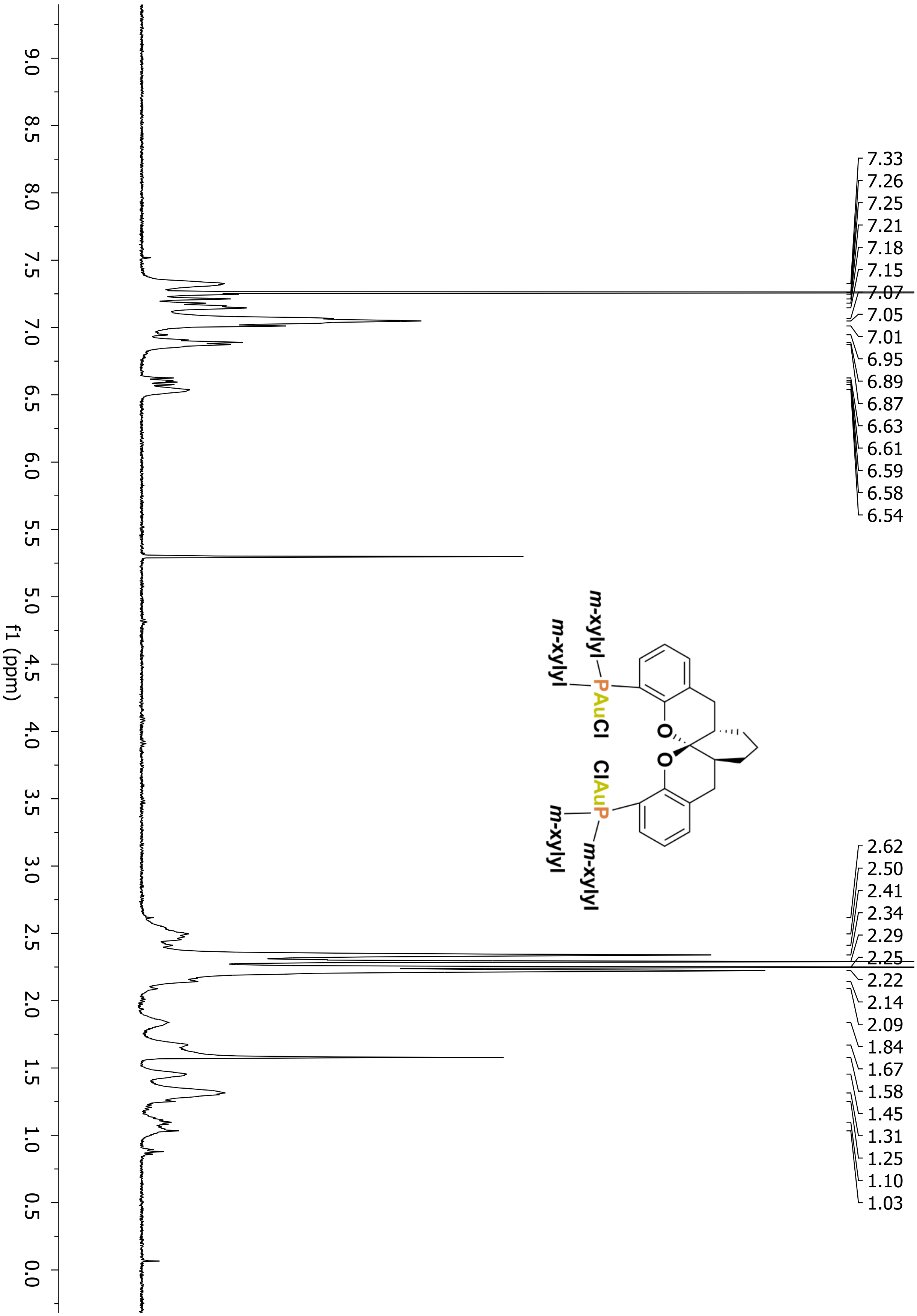

176.66
151.62
140.46
138.09
134.19
133.59
129.44
129.17
128.83
128.76
121.85
77.41
77.16
76.91
73.99
57.46
44.22
37.61
29.63
28.30
27.32
26.30
26.02
25.84
Cl
Cl
O
O
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


7.38
7.38
7.37
7.37
7.37
7.37
7.36
7.36
7.35
7.31
7.31
7.30
7.30
7.30
7.29
7.26
5.30
5.30
5.30
5.28
5.28
5.28
5.28
5.22
5.21
5.21
5.20
5.20
5.19
5.19
5.18
3.91
3.89
3.88
3.86
3.72
3.69
2.79
2.78
2.78
2.77
2.77
2.76
2.75
2.74
2.72
2.18
2.16
2.15
2.13
2.13
2.10
1.81
1.80
1.79
1.79
1.78
1.75
5.27
0.99
1.01
1.00
1.08
1.09
3.01
3.02
f1 (ppm)
Ph
O

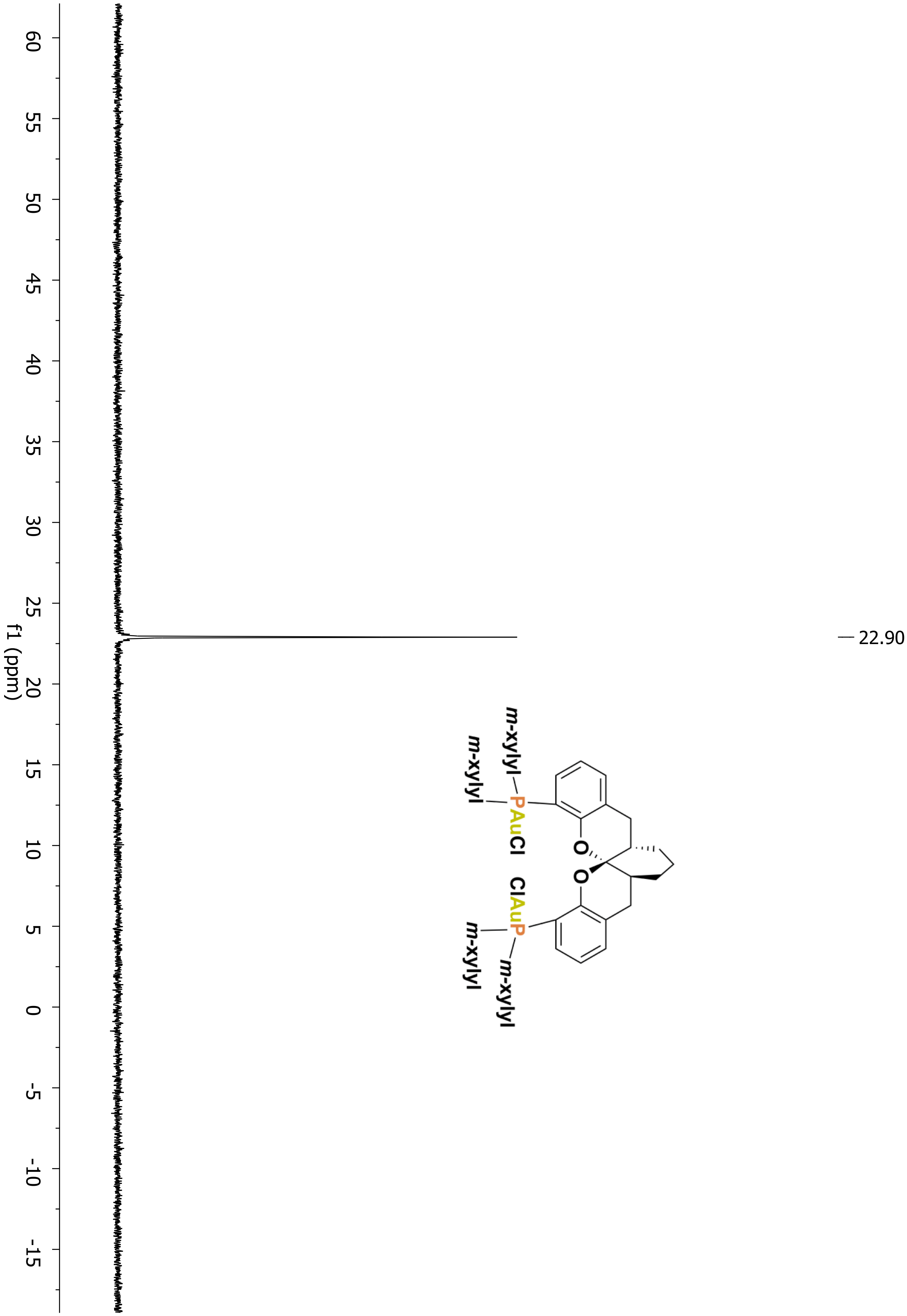

176.90
140.75
136.65
129.12
128.97
128.26
127.73
122.57
77.40
77.15
76.89
75.41
47.59
39.01
25.95
18.66
f1 (ppm)
Ph
O
O



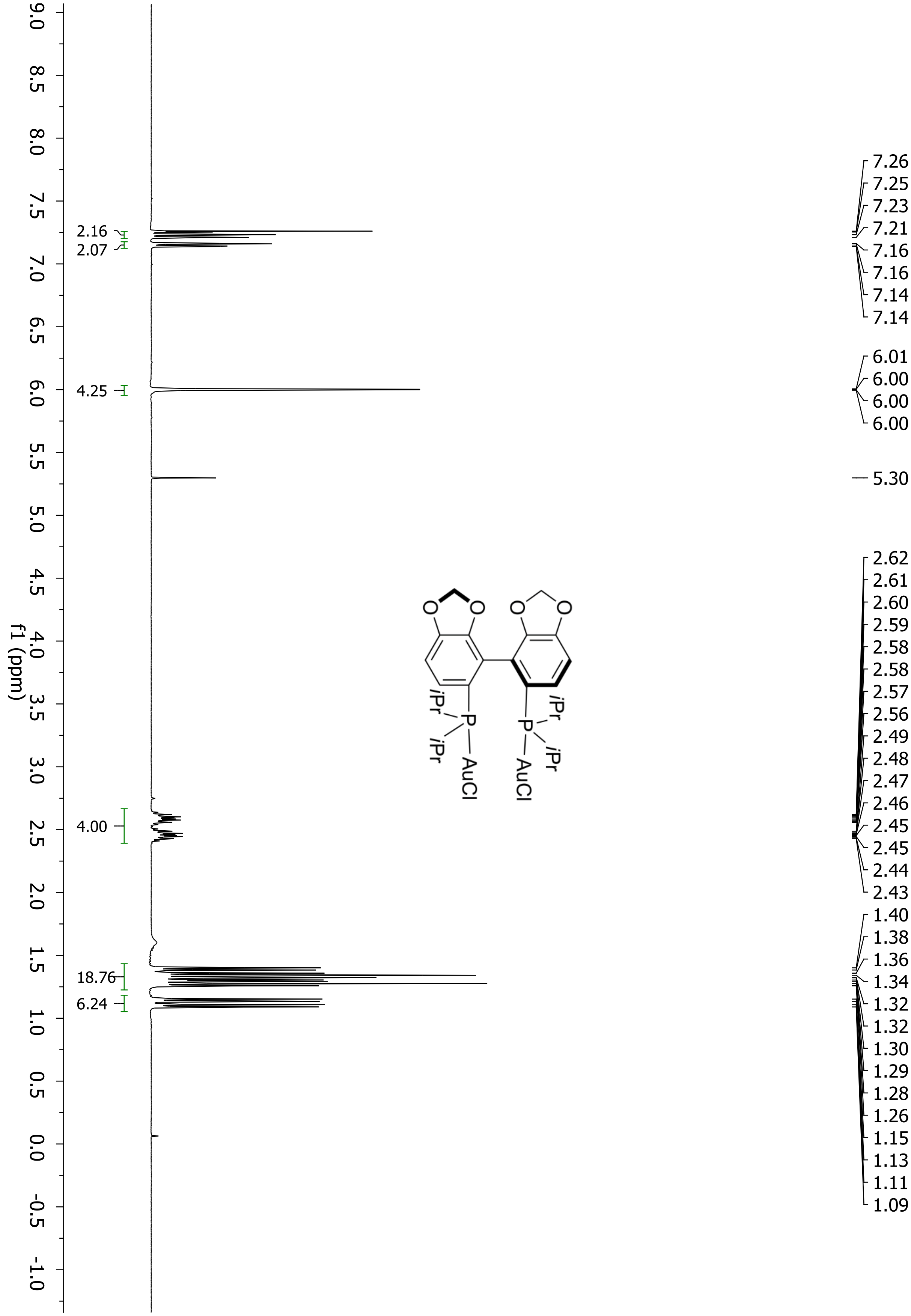
7.39
7.38
7.37
7.36
7.34
7.34
7.33
7.32
7.32
7.31
7.30
7.29
7.29
7.27
7.26
7.20
7.20
7.18
7.18
7.16
7.15
7.14
7.13
7.12
7.11
7.10
7.08
3.16
3.13
3.11
3.10
2.86
2.85
2.82
2.38
2.35
2.34
2.32
1.97
1.96
1.95
1.92
1.91
1.89
1.83
1.82
1.80
1.79
1.77
1.76
1.75
1.74
1.73
1.72
1.70
1.68
1.66
1.56
19.80
14.28
10.32
2.00
2.02
2.03
9.89
f1 (ppm)



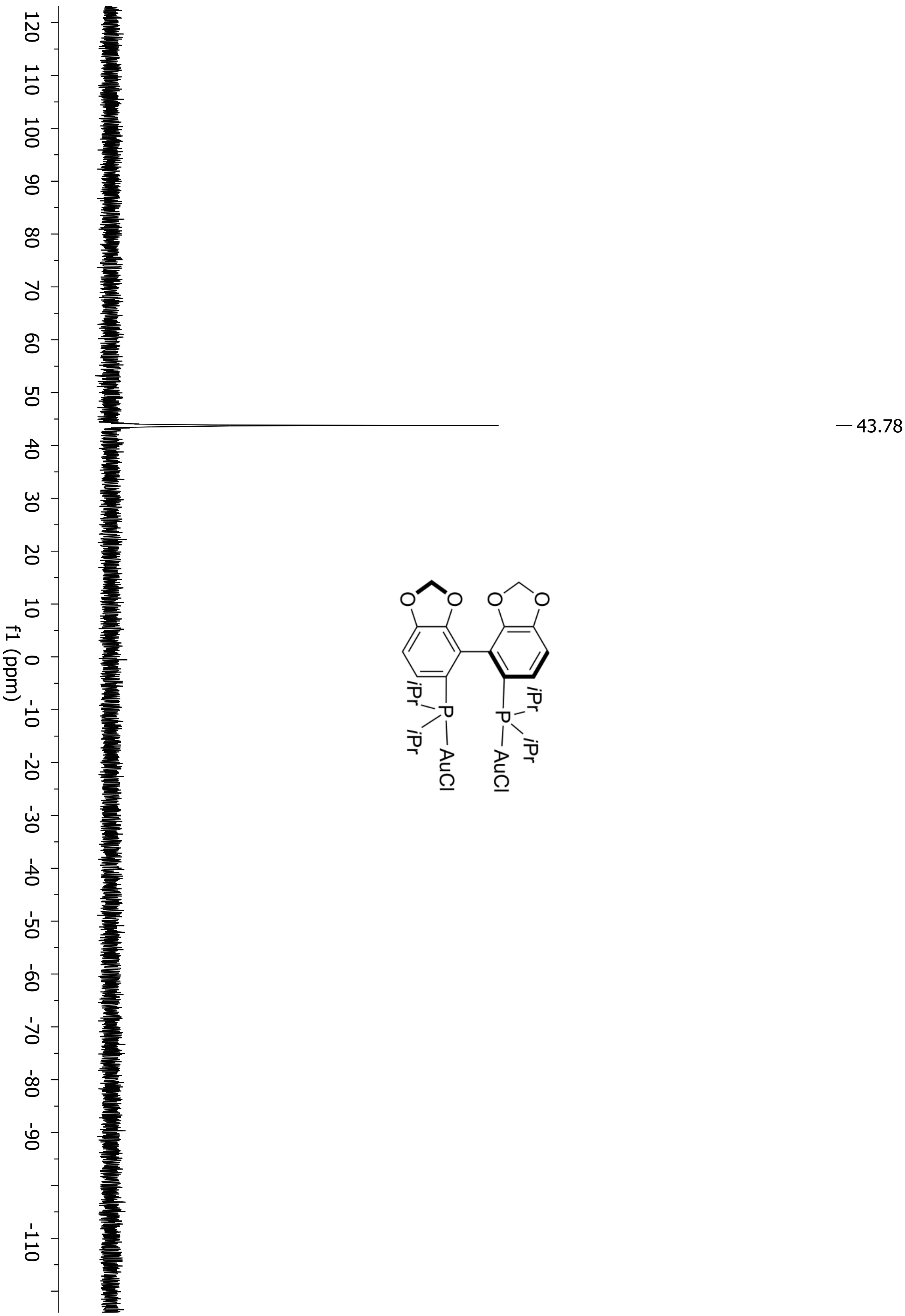
7.33
7.26
7.25
7.21
7.18
7.15
7.07
7.05
7.01
6.95
6.89
6.87
6.63
6.61
6.59
6.58
6.54
2.62
2.50
2.41
2.34
2.29
2.25
2.22
2.14
2.09
1.84
1.67
1.58
1.45
1.31
1.25
1.10
1.03
m-xylyl
m-xylyl
PAuCl
ClAuP
m-xylyl
m-xylyl
O
O
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

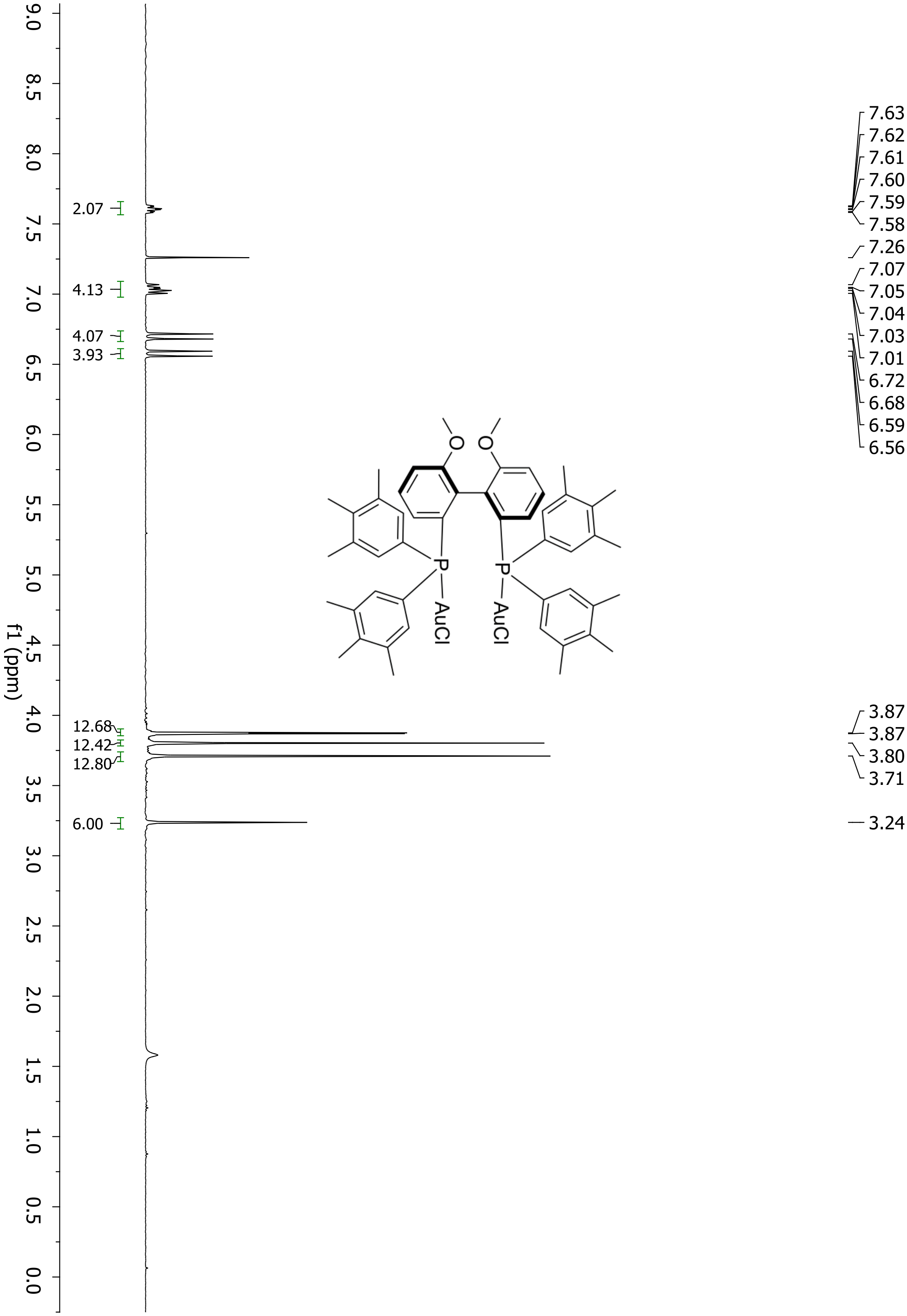


22.90
f1 (ppm)
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10
-15
m-xylyl
m-xylyl
PAuCl
O
O
ClAuP
m-xylyl
m-xylyl

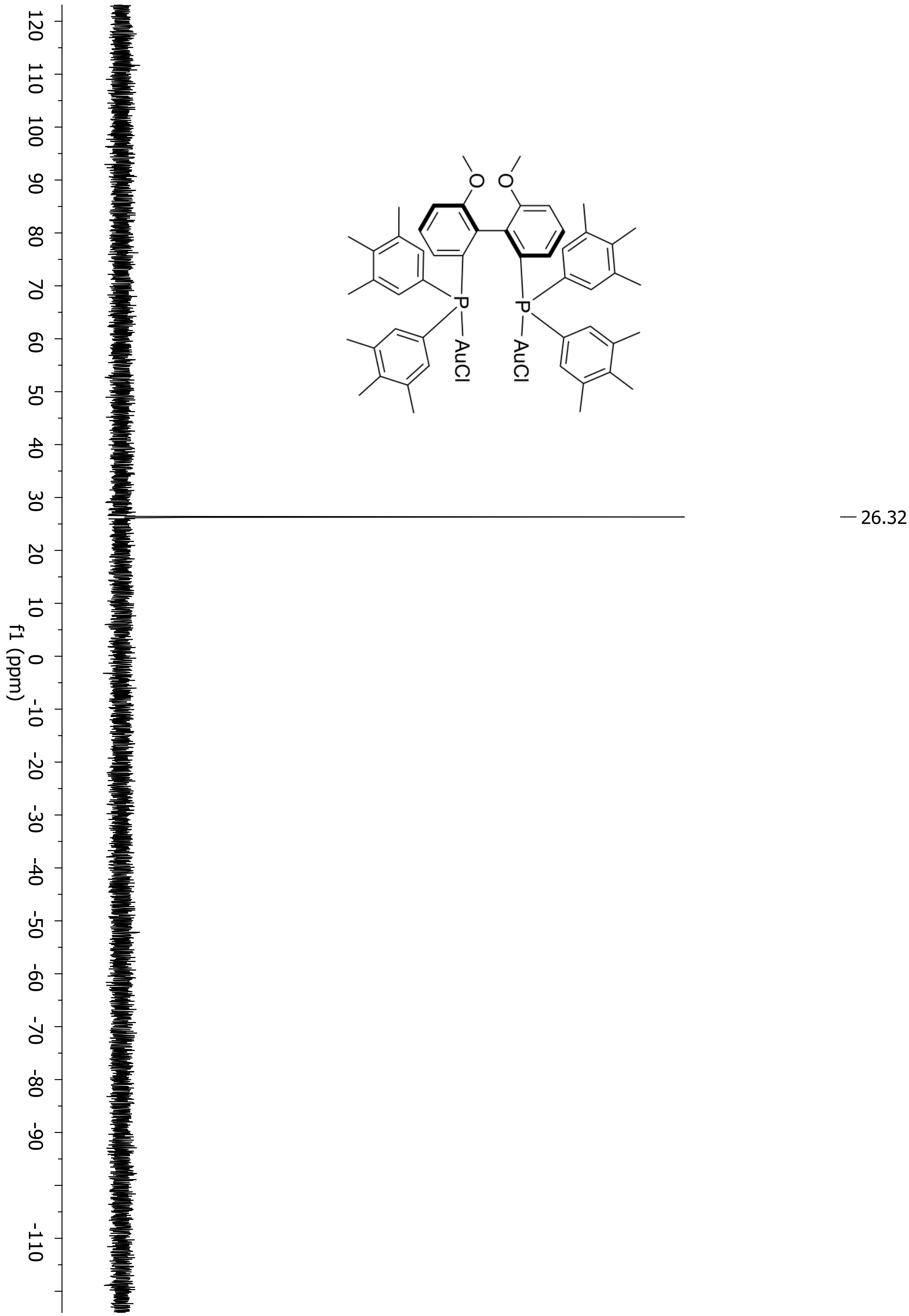


f1 (ppm)
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
2.16
2.07
4.25
4.00
18.76
6.24
7.26 7.25 7.23 7.21 7.16 7.16 7.14 7.14
6.01 6.00 6.00 6.00
5.30
2.62 2.61 2.60 2.59 2.58 2.58 2.57 2.56 2.49 2.48 2.47 2.46 2.45 2.45 2.44 2.43
1.40 1.38 1.36 1.34 1.32 1.32 1.30 1.29 1.28 1.26 1.15 1.13 1.11 1.09
iPr
P
AuCl

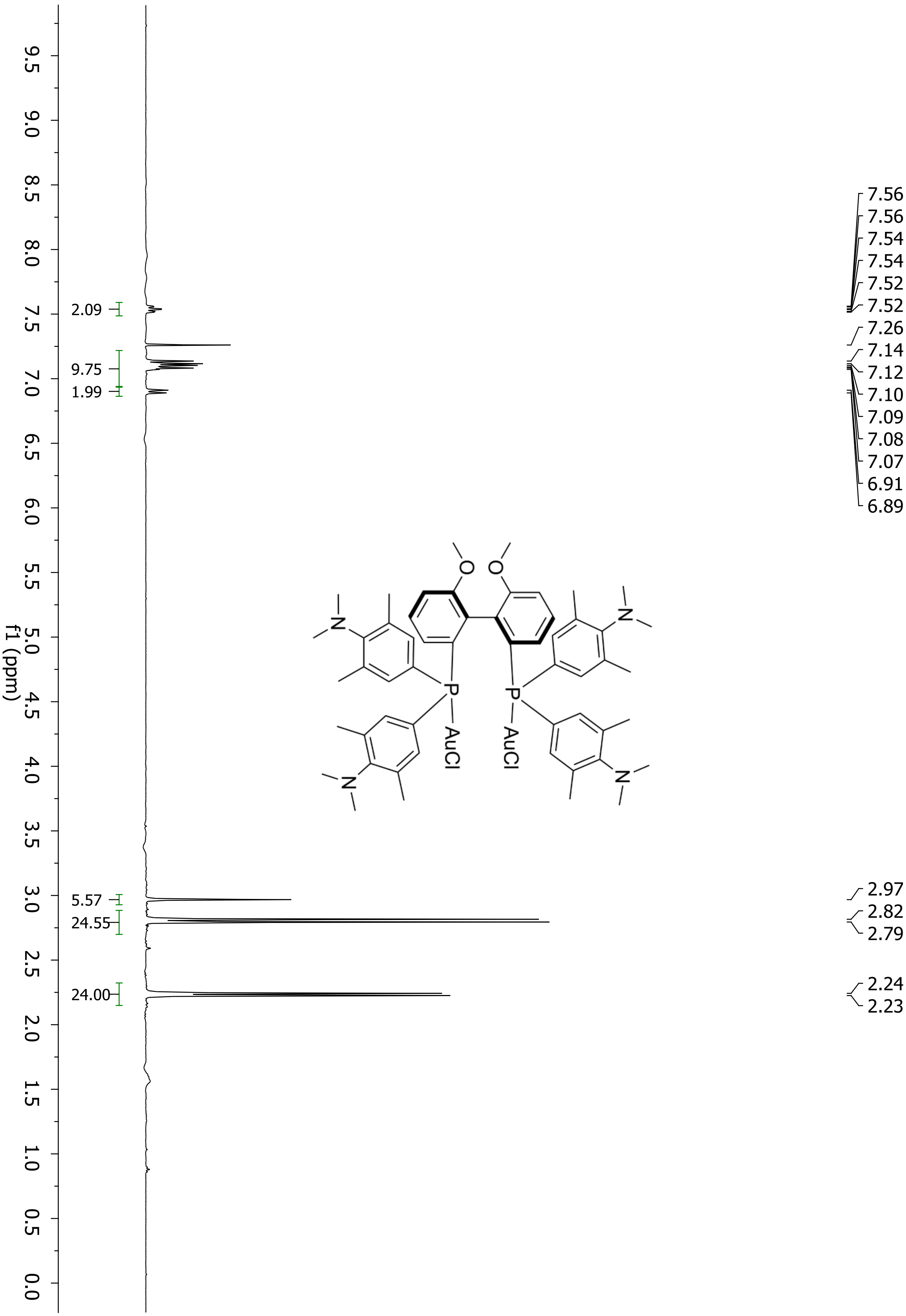

43.78
f1 (ppm)
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
O
O
O
O
iPr
iPr
iPr
iPr
P
P
AuCl
AuCl

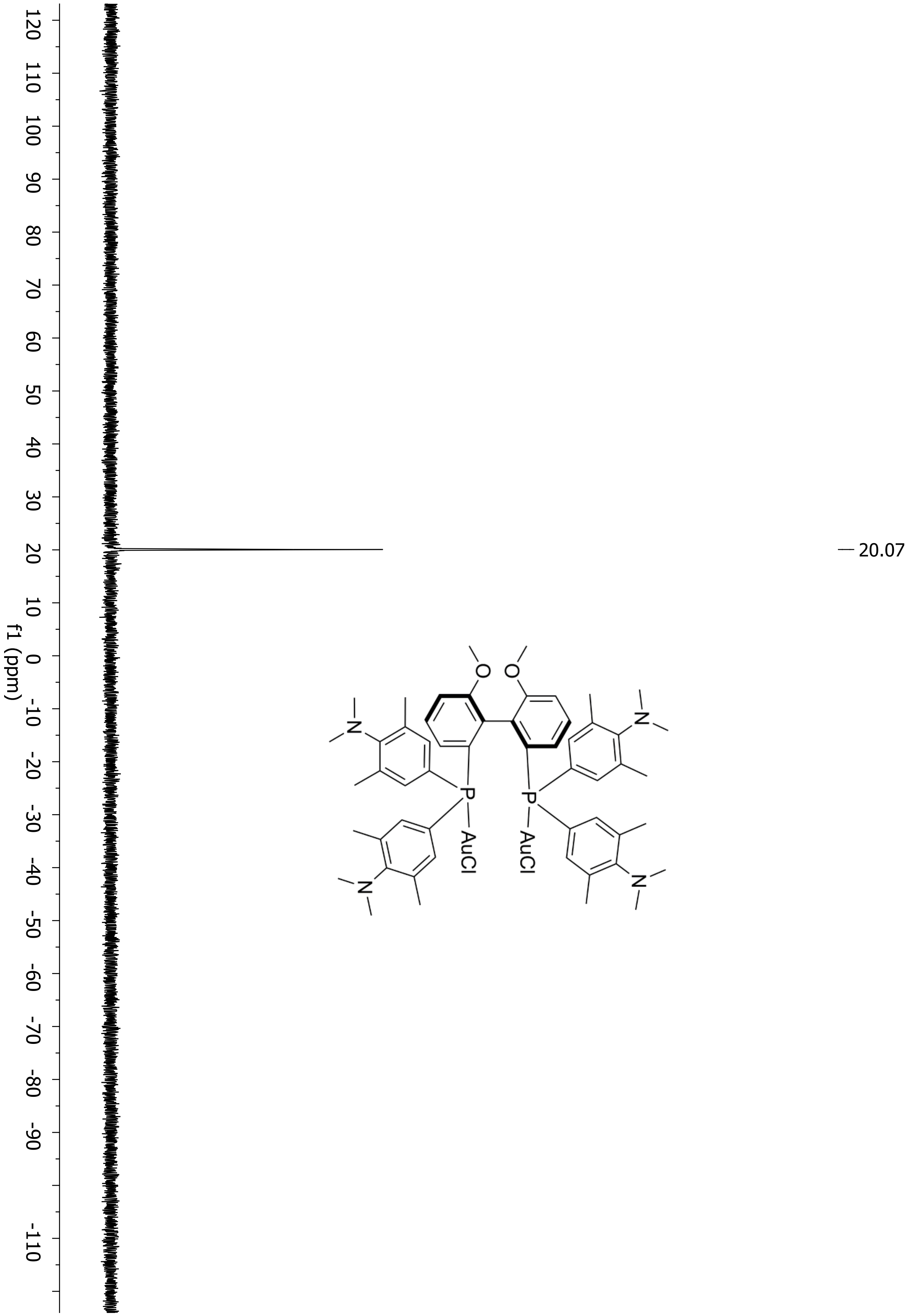


7.63
7.62
7.61
7.60
7.59
7.58
7.26
7.07
7.05
7.04
7.03
7.01
6.72
6.68
6.59
6.56
3.87
3.87
3.80
3.71
3.24
2.07
4.13
4.07
3.93
12.68
12.42
12.80
6.00
P
AuCl
P
AuCl
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

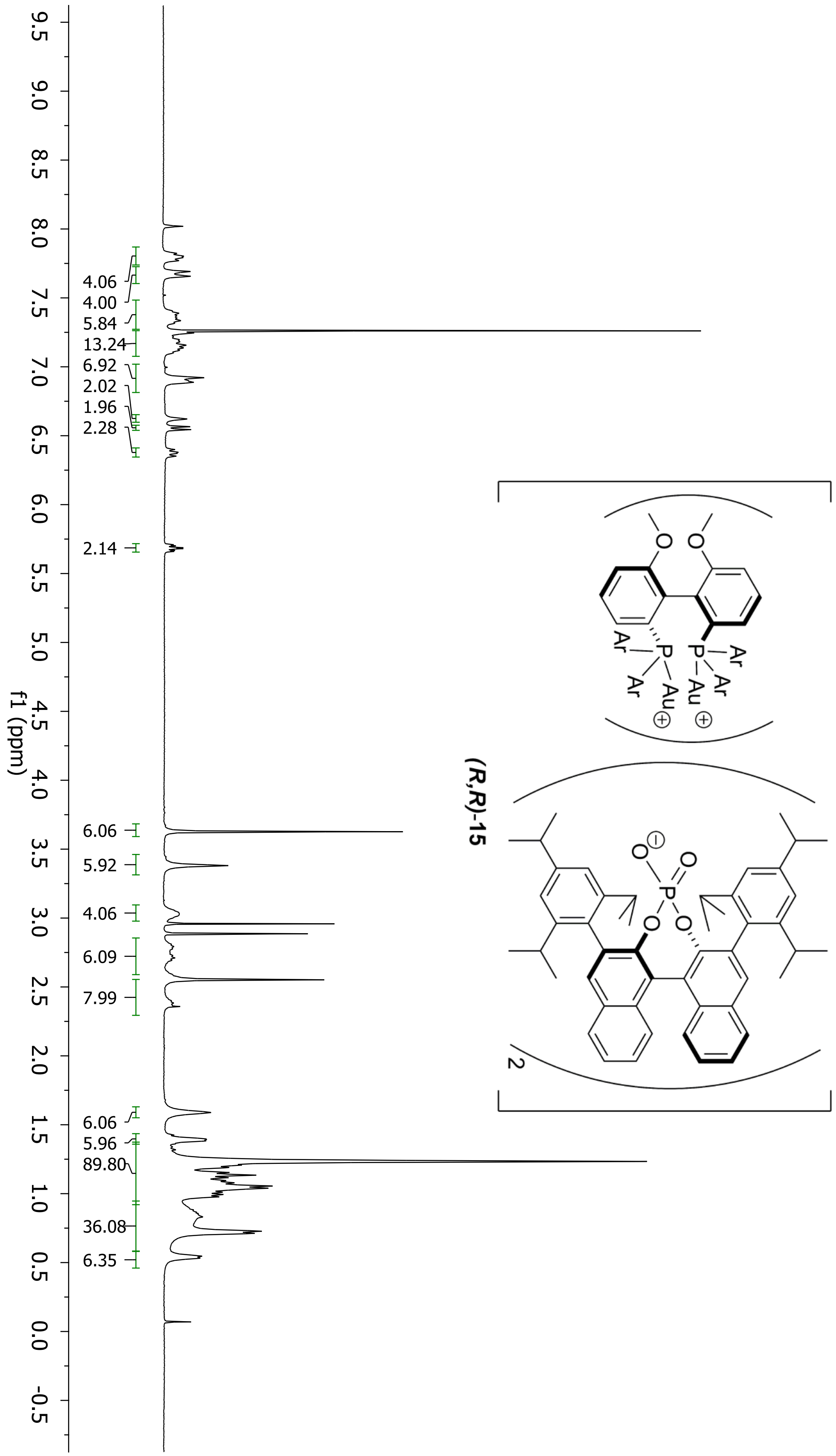


26.32
f1 (ppm)
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110
O
O
P
P
AuCl
AuCl

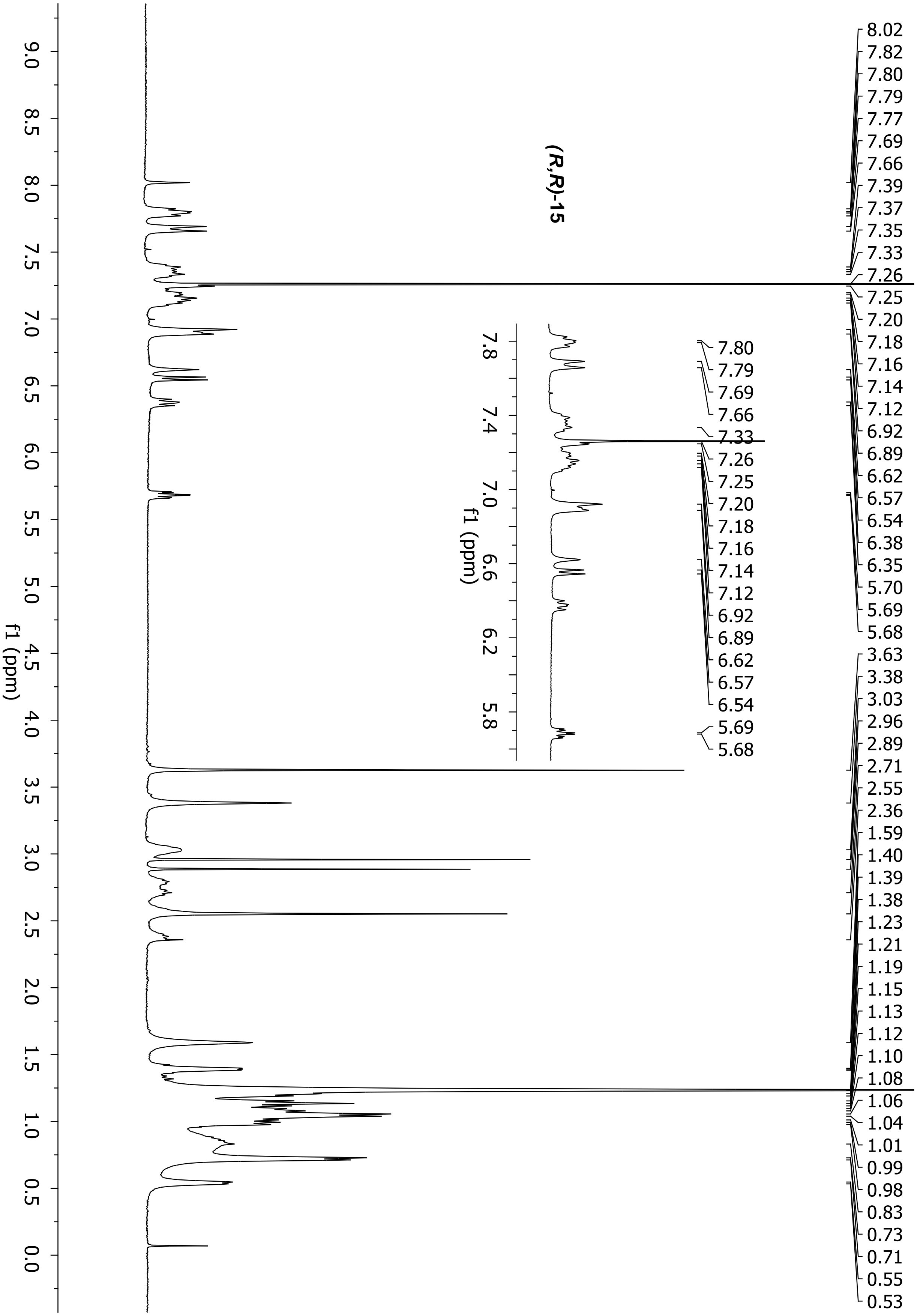

7.56
7.56
7.54
7.54
7.52
7.52
7.26
7.14
7.12
7.10
7.09
7.08
7.07
6.91
6.89
2.97
2.82
2.79
2.24
2.23
2.09
9.75
1.99
5.57
24.55
24.00
AuCl
AuCl
f1 (ppm)

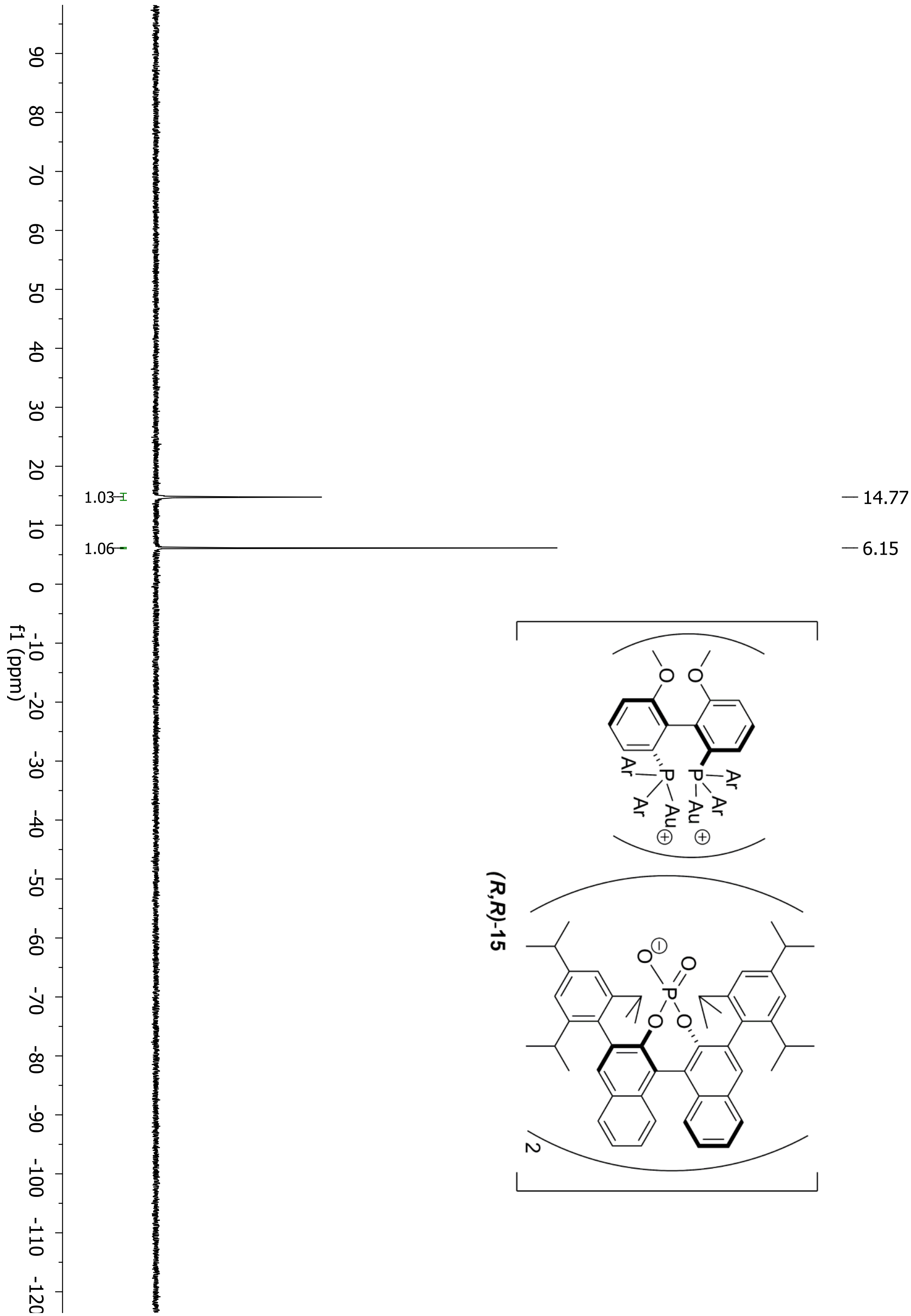


20.07
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
f1 (ppm)
O
O
N
N
N
N
P
P
AuCl
AuCl


f1 (ppm)
4.06
4.00
5.84
13.24
6.92
2.02
1.96
2.28
2.14
6.06
5.92
4.06
6.09
7.99
6.06
5.96
89.80
36.08
6.35
Ar
P
Au
O
2

(R,R)-15


(R,R)-15
f1 (ppm)
8.02 7.82 7.80 7.79 7.77 7.69 7.66 7.39 7.37 7.35 7.33 7.26 7.25 7.20 7.18 7.16 7.14 7.12 6.92 6.89 6.62 6.57 6.54 6.38 6.35 5.70 5.69 5.68 3.63 3.38 3.03 2.96 2.89 2.71 2.55 2.36 1.59 1.40 1.39 1.38 1.23 1.21 1.19 1.15 1.13 1.12 1.10 1.08 1.06 1.04 1.01 0.99 0.98 0.83 0.73 0.71 0.55 0.53
7.80 7.79 7.69 7.66 7.33 7.26 7.25 7.20 7.18 7.16 7.14 7.12 6.92 6.89 6.62 6.57 6.54 5.69 5.68


14.77
6.15
1.03
1.06
f1 (ppm)
(R,R)-15
Ar
Au
O
P
2

SECTION II. COMPUTATIONAL DETAILS

Part 1. Computational Results

Theoretical Methods. For molecules with no gold, complete geometry optimizations were carried out using density functional theory (DFT) methods using the B3LYP/6-311G(d,p),[1] M06/6-31+G(d,p), and M06/6-311+G(d,p) levels.[2] For organogold compounds, calculations were carried out using the B3LYP and PBE1PBE methods and the M06 method, shown to be optimal for metals.[2] The basis sets used for gold species were the LANL2DZ, LANL2TZ(f), SDD,[3,4] and aug-cc-pVXZ-PP[4,5] effective-core potentials. M06/6-31+G(d,p)(C,H,O,P)/SDD(Au) level geometry optimizations and frequency calculations were carried out in order to verify that the stationary points thus obtained were true minima and to determine thermodynamic parameters for the determination of reaction energetics. M06 single-point calculations were done with the 6-311+G(d,p)(C,H,O,P)/ LANL2TZ(f)(Au), aug-cc-pVDZ-PP, and aug-cc-pVTZ-PP basis sets using M06/6-31+G(d,p)(C,H,P)/SDD(Au) geometries. All M06 calculations were done with the Gaussian 'int=ultrafine' option. For non-gold species, 6-31 basis sets were used with the 5d option when energies are compared with calculations using 6-31 basis sets and effective-core potentials with gold species.

Thermochemical data were calculated with zero-point energy corrections from scaled M06 frequencies using a scaling factor of 0.99 for zero-point energies.[6] A scaling factor of 1.00 for M06 frequencies for the thermal and entropy terms was used.[6ab] The quasiharmonic approximation was used for low frequencies to calculate entropies to avoid the large distortions found when many low-frequency vibrations are present in organometallic compounds.[6c] Thus, frequencies below 100 cm-1 were rounded up to 100 cm-1 in calculating entropies. Intrinsic reaction coordinate (IRC) calculations[7] were carried out on transition-state structures to assure that the calculated transition states lead to the expected products and starting materials.

To establish confidence in the computational methods employed here in the analysis of the energies of organogold compounds, we have calculated energies at a variety of theoretical levels on smaller molecules to try to estimate the limits of accuracy of the methods used using CCSD(T)-F12 methods with aug-PVXZ-PP basis sets, which have been shown to agree well with experiment for gold, silver and copper.[8] These results show generally good agreement for the DFT methods and basis sets employed. We have chosen a polarized continuum model in ether solvent for our calculations using the SMD method of Truhlar and Cramer.[9] Solvent effects by similar methods have been treated successfully for cases where quantitative comparison with experiment is possible.[10] Preliminary Born-Oppenheimer molecular dynamics (BOMD) calculations[11] were carried out at the B3LYP/6-31G(d)/SDD(Au) level to compute reaction trajectories. BOMD calculations were used for these organonometallic compounds, since they could be done with larger step sizes(2500) than the, normally more efficient, atom-centered density matrix propagation molecular dynamics (ADMP) calculations.[12] All calculations were performed using the Gaussian 09 program suites.[13]

Theoretical Results. The mechanism by which these gold-catalyzed reactions might proceed has been investigated using DFT calculations with a PH3 ligand with the carboxylic acid precursor to product **19**, but without the phenyl substituents. Figure S1 shows two reaction mechanisms that have been considered with the terminal cyclopentano substituent. (1) One mechanism involves a strongly exothermic complexation of PH_3Au+ with the allene carboxylic acid to form **SM+** in Figure S1 followed by attack of the carboxylic acid oxygen at an allenic carbon. This reaction can occur with four regioisomeric outcomes, the most favorable experimentally being the 5-exo-trig attack to form **5-exo-trig prodH$^+$**. This intermediate may then undergo protodeauration via **5-exo-trig prod** to eventually form the final five-membered ring lactone product. The other regioisomeric products studied are also shown in Figure S1. (2) The alternative mechanism studied was one in which the carboxylic acid group is deprotonated before attack on the gold-allene moiety via **SM**, which results in direct formation of **5-exo-trig prod**, which could then undergo protodeauration, similar mechanisms can lead to the other three regioisomers, but are not shown in Figure S1.

Relative free energies of reaction and transition-state free energies in the gas phase and in solvent from quantum calculations are reported for the numerous reactions in Tables S1 and S2 for the cyclopentano substituent and Tables S3 and S4 without that substituent. Figure S2 shows structures of the transition states and intermediates. Thermochemical data and structures are reported for selected compounds in Table S5.

Table S1 contains differences in free energies for reactions of cyclopentano-4,5-hexadienoic acid with PH_3Au^+ at the M06/6-31+G(d,p)/SDD(Au) level in the gas phase and in chloroform and at the PBE1PBE/6-31+G(d,p)/SDD(Au)/SMD(toluene) level with geometries optimized with toluene solvent. These results show that the formation of **5-exo-trig prodH$^+$** and its regioisomers was endoergonic in all cases, with free-energy barriers slightly larger than the endoergonicity. The **5-exo-trig prodH$^+$** intermediate appeared not to be at a minimum in the gas-phase calculations, but was found in toluene solution calculations. The 5-exo-trig and 6-endo-dig products are favored thermodynamically in toluene. Solvation is expected to play a very large role for these ionic species, generally favoring smaller ions with high charge density such as PH_3Au^+.[14] This effect is seen clearly in the effect of solvent on the free energy of the complexation reaction of PH_3Au^+ with the allene carboxylic acid in Table S1. Similarly the **SM+** appears to have a somewhat higher charge density than the ring-closing products like **6-endo-dig prodH$^+$**, with correspondingly smaller solvation effects in Table S1 (and Table S3). It is not certain what polarity to expect for the medium in the interior of the micelles containing these gold complexes. Some experiments to probe this issue were carried out with the commercially available 2,6-di-t-butyl-4(2,4,6-triphenyl-1-pyridino) phenolate E_T dye[15] dissolved in the TPGS-750-M micelle used in this work. These experiments gave an E_T value similar to n-propanol. This is more polar than we would expect for the hydrophobic region of the micelle. Despite the t-butyl groups encumbering the phenoxy anion end of the dye, it appears that the phenoxy group is attracted to the polar interface of the micelle by hydrogen bonding to water in that region as seen to a greater extent for the less encumbered 2,6-di-t-butyl-4(2,4,6-triphenyl-1-pyridino) phenolate $E_T(30)$ dye.[16] It is likely that toluene solvent best mimics the micellar environment of our gold complexes, but comparing data in different solvents shows that the trends in relative reaction energies in Tables S1 and S2 are similar in all solvents tried.

Results of calculations on reactions without the cyclopentano substituent in Table S3 are rather similar to those with the ring in Table S1. The most complete set of transition-state energies that we obtained were in toluene solvent at the PBE1PBE/6-31+G(d,p)/SDD(Au)/SMD(toluene) level, showing the lowest energy transition state is for 5-exo-trig product, rather than the 6-exo-dig pathway, as observed experimentally. The other regioisomers have higher, but similar, transition-state energies that run mainly parallel to the order of the product energies. The electronic energies of these reactions at the M06/6-31+G(d,p))/SDD(Au) and PBE1PBE/6-31+G(d,p)/SDD(Au) levels compare closely with M06/aug-cc-pVTZ-PP calculations using a much larger basis set in Table S3.

Concern that the calculated reaction paths did not clearly fit experiment and the fact that transition-state energies were similar and in a potentially flat energy surface, led us to consider the possibility that these reactions might be complicated by bifurcation mechanisms. We and others have seen such mechanisms in similar situations in gold chemistry.[17] This idea was tested by doing preliminary BOMD trajectory calculations in toluene at the PBE1PBE/6-31+G(d,p)(C,H,O,P)/SDD(Au)/SMD level starting from the optimized **5-exo-trig TSH$^+$** (100 trajectories) and **6-endo-dig TSH$^+$** (50 trajectories) structures with the cyclopentano substituent. The **5-exo-trig TSH$^+$** trajectories all led back to **SM+** or it's slightly more stable Au-slipped allylic cation isomer.[18] The **6-endo-dig TSH$^+$** trajectories led primarily again to **SM+** and 10% of **6-endo-dig prodH$^+$**. No crossover to 5-membered products that would suggest a bifurcation have been seen thus far. Another concern in probing the preference for 5-membered ring lactones, as well as the stereochemical selectivity, found experimentally for these reactions is whether protodeauration might be the rate-limiting, and product-determining, step in these reactions. Experimental evidence for such a mechanism has been found by Widenhoefer[19] for allenic alcohols. Experimental[20] and computatuional[21] studies of the protodeauration reaction does not offer a clear general answer to whether it would be rate determining for other reactions.

Experiments with small amounts(0.10 equiv.) of added base, triethylamine or tetrabutylammonium hydroxide, in our reactions led, in fact, to accelerated reaction rates which does not appear to be consistent with a rate-determining protodeauration. In light of these experiments, we considered the possibility that the reaction mechanisms might proceed through a deprotonated carboxylic acid **SM** in Figure S1. While the rate acceleration certainly implicates a carboxylate intermediate **SM**, it is difficult, theoretically, to ascertain the thermodynamics of such a deprotonation step within the micelle. Determining the magnitudes of solvent effects and ion-paring effects in the micelle is problematic. We did, however, estimate the energy required for this deprotonation step within the micelle with triethylamine as base using calculated deprotonation energies in both dichloromethane and toluene, which likely spans the polarity range within the micelle. The deprotonation step was estimated at 10-27 kcal/mol uphill in free energy (see Table S2), and we expect that ion-pairing effects would lower the reaction energy to make this a quite feasible reaction pathway.

In Table S2, we see calculations showing that the 5-exo-trig and 6-endo-dig products from this reaction in base are the most stable of the four possible regioisomers in three different solvents. For the allene without a cyclpentano substituent, the calculations showed some complications with the 6-exo-dig product favored thermodynamically in the gas–phase and solution. At some levels of theory, low-barrier transition states in dichloromethane could be found for some product-forming reactions from the extended conformation of the starting carboxylate, but in toluene these transition states were barely higher in energy than the starting conformation. The significance of such transition states is not clear at this point. Calculations in solution showed that there was no minimum that could be detected for the starting material **SM**, unless it was in an extended conformation with the carboxylate ion far from the allene-gold moiety, or in a cyclic form with weak complexation of the carboxylate group to gold (ΔG° = -4.7 kcal/mol in CH_2Cl_2 and -13.3 kcal/mol in toluene, PBE1PBE/6-

31+G(d,p)/SDD(Au)/SMD(toluene)). Whenever the conformation was changed to bring the carboxylate closer in the gas phase, 5-exo-trig and/or 6-endo-dig products were formed without a barrier. This sort of reaction mechanism is akin to ridge-valley inflection bifurcation reactions,[17a] where a conformational change leads to a conformation of the starting material that can then proceed downhill to products with little or no further barrier. This process was modeled with preliminary BOMD trajectories at the B3LYP/6-31G(d)(C,H,O,P)/SDD(Au)/SMD level starting at various conformations of the carboxylate starting material as the carboxylate closely approaches the gold-allene group from the backside in the gas phase and in toluene solution. The trajectories mainly gave **SM** and the 5-exo-trig product, opt=calcall calculations from such conformations similarly favored the 5-exo-trig product. While the selection of starting geometries for the trajectories has been somewhat arbitrary at this point, the results do show that preferred formation of the 5-exo-trig product is conceivable in this sort of mechanism.

In the absence of added base, the deprotonation step would be more difficult and the reaction mechanism might proceed by direct attack of the carboxylic acid carbonyl group on the bridged gold complex, for which we found reasonably small free-energy barriers of less than 20 kcal/mol and predictions of the experimental regiochemistry. Curiously, the addition of triethylamine base seriously lowers the %ee observed in the reaction to the same levels as observed without a chiral counterion. Furthermore, the %ee does not depend upon which enantiomeric form of the counterion is used when base is added. These observations could be understood in terms of a change in mechanism, wherein we might expect the counterion to be less tightly bound to gold after deprotonation.

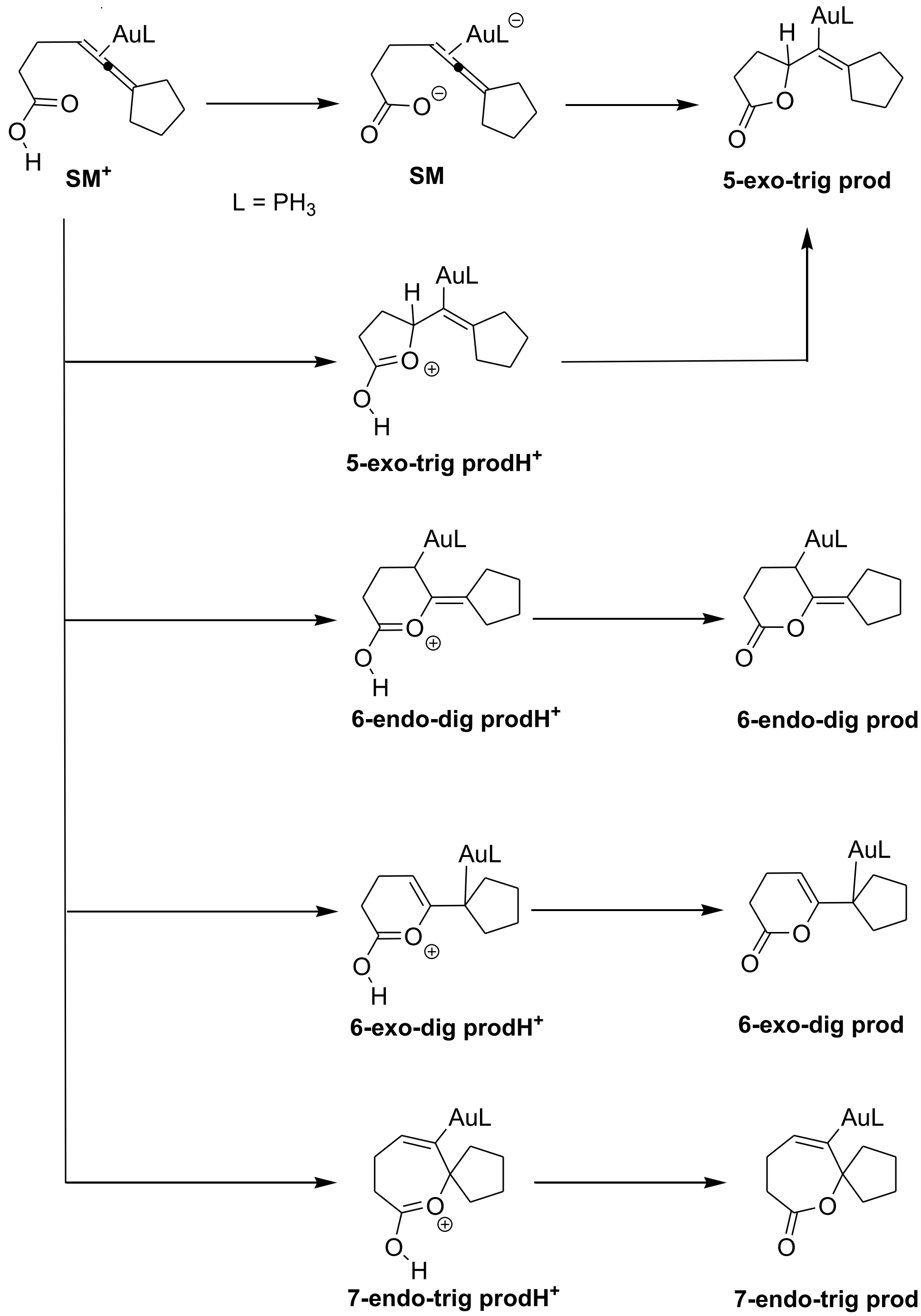


Fig S1. Possible reaction pathways.

Table S1. Relative free energies of transition states and products in the reaction of 6,6-cyclopentano-4,5-hexadienoic acid with PH_3Au^+ from quantum calculations at 298K at M06/6-31+G(d,p)/SDD(Au) level and at PBE1PBE/6-31+G(d,p)/SDD(Au)/SMD(toluene) level. (All values in kcal/mol).

	M06/6-31+G(d,p)/SDD(Au)[a,b]		PBE1PBE/6-31+G(d,p)/SDD(Au)/SMD SMD geom[c]
Structure:	$\Delta G^o_{g,298}$	ΔG^o_{CHCl3}	ΔG^o_{tol}
Au complexation to allene to form **SM⁺**	-42.72	-18.28	
allene-gold complex, **SM⁺**	0.00	0.00	0.00
5-exo-trig TSH⁺			12.89
6-endo-dig TSH⁺	11.71	16.87	14.28
6-exo-dig TSH⁺	21.85	25.86	23.54
7-endo-trig TSH⁺	12.81		
5-exo-trig prodH⁺			13.17
6-endo-dig prodH⁺	9.95	14.87	10.69
6-exo-dig prodH⁺	21.99	25.25	22.60
7-endo-trig prodH⁺	12.70	17.04	18.31

a) Geometry optimized at the M06/6-31+G(d,p)/SDD(Au) level.
b) Solvation energy term from the difference in free energies of solvation from SMD model at M06/6-31+G(d,p)/SDD(Au) level in chloroform. (Ref. 9)
c) Geometry optimized at PBE1PBE/6-31+G(d,p)/SDD(Au)/SMD(toluene) level.

Table S2. Relative free energies of starting material and products in the reaction of 6,6-cyclopentano-4,5-hexadienoate with PH_3Au^+ from quantum calculations at 298K at M06/6-31+G(d,p)/SDD(Au) level and at PBE1PBE/6-31+G(d,p)/SDD(Au)/SMD(toluene) level. (All values in kcal/mol).

	M06/6-31+G(d,p)/SDD(Au)[a,b]			PBE1PBE/6-31+G(d,p)/SDD(Au)/SMD at SMD geom in CH_2Cl_2 (in toluene)[c]
Structure:	$\Delta G^o_{g,298}$	ΔG^o_{CHCl3}	ΔG^o_{tol}	ΔG^o_{CH2Cl2}
extended allene-gold complex, **SM**	0.00	0.00	0.00	0.00 (0.0)
5-exo-trig prod	-56.89	-24.90	-36.18	-22.12 (-34.61)
6-endo-dig prod	-58.13	-24.99	-36.85	-21.85 (-35.19)
6-exo-dig prod	-53.69	-20.07	-31.85	-16.00 (-29.33)
7-endo-trig prod	-51.23	-18.87	-30.07	-13.89 (26.28)
SM$^+$ + Et_3N to **SM** + Et_3NH^+ (deprotonation step, see Figure S1)	58.25	15.58	29.30	10.2 (27.0)

a) Geometry optimized at the M06/6-31+G(d,p)/SDD(Au) level.
b) Free energies in solution combine the gas-phase free energies and the SMD free energies of solvation computed with gas-phase geometries at M06/6-31+G(d,p)/SDD(Au) level in chloroform and toluene. (Ref. 9).
c) Geometry optimized at PBE1PBE/6-31+G(d,p)/SDD(Au)/SMD(CH_2Cl_2) and PBE1PBE/6-31+G(d,p)/SDD(Au)/SMD(toluene) levels.

Table S3. Relative free energies and electronic energies of transition states and products in the reaction of 4,5-hexadienoic acid with PH_3Au^+ from quantum calculations at 298K at M06/6-31+G(d,p)/SDD(Au) level. (All values in kcal/mol).[a]

	M06/6-31+G(d,p)/SDD(Au)[b]			M06/ ATZ-PP[c]
Structure:	$\Delta G^o_{g,298}$	ΔG^o_{THF}	ΔE^o_e	ΔE^o_e
Au complexation to allene to form **SM**$^+$	-38.15			
allene-gold complex, **SM**$^+$	0.00	0.00	0.00	0.00
5-exo-trig TSH$^+$	9.98	14.04	8.50	9.21
6-endo-dig TSH$^+$	10.92	16.97	9.62	10.87
6-exo-dig TSH$^+$	7.41	13.23	6.43	7.41
7-endo-trig TSH$^+$	13.02	17.92	11.11	12.13
5-exo-trig prodH$^+$	10.56	13.82	7.81	8.12
6-endo-dig prodH$^+$	8.57	14.48	5.81	6.51
6-exo-dig prodH$^+$	6.38	11.34	4.23	4.59
7-endo-trig prodH$^+$	12.70	16.95	9.33	9.87

a) Geometries all optimized at the M06/6-31+G(d,p)/SDD(Au) level.
b) Solvation energy terms from the difference in free energies of solvation from SMD model at M06/6-31+G(d,p)/SDD(Au) level in tetrahydrofuran. (Ref. 9)
c) Electronic energy at M06/aug-cc-PVTZ-PP level (effective core potential on Au).

Table S4. Relative free energies of transition states and products in the reaction of 4,5-hexadienoate with PH_3Au^+ from quantum calculations at 298K at M06/6-31+G(d,p)/SDD(Au) level and at PBE1PBE/6-31+G(d,p)/SDD(Au)/SMD(CH2Cl2) level. (All values in kcal/mol).

	M06/6-31+G(d,p)/SDD(Au)[a,b]		PBE1PBE/6-31+G(d,p)/SDD(Au)/SMD SMD geom[c]
Structure:	$\Delta G^o_{g,298}$	ΔG^o_{CHCl3}	ΔG^o_{CH2Cl2}
allene-gold complex, **SM**	0.00	0.00	0.00
5-exo-trig TS			
6-endo-dig TS	-0.77		6.0
6-exo-dig TS	-1.53		2.9
7-endo-trig TS	-0.7		5.7
5-exo-trig prod	-50.75	-20.38	
6-endo-dig prod	-49.17	-17.75	-22.6
6-exo-dig prod	-53.84	-11.11	
7-endo-trig prod	-43.71	-13.57	-19.8

a) Geometry optimized at the M06/6-31+G(d,p)/SDD(Au) level.
b) Solvation energy terms from the difference in free energies of solvation from SMD model at M06/6-31+G(d,p)/SDD(Au) level in chloroform. (Ref. 9)
c) Geometry optimized at PBE1PBE/6-31+G(d,p)/SDD(Au)/SMD(CH2Cl2) level.

Acknowledgments. We are pleased to acknowledge support from the Center for Scientific Computing at the CNSI and MRL: an NSF MRSEC (DMR-1121053) and NSF CNS-0960316. We also acknowledge NSF support from the National Center for Supercomputing Applications (NSF TG-CHE100123) utilizing the NCSA Gordon and Blacklight systems, and the use of software for 3-D drawings from CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org).

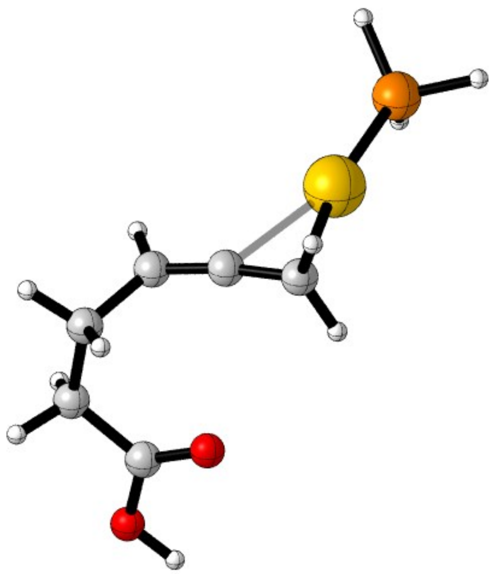
Part 2. References:

[1] A. D. Becke *J. Chem. Phys*. **1993**, *98*, 5648.
[2] Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215-241.
[3] P. J. Hay and W. R. Wadt, *J. Chem. Phys*. **1985**, *82*, 299.
[4] From EMSL Library of Basis Set Exchange: Schuchardt, K.L., Didier, B.T., Elsethagen, T., Sun, L., Gurumoorthi, V., Chase, J., Li, J., and Windus, T.L. *J. Chem. Inf. Model*. **2007**, *47*, 1045-1052.
[5] K.A. Peterson and C. Puzzarini, *Theor. Chem. Acc*., **2005**, *114*, 283.
[6] (a) A. P. Scott, L. Radom *J. Phys. Chem*. **1996**, *100*, 16502. (b) Alecu, I. M.; Zheng, J.; Zhao, Y. and Truhlar, D. G. *J. Chem. Theory Comput.* **2010,** *6,* 2872–2887. (c) Raphael F. Ribeiro, Aleksandr V. Marenich, Christopher J. Cramer,* and Donald G. Truhlar *J. Phys. Chem*. *A* **2011**, *115*, 14556-14562. (d) D. H. Aue, to be published. We have evaluated optimum scale factors for experimental fundamental frequencies for numerous organic molecules and find that the DFT scale factors differ with basis set between 0.96 for the B3LYP/6-31G(d) and M06-2X/ 6-311+G(d,p) levels to 0.97 for the B3LYP/ 6-311G(d,p) level. For thermal terms and entropies, such variation has little effect, and one may argue that a scaling factor close to 1.00 might be best for the dominant low frequencies (we get 1.005 for 111 frequencies below 150 cm^{-1})(see also ref. 6a). For zero point energies, the 0.99 scale factor fits experimental zero-point energies for organic molecules reasonably well.
[7] C. Gonzalez, H. B. Schlegel *J. Phys. Chem.* **1990**, *94*, 5523.
[8] Hill, J. G.; Peterson, K. A. *J. Chem. Theory Comput*. **2012**, *8*, 518−526.
[9] A. V. Marenich, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378-96.
[10] a) K. S. Raymond, A. K. Grafton, R. A. Wheeler, *J. Phys. Chem. B* **1997**, *101*, 623 (and references therein); b) M. Namazian, P. Norouzi, *J. Electroanal. Chem*. **2004**, *573*, 49.
[11] Li, X.; Millam, J. M.; Schlegel, H. B. *J. Chem. Phys.* **2000**, *113*, 10062-67.
[12] H. B. Schlegel, S. S. Iyengar, X. Li, J. M. Millam, G. A. Voth, G. E. Scuseria, and M. J. Frisch, *J. Chem. Phys.* **2002**, *117*, 8694-704.
[13] Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

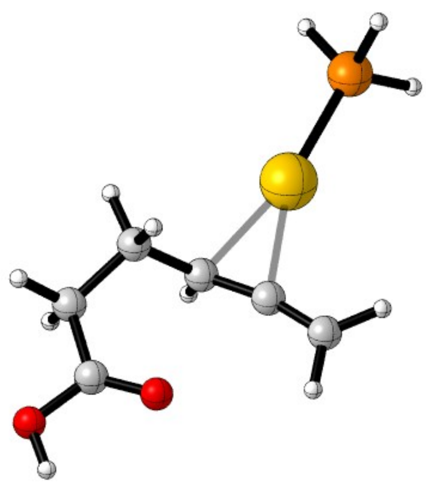
[14] (a) D. H. Aue, H. M. Webb, and M. T. Bowers, *J. Am. Chem. Soc*. **1976**, *98*, 318. (b) H. P. Hopkins Jr., D. V. Jahagirdar, S. P. Moulik, D. H. Aue, H. M. Webb, W. R. Davidson, and M. D. Pedley, *J. Am. Chem. Soc*. **1984**, *106*, 4341. (c) D. H. Aue, H. M. Webb, W. R. Davidson, P. Toure, H. P. Hopkins, Jr., S. P. Moulik, and D. V. Jahagirdar, *J. Am. Chem. Soc*. **1991**, *113*, 1770.
[15] Reichardt, C. *Chem. Rev*. **1994**, *94,* 2319-2358.
[16] Das, P. K.; Pramanik, R.; Bagchi, S. *Spectrochimica Acta A* **2003**, *59*, 1681-1688.
[17] (a) Ye, L.; Wang, Y.; Aue, D. H.; Zhang, L. *J. Am. Chem. Soc.* **2012**, *134,* 31-34. (b) Lu, B.; Li, Y.; Wang, Y.; Aue, D. H.; Luo, Y.; Zhang, L. *J. Am. Chem. Soc.* **2012**, *135,* 8512-8524. (c) Wang, Y.; Yepremyan, A.; Ghorai, S.; Todd, R.; Aue, D. H.; Zhang, L. *Angew. Chem., Int. Ed*. **2013**, *52*, 7795-7799**.**
[18] "Computational Mechanisms of Au and Pt Catalyzed Reactions", *Topics in Current Chemistry* **2011** Soriano, E; Marco-Contelles, J., Eds., Springer, Berlin.
[19] Brown, T. J.; Weber, D.; Gagné, M. R.; Widenhoefer, R. A. J. *Am. Chem. Soc*. **2012**, *134*, 9134−9137.
[20] Roth, K. E.; Blum, S. A. *Organometallics* **2010**, *29*, 1712–1716.
[21] (a) Dudnik, A. S.; Xia, Y.; Li, Y.; Gevorgyan, V. *J. Am. Chem. Soc*. **2010**, *132*, 7645–7655. (b) LaLonde, R. L.; Brenzovich, W. E. Jr.; Benitez, D.; Tkatchouk, E.;Kelley, K.; Goddard, W. A. III; Toste, F. D. *Chem. Sci*., **2010**, *1*, 226–233.

Part 3. Drawings of some structures

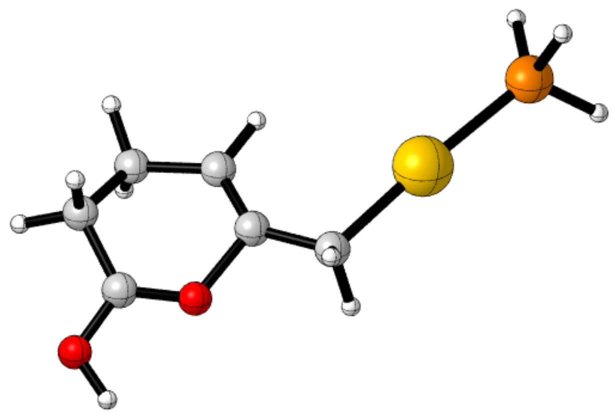
Figure S2. Structures of some intermediates and transition states.



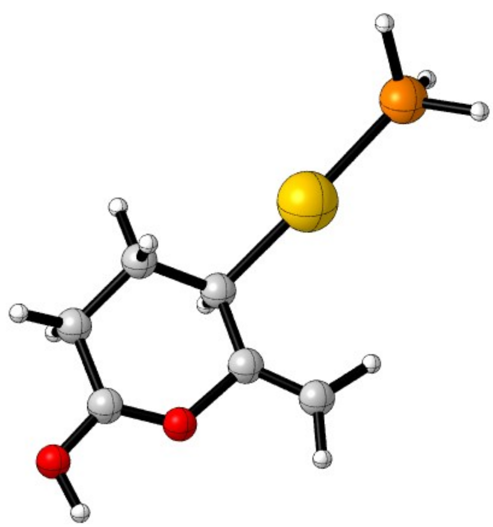
5,6-complex of PH3Au hexa-4,5-dienoic acid



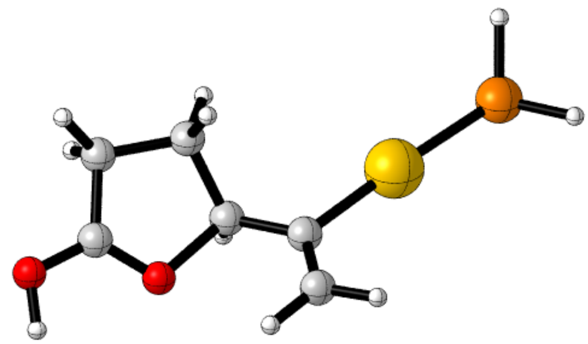
4,5-complex of PH3Au hexa-4,5-dienoic acid



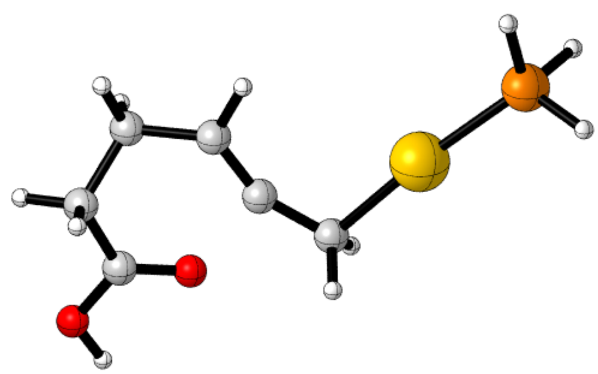
5,6-PH3Au complex of hexa-4,5-dienoic acid 6-exo-dig-ring closure product



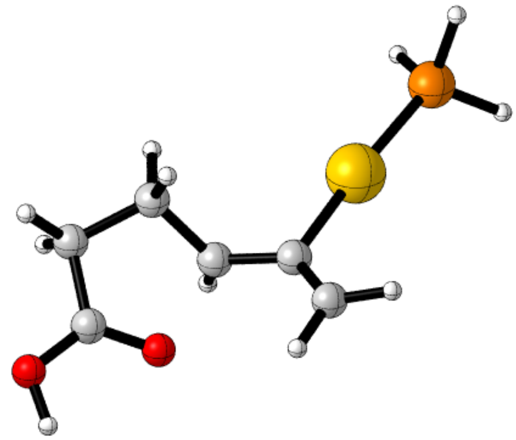
4,5-PH3Au complex of hexa-4,5-dienoic acid 6-endo-dig-ring closure product



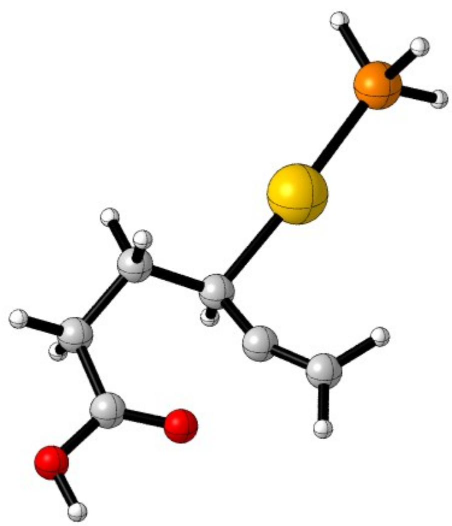
4,5-PH3Au complex of hexa-4,5-dienoic acid 5-exo-trig-ring closure product



5,6-PH3Au complex of hexa-4,5-dienoic acid - 6-exo-dig-6-ring closure TS (-161.5 cm-1)



4,5-PH3Au complex of hexa-4,5-dienoic acid - 6-exo-trig-5-ring closure TS (-120.7 cm-1)



4,5-PH3Au complex of hexa-4,5-dienoic acid - 6-endo-dig-6-ring closure TS (-238.6 cm-1)

Part 4. Calculated geometries, thermochemical data, and vibrational frequencies

Table S5. Calculated geometries, thermochemical data, and vibrational frequencies.

SM for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid carboxylate:

Processing aupcphexdienoat5sm26psd1pbedcms.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-1017.4850081

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
149.83848	160.832	145.783	133.765	160.895	43.821	34.015

30

C	4.463068	-1.087985	0.511794
C	3.118896	-0.352773	0.595454
C	2.149606	-1.277045	-0.116531
C	2.826889	-2.618640	-0.365245
C	4.068051	-2.565699	0.532629
C	0.913462	-1.019947	-0.484066
C	-0.358310	-1.119318	-0.944612
C	-1.501684	-1.748135	-0.186068
C	-2.831006	-1.011546	-0.358951
C	-3.957713	-1.742756	0.399031
O	-4.668460	-2.535223	-0.272649
Au	0.005725	1.008074	-0.200733
P	-0.261039	3.227495	0.403721
O	-4.045474	-1.499745	1.631854
H	-0.885002	4.056859	-0.543125
H	-1.024885	3.464966	1.558396
H	0.921751	3.934407	0.679357
H	-0.537339	-0.919923	-2.006234
H	-1.243945	-1.837120	0.873622
H	-1.600717	-2.769053	-0.584831
H	-3.077146	-0.947819	-1.425145
H	-2.727547	0.007337	0.035842
H	2.164617	-3.465601	-0.164784
H	3.125331	-2.673860	-1.420634
H	3.136323	0.650179	0.158539
H	2.806151	-0.249757	1.643026
H	3.803252	-2.867063	1.553964
H	4.863718	-3.230776	0.182957
H	4.960771	-0.849970	-0.436787

H 5.141932 -0.810236 1.323683

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3144.0345	47.7292	253.2427	0.7463	0.8547	27.6112
A	3140.5554	38.8702	114.8955	0.4245	0.5960	
A	3140.2794	1.8068	210.2876	0.6876	0.8149	
A	3135.1224	39.2262	324.9062	0.2762	0.4329	
A	3132.6344	23.0715	298.7865	0.1643	0.2822	
A	3129.2874	11.7770	251.2478	0.2830	0.4412	
A	3112.4145	31.4808	293.4904	0.6730	0.8045	
A	3074.5815	54.9711	89.7868	0.5989	0.7491	
A	3071.2966	38.5918	319.4854	0.1244	0.2214	
A	3067.6557	3.3316	587.4611	0.0543	0.1030	
A	3065.6411	28.5672	203.5770	0.1607	0.2769	
A	3056.3776	57.0605	82.3918	0.0668	0.1252	
A	3046.0464	3.1439	723.4130	0.1268	0.2250	
A	2562.5348	0.2078	312.9224	0.7445	0.8535	
A	2560.5468	0.2929	314.5700	0.7425	0.8522	
A	2539.2924	11.2046	896.7178	0.0189	0.0371	
A	1964.8742	29.3198	81.5214	0.5611	0.7188	
A	1666.2646	987.2766	25.5582	0.5959	0.7468	
A	1489.5556	0.3886	2.9416	0.7458	0.8544	
A	1475.3138	8.5691	28.0912	0.7475	0.8555	
A	1471.1298	45.5524	17.2829	0.4729	0.6422	
A	1452.9033	10.7020	30.1714	0.6942	0.8195	
A	1449.5159	12.4493	8.7346	0.7157	0.8343	
A	1446.4868	25.0112	37.3552	0.6924	0.8183	
A	1432.5168	63.2409	38.8078	0.2072	0.3433	
A	1416.3718	376.5706	41.4359	0.7433	0.8528	
A	1350.0770	6.9972	2.7039	0.7339	0.8465	
A	1341.3399	2.2004	6.4179	0.2157	0.3548	
A	1331.3565	1.8322	4.8394	0.7406	0.8510	
A	1323.8598	4.1222	27.5291	0.6173	0.7633	
A	1296.2376	2.0431	6.9921	0.7120	0.8318	
A	1285.1179	8.5705	26.0429	0.4860	0.6541	
A	1252.3025	3.2297	25.1427	0.7108	0.8310	
A	1240.3418	8.3200	8.1795	0.3171	0.4815	
A	1233.1649	6.7354	7.3467	0.7342	0.8467	
A	1228.3055	9.1323	57.1371	0.1454	0.2539	
A	1169.3614	10.0746	8.5716	0.4927	0.6602	
A	1167.8889	3.9473	2.4576	0.6365	0.7779	
A	1145.2247	1.9626	2.1039	0.3667	0.5366	
A	1142.7224	1.0464	24.4544	0.4447	0.6156	
A	1115.1978	9.1382	38.2285	0.7477	0.8556	
A	1114.0927	9.0867	42.5666	0.7468	0.8550	
A	1068.4439	5.0393	5.9009	0.5426	0.7035	

A	1064.1796	8.5168	20.0424	0.2854	0.4441
A	1042.4007	4.7982	28.9614	0.6881	0.8152
A	1033.4355	5.4610	13.8667	0.2549	0.4062
A	991.9707	26.8381	16.9489	0.5502	0.7099
A	974.4935	226.8749	29.3539	0.7471	0.8552
A	970.4028	11.4723	3.4266	0.7433	0.8527
A	928.6320	10.8509	34.7065	0.0539	0.1023
A	927.4547	46.6606	35.1068	0.2192	0.3596
A	917.3651	1.3294	2.2516	0.6902	0.8167
A	890.9760	26.6162	15.6479	0.7358	0.8478
A	876.3082	4.7533	3.5753	0.4864	0.6545
A	847.8483	8.6112	32.0790	0.1756	0.2988
A	782.8250	7.6437	6.3016	0.0856	0.1577
A	769.7159	10.9080	8.4757	0.4790	0.6477
A	719.5607	15.5426	14.3994	0.0935	0.1710
A	664.3594	44.7681	3.0339	0.6946	0.8198
A	584.8911	6.9557	7.1549	0.5160	0.6808
A	565.3080	12.1213	5.7435	0.6857	0.8136
A	552.7341	40.5186	22.0946	0.4357	0.6070
A	499.5909	1.4026	1.7293	0.7500	0.8571
A	484.6605	0.6203	0.8226	0.7476	0.8556
A	477.3253	0.9179	15.4290	0.3361	0.5031
A	457.2664	1.7914	2.4498	0.6924	0.8183
A	396.4475	7.5428	8.7516	0.5619	0.7195
A	371.6554	17.5142	39.5445	0.2727	0.4285
A	308.6586	6.5045	11.6048	0.3455	0.5135
A	262.8628	0.3448	2.7242	0.3976	0.5690
A	237.4039	17.8842	7.4596	0.7500	0.8571
A	199.5231	7.8977	2.1256	0.4105	0.5821
A	183.8538	8.8521	4.7187	0.4669	0.6365
A	166.7698	3.5910	9.4917	0.5016	0.6681
A	102.6262	5.9004	1.4906	0.7348	0.8471
A	91.9598	0.0609	0.0210	0.6731	0.8046
A	88.7824	1.3852	0.7894	0.4194	0.5909
A	78.5907	1.6220	0.8819	0.6617	0.7964
A	65.0798	2.7442	3.5392	0.7488	0.8564
A	58.8202	3.2346	0.9237	0.6611	0.7960
A	43.9501	16.6392	1.3633	0.7190	0.8365
A	35.8227	9.2033	1.9025	0.7479	0.8558
A	28.2244	3.6856	3.6376	0.7405	0.8509
A	20.5361	1.0803	0.9494	0.7492	0.8566

5-exo-trig prod for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid carboxylate:

Processing aupcphexdienoat5prod6psdm6.log

PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-1017.8854422

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
150.42131	160.671	137.449	128.374	160.720	43.821	33.781

30

C	1.066144	1.362538	0.004219
C	0.545418	0.130332	-0.127553
Au	-1.494717	-0.194573	-0.057197
P	-3.853012	-0.574948	0.006143
C	1.364971	-1.120516	-0.236500
C	1.690615	-1.783106	1.107766
C	2.972537	-2.536109	0.798789
C	3.605893	-1.701609	-0.294616
O	4.753181	-1.709014	-0.661645
O	2.669256	-0.905704	-0.845808
H	-4.334278	-1.859777	-0.321806
H	-4.558152	-0.388572	1.214106
H	-4.686327	0.184347	-0.842186
C	0.240958	2.627832	0.166667
C	2.533395	1.771397	0.024063
H	0.857018	-1.846486	-0.891981
H	1.865212	-0.999710	1.857676
H	0.864311	-2.407621	1.462558
H	3.667162	-2.659386	1.633511
H	2.776999	-3.534070	0.381861
C	2.525726	3.237545	0.463592
H	3.148057	1.132996	0.670304
H	2.959559	1.673429	-0.984328
C	1.216554	3.770544	-0.112239
H	-0.645352	2.633049	-0.479605
H	-0.119208	2.696551	1.207021
H	2.494414	3.302630	1.561832
H	3.411453	3.789680	0.129123
H	1.322524	3.915824	-1.197564
H	0.901676	4.727232	0.320411

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3136.4032	7.7048	94.7296	0.4832	0.6516	9.7738

A	3117.3616	14.7994	45.9868	0.3345	0.5013
A	3098.9988	42.7392	144.1793	0.6871	0.8145
A	3094.0187	53.5109	173.5717	0.3510	0.5196
A	3088.5066	23.3411	95.4378	0.2786	0.4358
A	3080.8062	23.9358	36.6293	0.2370	0.3832
A	3051.2643	23.3125	22.7852	0.7482	0.8560
A	3047.2641	6.0542	158.7008	0.0673	0.1262
A	3039.9025	15.6879	106.5308	0.0740	0.1377
A	3027.3763	46.9670	58.8713	0.4435	0.6145
A	3018.7409	40.9215	180.7187	0.0933	0.1707
A	3003.2348	24.4149	76.9540	0.1811	0.3067
A	2995.9499	19.8879	92.9868	0.1267	0.2250
A	2496.9926	15.8983	133.9523	0.7498	0.8570
A	2493.6999	19.2593	150.4897	0.6884	0.8154
A	2481.5663	112.7523	701.5440	0.1013	0.1840
A	1887.2468	549.9499	12.9062	0.5336	0.6959
A	1701.2850	19.5040	76.8850	0.2484	0.3980
A	1476.0653	2.0322	0.8996	0.7188	0.8364
A	1462.5573	7.8767	3.2669	0.7465	0.8548
A	1460.4086	7.4250	12.8950	0.7463	0.8547
A	1438.7962	6.4083	4.4556	0.6810	0.8103
A	1432.3242	4.0925	9.5117	0.7478	0.8557
A	1431.3492	8.4038	5.6326	0.6221	0.7671
A	1377.4735	5.0370	8.0978	0.2120	0.3498
A	1344.2934	67.4587	9.1207	0.7493	0.8567
A	1330.9369	4.8725	2.5107	0.3807	0.5515
A	1320.4507	0.2430	3.3396	0.5914	0.7432
A	1310.3757	2.8311	6.6541	0.7378	0.8491
A	1306.3140	97.6906	4.0132	0.4029	0.5744
A	1287.7047	1.4001	4.4878	0.3782	0.5489
A	1285.3600	7.5866	1.5437	0.7349	0.8472
A	1245.8050	13.3275	13.6669	0.5593	0.7174
A	1236.1163	64.5277	10.0418	0.4430	0.6140
A	1228.2478	5.1044	3.4415	0.6859	0.8137
A	1208.2083	152.3642	7.0771	0.3876	0.5586
A	1191.4193	18.2430	15.6444	0.1173	0.2100
A	1179.1773	1.5531	2.7042	0.6207	0.7659
A	1145.8310	45.7867	6.4796	0.0627	0.1180
A	1133.4144	4.5102	14.2783	0.7195	0.8369
A	1131.5480	5.5763	2.9888	0.3994	0.5708
A	1129.6168	3.6445	18.9014	0.7314	0.8449
A	1104.0639	34.6267	19.5583	0.4613	0.6313
A	1069.3880	35.4820	3.6124	0.6380	0.7790
A	1053.8973	35.9169	7.1205	0.3200	0.4848
A	1038.6681	1.4854	11.3457	0.5695	0.7257
A	1016.0689	206.0075	28.8757	0.6741	0.8053
A	1009.2122	7.6951	3.4158	0.7053	0.8272

A	995.7032	11.6190	4.3465	0.3054	0.4679
A	976.3816	15.0356	3.2383	0.3269	0.4927
A	940.2613	73.0472	6.8982	0.2379	0.3844
A	929.3069	0.7489	11.4716	0.0939	0.1717
A	907.7246	0.0429	0.6280	0.4116	0.5831
A	879.0701	0.6502	8.3355	0.1805	0.3058
A	867.4051	0.9805	1.3482	0.7447	0.8537
A	853.0807	1.4889	5.8185	0.2052	0.3406
A	820.2242	2.0656	17.7966	0.1770	0.3007
A	815.1145	7.8736	3.2983	0.3191	0.4838
A	714.0186	11.6075	9.5122	0.1019	0.1849
A	674.4740	13.9963	2.6541	0.4107	0.5823
A	632.5733	0.1384	0.9519	0.7116	0.8315
A	593.3235	1.0574	0.8051	0.7402	0.8507
A	559.6793	1.7798	1.0206	0.4466	0.6174
A	533.4124	5.4244	1.2664	0.4168	0.5884
A	516.6461	7.3849	1.6947	0.7071	0.8284
A	477.5407	5.4509	2.1783	0.2207	0.3615
A	419.6410	0.5918	1.4292	0.4583	0.6286
A	415.6496	0.6675	1.8582	0.4232	0.5948
A	367.7429	9.4461	3.2704	0.1209	0.2157
A	302.5689	1.8502	1.3737	0.7421	0.8519
A	275.1916	0.4504	0.7588	0.1986	0.3314
A	259.7593	1.0341	0.3360	0.7052	0.8271
A	248.9163	0.2689	12.4692	0.1498	0.2606
A	179.6850	1.4170	1.0158	0.6607	0.7957
A	165.7487	4.1847	1.3997	0.2429	0.3909
A	141.2622	2.1604	0.8153	0.5293	0.6922
A	116.6708	0.3499	0.1544	0.3299	0.4962
A	94.8479	0.9207	0.3322	0.6762	0.8069
A	85.2097	0.8820	0.3291	0.6460	0.7850
A	59.7058	5.4680	2.5288	0.7435	0.8529
A	50.0672	2.5529	1.0241	0.7492	0.8566
A	45.3571	0.4082	0.9512	0.6545	0.7912
A	36.9474	0.2374	0.2955	0.6496	0.7876
A	24.6185	2.3291	0.8564	0.7310	0.8446

Processing aupcphexdienoat5prod6psd1pbedcms.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-1017.5249201

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
151.84527	161.953	136.125	127.711	161.999	43.821	33.788

30

C	1.068615	1.425057	0.026758
C	0.559502	0.185884	-0.128686
Au	-1.466071	-0.184392	-0.055899
P	-3.758184	-0.623316	0.006121
C	1.364445	-1.065977	-0.319113
C	1.485796	-1.955622	0.927647
C	2.769796	-2.727171	0.660906
C	3.563383	-1.780043	-0.205732
O	4.749803	-1.814922	-0.460657
O	2.759896	-0.836997	-0.711992
H	-4.171375	-1.946438	-0.242680
H	-4.451066	-0.371380	1.206455
H	-4.584539	0.066319	-0.902406
C	0.215154	2.667875	0.248230
C	2.528706	1.880028	0.004138
H	0.937778	-1.651971	-1.144083
H	1.592053	-1.323408	1.816061
H	0.604545	-2.587702	1.057500
H	3.341467	-3.007000	1.548265
H	2.590958	-3.637504	0.073612
C	2.493962	3.363223	0.397557
H	3.168160	1.284494	0.662311
H	2.939532	1.765565	-1.006654
C	1.131471	3.840706	-0.105801
H	-0.715459	2.640800	-0.327602
H	-0.065636	2.736945	1.310430
H	2.533812	3.463475	1.490641
H	3.335175	3.930897	-0.014794
H	1.163757	3.976097	-1.195465
H	0.810643	4.789087	0.338428

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3169.6904	14.0004	170.9651	0.6911	0.8173	13.0535
A	3163.0937	12.0967	186.7098	0.2623	0.4156	
A	3128.9804	59.4679	239.1762	0.6831	0.8117	
A	3123.0037	60.1669	257.1699	0.7419	0.8518	
A	3117.3049	37.7793	212.0460	0.1738	0.2961	
A	3115.7189	72.9136	413.2311	0.2283	0.3717	
A	3093.8789	27.5400	107.6441	0.1441	0.2519	
A	3084.6000	8.1396	320.7159	0.1015	0.1842	
A	3070.4515	25.4805	317.3280	0.0896	0.1644	

A	3060.8502	27.9147	350.0846	0.1847	0.3118
A	3058.2819	68.7035	88.4271	0.7078	0.8289
A	3056.1714	55.0356	427.6548	0.1165	0.2087
A	3031.1349	32.1430	295.7937	0.1336	0.2357
A	2530.2860	8.3465	319.4453	0.7495	0.8568
A	2529.1045	9.0907	336.7982	0.7481	0.8559
A	2513.9833	63.0994	1162.7460	0.0457	0.0875
A	1825.7553	809.6191	29.4867	0.4443	0.6152
A	1698.0284	25.6539	243.5885	0.2522	0.4029
A	1488.4678	0.6506	2.0035	0.5517	0.7111
A	1476.1317	9.1578	11.3902	0.7348	0.8471
A	1473.0984	7.3135	29.5990	0.7491	0.8566
A	1454.7292	10.4423	14.0031	0.7448	0.8537
A	1448.9041	7.3563	16.0570	0.6417	0.7817
A	1439.1274	12.5885	17.3052	0.7402	0.8507
A	1387.7114	18.5670	18.3867	0.2192	0.3596
A	1356.8614	85.7420	26.8719	0.7236	0.8396
A	1342.3110	4.8108	5.7313	0.3158	0.4800
A	1332.3075	1.0153	4.0319	0.6757	0.8065
A	1324.8920	140.7617	7.1606	0.3705	0.5407
A	1320.9213	3.2559	13.1103	0.6952	0.8202
A	1299.8236	21.2311	1.9689	0.7263	0.8415
A	1295.9385	1.6373	12.0458	0.6331	0.7753
A	1256.4708	121.8441	30.1137	0.4507	0.6214
A	1250.0174	21.3515	13.2518	0.7416	0.8516
A	1234.7606	4.2300	9.6451	0.7359	0.8479
A	1214.6715	243.9037	11.0601	0.6350	0.7768
A	1193.4498	3.0595	27.3819	0.0657	0.1233
A	1187.1556	4.3913	7.9522	0.6836	0.8121
A	1159.5584	50.6868	8.2080	0.2600	0.4127
A	1141.6898	7.6319	5.2951	0.1976	0.3300
A	1122.7433	9.1473	37.9334	0.7235	0.8396
A	1120.5298	9.3059	43.1282	0.7432	0.8527
A	1101.5859	32.5744	39.7016	0.4919	0.6594
A	1076.2004	33.9462	7.9478	0.7452	0.8540
A	1045.7639	83.7894	30.9282	0.3304	0.4966
A	1043.0933	10.0267	31.1309	0.7178	0.8357
A	1019.9055	1.1878	7.9791	0.5866	0.7394
A	1003.2440	36.5814	2.8024	0.2943	0.4548
A	993.9584	225.4884	81.5081	0.7231	0.8393
A	978.0057	30.7088	3.9348	0.4760	0.6450
A	946.6381	129.8963	12.1383	0.1834	0.3099
A	932.7352	3.6142	24.6983	0.1072	0.1936
A	919.5096	0.2805	2.9827	0.3885	0.5596
A	881.3375	6.4654	16.1626	0.1745	0.2971
A	874.0448	5.5899	3.2538	0.5977	0.7482
A	859.0537	4.2144	7.8801	0.2345	0.3799

A	828.8545	4.5912	31.1947	0.1058	0.1913
A	819.7872	20.7345	3.8202	0.2674	0.4220
A	721.1756	16.5140	12.1313	0.1159	0.2078
A	674.2847	37.6904	13.0624	0.4269	0.5984
A	639.0223	0.2633	2.9334	0.7153	0.8340
A	606.3023	5.0154	4.1669	0.6925	0.8183
A	569.9399	2.3569	2.9056	0.4794	0.6481
A	540.6106	5.4024	3.8116	0.2513	0.4016
A	529.7889	15.6907	4.2625	0.7489	0.8564
A	488.7266	5.1124	2.4713	0.4453	0.6162
A	466.7071	0.0481	1.7896	0.5273	0.6905
A	463.1325	2.5623	7.1339	0.3996	0.5710
A	366.9616	19.5509	6.6010	0.1959	0.3276
A	299.0051	3.2315	2.9036	0.6225	0.7673
A	292.6666	1.0374	13.7204	0.1347	0.2374
A	265.4554	1.1566	1.7670	0.1879	0.3163
A	244.6324	2.5534	6.0711	0.1372	0.2413
A	186.5233	6.9038	2.1773	0.6884	0.8155
A	166.4947	1.5785	0.9503	0.7500	0.8571
A	142.5557	3.3522	1.4146	0.6544	0.7911
A	116.8720	0.4677	0.3891	0.6473	0.7859
A	89.3767	3.7264	0.6570	0.7439	0.8532
A	78.4131	3.2988	1.0224	0.7238	0.8398
A	70.7273	0.2893	0.2011	0.7484	0.8561
A	64.7428	4.8156	2.8494	0.7464	0.8548
A	51.6850	3.0197	0.6828	0.7498	0.8570
A	47.5445	1.4271	0.7189	0.6210	0.7662
A	17.6595	6.4339	0.7740	0.7157	0.8343

6-endo-dig prod for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid carboxylate:

Processing aupcphexdienoat6prod6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-1017.8876449

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
150.37809	160.515	135.392	127.377	160.563	43.821	33.687

30

C	1.988720	1.061497	-0.043291
C	1.526396	-0.195453	-0.039916
C	0.419466	-0.740887	-0.875178

C	0.503286	-2.266348	-1.004379
C	1.960234	-2.711900	-0.874954
C	2.440800	-2.332061	0.497234
O	3.026423	-3.055223	1.263342
Au	-1.443944	-0.088140	-0.119205
P	-3.540138	0.649074	0.783289
O	2.118807	-1.070578	0.881954
H	-4.222118	1.709639	0.149728
H	-4.605971	-0.272274	0.856864
H	-3.584648	1.130290	2.109005
C	1.409115	2.164995	-0.890184
C	3.107948	1.602802	0.808955
H	0.497654	-0.284451	-1.872656
H	-0.078796	-2.776977	-0.225265
H	0.077852	-2.586989	-1.962484
H	2.101160	-3.790033	-0.992305
H	2.576948	-2.197953	-1.627586
C	2.052760	3.437469	-0.325913
H	1.681566	2.031757	-1.950875
H	0.306862	2.183778	-0.858751
C	3.417348	2.959873	0.169866
H	2.766524	1.738778	1.848551
H	3.971040	0.928883	0.856753
H	3.902156	3.663098	0.856748
H	4.091668	2.820131	-0.688170
H	2.111195	4.253571	-1.055327
H	1.462315	3.802189	0.527810

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3127.3749	17.4269	8.2974
A	3098.6337	45.1524	
A	3093.7411	54.5674	
A	3092.5455	25.2540	
A	3089.7917	23.9469	
A	3039.2963	3.9541	
A	3038.7652	24.0212	
A	3029.9062	47.3516	
A	3029.2831	26.6693	
A	3024.0553	25.9417	
A	3013.2196	19.0541	
A	3001.1641	30.1173	
A	2981.0054	29.7985	
A	2500.4131	14.9512	
A	2498.5184	16.4169	
A	2483.2550	122.3795	
A	1873.3771	533.1264	

A	1753.1369	97.6053
A	1476.4603	3.5559
A	1469.6531	6.0997
A	1459.4066	6.9001
A	1447.1943	5.3032
A	1443.5202	2.6270
A	1437.8040	23.3733
A	1349.5603	85.9086
A	1341.5989	23.5298
A	1332.5894	21.5373
A	1327.0023	14.2589
A	1318.0470	0.0481
A	1310.0201	23.7028
A	1298.3343	11.5195
A	1278.7659	40.7485
A	1256.5231	118.3757
A	1240.5039	1.4081
A	1221.7214	4.6143
A	1204.2769	16.9407
A	1191.6686	7.0091
A	1175.4166	116.1425
A	1158.0658	162.4659
A	1132.3262	4.1951
A	1131.0038	2.5613
A	1129.7370	1.9133
A	1084.2853	4.7943
A	1081.1117	41.6889
A	1037.2373	2.3407
A	1023.5939	9.4095
A	1017.4762	189.3099
A	1007.1596	29.6974
A	986.0354	12.8759
A	963.7605	1.2486
A	953.3128	10.7527
A	922.2352	0.7685
A	918.7428	2.7530
A	905.2069	1.0689
A	868.7761	4.0793
A	866.9164	0.2481
A	821.2067	2.0082
A	763.5595	0.7265
A	703.7316	1.1721
A	672.0118	19.0801
A	637.7437	0.3736
A	612.1519	9.6139
A	554.5769	1.4671
A	516.6785	8.6861

A	482.4747	1.4585
A	441.7711	1.1649
A	413.3041	1.6191
A	407.8868	1.9375
A	372.4668	2.1831
A	338.5910	3.7008
A	319.4682	0.9591
A	263.2321	0.2379
A	245.6969	2.5156
A	204.3578	2.4514
A	187.9313	0.4376
A	144.4661	1.0649
A	130.8926	2.7518
A	92.1995	0.7898
A	82.5772	0.1107
A	69.5858	3.7476
A	62.5027	1.6061
A	50.8246	0.1997
A	37.8423	2.1861
A	26.7431	1.6269

Processing aupcphexdienoat6prod6psd1pbedcms.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-1017.5246673

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
151.77127	161.724	133.863	126.558	161.763	43.821	33.688

30

C	2.024361	1.024908	-0.044745
C	1.514000	-0.215502	-0.045670
C	0.376306	-0.732380	-0.863789
C	0.439360	-2.261876	-1.013495
C	1.888997	-2.744410	-0.892117
C	2.383017	-2.372490	0.472596
O	2.962276	-3.108678	1.245547
Au	-1.460663	-0.056098	-0.104637
P	-3.504118	0.680647	0.753761
O	2.101518	-1.113896	0.868525
H	-4.127745	1.778157	0.128759
H	-4.572916	-0.236807	0.761133
H	-3.539142	1.108303	2.095441

C	1.476905	2.154207	-0.885624
C	3.174917	1.525248	0.799637
H	0.469361	-0.277006	-1.858716
H	-0.153096	-2.775996	-0.248040
H	0.022885	-2.560780	-1.980508
H	1.997023	-3.824432	-1.013998
H	2.516450	-2.244716	-1.643254
C	2.166925	3.405755	-0.322458
H	1.739891	2.015653	-1.945517
H	0.379689	2.209237	-0.843359
C	3.518174	2.884178	0.173755
H	2.856401	1.661443	1.844663
H	4.023201	0.832640	0.819902
H	4.013453	3.564735	0.874418
H	4.193206	2.738340	-0.680165
H	2.257266	4.211743	-1.058304
H	1.590115	3.796315	0.526350

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3160.4914	22.5345	338.4139	0.4228	0.5943	10.8983
A	3129.7340	30.8686	265.4925	0.3765	0.5470	
A	3128.5308	83.3465	260.6405	0.7440	0.8532	
A	3122.1753	68.7059	411.6399	0.3377	0.5049	
A	3112.0073	40.6305	322.3525	0.2706	0.4260	
A	3075.8350	29.6375	49.7728	0.4406	0.6117	
A	3071.9485	52.7996	149.1493	0.0605	0.1142	
A	3067.4068	3.0141	464.3070	0.0489	0.0932	
A	3064.6455	59.0510	83.7015	0.5773	0.7320	
A	3060.8235	35.0914	221.0245	0.1810	0.3065	
A	3055.1908	25.4451	389.6120	0.4467	0.6176	
A	3030.5161	38.5437	634.2656	0.0945	0.1726	
A	3025.2287	59.6779	288.8783	0.1061	0.1918	
A	2529.8654	7.4789	282.5285	0.7495	0.8568	
A	2527.7426	10.0410	328.8056	0.7019	0.8249	
A	2511.4694	72.3003	1267.5407	0.0549	0.1041	
A	1814.9583	731.6183	173.0550	0.1195	0.2135	
A	1746.6282	232.5943	1079.3458	0.2333	0.3784	
A	1490.8851	1.9412	2.9823	0.7072	0.8285	
A	1483.1260	10.6079	23.0362	0.7254	0.8409	
A	1474.1132	7.1985	31.2001	0.7469	0.8551	
A	1462.4819	5.9357	29.5613	0.5486	0.7085	
A	1459.5912	5.8120	13.8782	0.6724	0.8041	
A	1450.7594	33.4693	18.9207	0.7287	0.8431	
A	1361.6956	189.6251	14.6446	0.1199	0.2141	

A	1348.9686	27.4325	28.0964	0.2965	0.4573
A	1344.6619	24.3202	4.5177	0.7358	0.8478
A	1337.4843	7.7456	11.0811	0.5178	0.6823
A	1329.4018	0.9628	8.5574	0.5949	0.7460
A	1313.9234	25.6928	6.0084	0.4463	0.6172
A	1304.7067	38.6638	23.6538	0.7269	0.8418
A	1292.3302	98.6585	5.9292	0.7257	0.8410
A	1258.6708	74.3450	37.7935	0.7124	0.8321
A	1247.3162	2.3682	50.0059	0.6785	0.8084
A	1231.5060	6.0660	16.0523	0.7400	0.8505
A	1202.8351	41.0334	3.4525	0.4206	0.5921
A	1195.1652	12.4875	81.5636	0.4556	0.6260
A	1175.6925	32.3836	16.3047	0.7264	0.8415
A	1160.2392	337.5483	97.8978	0.1130	0.2030
A	1142.0202	1.7843	2.1793	0.6937	0.8192
A	1124.0716	12.3026	41.0309	0.7010	0.8242
A	1120.8125	8.4426	38.6493	0.7426	0.8523
A	1093.3790	27.0836	275.8681	0.1942	0.3252
A	1079.4438	137.4578	178.9165	0.4393	0.6104
A	1043.6702	4.6856	28.2503	0.7315	0.8449
A	1036.6336	8.5384	13.1378	0.3021	0.4640
A	1012.4653	17.7327	158.3161	0.3097	0.4730
A	992.6764	96.7297	64.1986	0.4683	0.6379
A	987.1703	193.3058	41.5206	0.7391	0.8500
A	969.3067	10.8795	14.4302	0.2412	0.3886
A	956.7693	15.7115	128.0888	0.1888	0.3177
A	926.8045	0.9490	5.0300	0.3066	0.4693
A	924.5017	7.0994	27.9906	0.0854	0.1573
A	919.9924	3.4185	5.2236	0.6148	0.7615
A	876.9908	5.2899	3.9891	0.5485	0.7084
A	873.1882	0.9545	8.5192	0.2098	0.3468
A	831.1110	5.4300	8.4645	0.0877	0.1613
A	772.3821	0.7144	12.4494	0.2696	0.4247
A	710.6703	2.7696	7.3632	0.1896	0.3188
A	681.9165	27.8322	20.7377	0.3633	0.5329
A	646.7602	0.8082	4.3358	0.2749	0.4312
A	619.8910	16.6120	40.4335	0.1603	0.2763
A	566.8974	5.1731	1.5312	0.7337	0.8464
A	521.1776	13.9115	5.8681	0.5344	0.6966
A	490.7142	3.0699	7.6426	0.7126	0.8322
A	471.8670	1.0489	8.7727	0.4721	0.6414
A	455.4517	1.5094	3.1293	0.4642	0.6341
A	425.7907	2.9117	6.7689	0.5020	0.6685
A	378.8879	5.7284	4.7085	0.6380	0.7790
A	340.1687	8.2278	8.3503	0.1453	0.2537
A	322.9496	2.8730	6.6192	0.3609	0.5304
A	287.6987	0.7189	33.2019	0.1705	0.2913

A	267.8031	0.4281	2.6928	0.2101	0.3473
A	202.3511	5.4209	4.2590	0.0864	0.1590
A	188.5129	2.2303	2.4129	0.7409	0.8511
A	147.8086	1.7918	2.9638	0.6652	0.7990
A	130.0635	5.2237	1.8355	0.6990	0.8228
A	98.8673	0.6632	1.4689	0.7096	0.8301
A	90.0205	0.3185	0.5616	0.7083	0.8292
A	83.4531	0.5876	2.3152	0.7464	0.8548
A	73.7675	4.4675	1.0368	0.6903	0.8168
A	57.9719	4.9857	0.9762	0.6781	0.8082
A	41.2257	4.8627	2.2713	0.7264	0.8415
A	18.7182	2.2316	3.9797	0.7461	0.8546

6-exo-dig prod for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid carboxylate:

Processing aupcphexdienoat6xprod6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-1017.8802510

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
150.35641	160.497	133.737	127.990	160.531	43.821	33.396

30

O	2.895399	0.430635	-0.172516
C	1.655512	-0.228507	-0.126202
C	1.617463	-1.564180	-0.197863
C	2.872236	-2.376822	-0.258589
C	3.976515	-1.639187	0.486001
C	4.074371	-0.202133	0.055226
C	0.536177	0.757732	-0.045765
Au	-1.358356	-0.206071	-0.000457
P	-3.533154	-1.225144	0.051580
O	5.102212	0.414161	-0.065013
H	-3.639030	-2.631991	0.009791
H	-4.452868	-0.918606	-0.973955
H	-4.372735	-0.988109	1.160985
C	0.661261	1.697735	1.168323
C	0.561161	1.783212	-1.195779
H	0.645865	-2.050678	-0.207543
H	2.718774	-3.366562	0.187316
H	3.172530	-2.557032	-1.303385
H	3.743408	-1.629486	1.561557

H	4.964915	-2.090380	0.364668
C	-0.335601	2.925600	-0.706445
H	1.593057	2.149525	-1.321274
H	0.245365	1.365385	-2.160013
C	-0.264823	2.874433	0.839119
H	0.423273	1.212423	2.123474
H	1.702350	2.055174	1.233177
H	-1.264729	2.704077	1.262344
H	0.103818	3.812004	1.271864
H	-1.369502	2.771726	-1.046351
H	-0.013537	3.893611	-1.108184

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3195.6901	13.4882	77.4463	0.2113	0.3489	9.2892
A	3131.3350	13.1599	135.8199	0.4122	0.5838	
A	3097.1430	86.6301	163.2962	0.4053	0.5768	
A	3082.4215	3.5773	76.9092	0.7304	0.8442	
A	3081.3805	22.1511	118.6329	0.4222	0.5938	
A	3079.0273	2.9021	125.5295	0.4919	0.6594	
A	3073.7944	41.3689	9.3583	0.6829	0.8116	
A	3035.1387	64.4756	170.8019	0.0574	0.1085	
A	3033.8135	12.8411	66.4800	0.1964	0.3284	
A	3023.0128	22.7936	40.3323	0.7500	0.8571	
A	3010.2667	42.5851	256.5637	0.1345	0.2371	
A	3005.6628	37.1365	220.3549	0.1629	0.2801	
A	3003.3663	38.9157	104.8644	0.2746	0.4309	
A	2498.3673	17.4646	134.7562	0.7307	0.8444	
A	2495.1544	20.3897	145.9143	0.5779	0.7325	
A	2480.7739	109.3360	619.7231	0.0926	0.1695	
A	1875.0066	493.8536	16.8433	0.4331	0.6045	
A	1743.3616	54.0600	73.1052	0.2405	0.3877	
A	1484.8475	4.2830	3.0061	0.7499	0.8571	
A	1464.5691	7.6192	7.3470	0.7499	0.8571	
A	1461.0152	10.7119	8.8925	0.7324	0.8455	
A	1460.2933	6.2715	16.7263	0.5227	0.6866	
A	1450.5886	0.0371	13.6523	0.7500	0.8571	
A	1432.0373	18.8637	7.0816	0.7498	0.8570	
A	1362.8849	98.0281	2.4857	0.6374	0.7786	
A	1335.6831	9.1075	23.2616	0.2019	0.3360	
A	1333.0675	5.7274	10.8066	0.1695	0.2898	
A	1319.4658	0.0245	0.6859	0.7498	0.8570	
A	1309.6521	7.6162	15.6077	0.3629	0.5326	
A	1299.6003	42.7946	34.9034	0.5481	0.7081	
A	1288.5508	0.1292	0.8039	0.7476	0.8556	
A	1253.6676	50.3200	9.6342	0.2549	0.4063	
A	1238.6134	18.1932	5.6676	0.7183	0.8361	

A	1238.5090	151.9928	5.4454	0.2527	0.4035
A	1220.0733	114.5241	36.2465	0.2574	0.4094
A	1197.8876	21.7814	58.0422	0.3801	0.5508
A	1194.0844	1.5179	1.3688	0.7260	0.8413
A	1165.4628	183.7787	12.8235	0.7237	0.8397
A	1157.2053	10.8474	3.7301	0.5809	0.7349
A	1132.9713	3.6753	16.7616	0.7500	0.8571
A	1132.6899	3.0909	15.9354	0.7498	0.8570
A	1106.9336	0.1125	4.3612	0.7497	0.8570
A	1071.2103	132.2683	3.4733	0.6763	0.8069
A	1064.7819	0.4750	11.5225	0.5805	0.7346
A	1037.1823	3.1877	1.6932	0.3356	0.5025
A	1036.7582	1.4578	1.6665	0.3293	0.4955
A	1021.8545	215.1361	15.3400	0.7500	0.8571
A	997.8921	26.5058	3.2753	0.4160	0.5876
A	977.2194	6.9823	46.6056	0.5353	0.6973
A	967.9178	1.5707	0.4226	0.6395	0.7801
A	950.0146	12.7421	1.9495	0.1193	0.2132
A	944.9362	16.2660	8.9662	0.5160	0.6807
A	910.8087	4.3061	46.5571	0.2540	0.4050
A	897.8274	0.0368	10.2646	0.4671	0.6367
A	825.7154	0.4195	1.0032	0.6745	0.8056
A	800.9871	1.1728	10.5890	0.1167	0.2090
A	793.5116	7.3346	2.3378	0.3064	0.4691
A	759.2199	8.9811	5.3089	0.6965	0.8211
A	733.8417	9.4725	16.9600	0.3355	0.5024
A	662.8936	2.0492	2.9369	0.1729	0.2948
A	655.0362	3.5690	10.0242	0.1101	0.1983
A	617.2459	0.1531	1.1741	0.6800	0.8095
A	587.4575	7.7200	17.6114	0.2039	0.3388
A	535.4023	6.4318	6.2316	0.2621	0.4153
A	490.2373	3.8767	2.1295	0.2509	0.4011
A	469.1163	2.0149	10.9085	0.4237	0.5952
A	418.1918	0.6231	0.8405	0.7096	0.8301
A	416.3015	0.6790	0.9522	0.7487	0.8563
A	341.2723	1.5739	4.7296	0.2069	0.3428
A	312.5658	0.8726	1.4653	0.4998	0.6665
A	283.4933	1.2373	0.5763	0.6583	0.7939
A	244.0969	1.6926	9.7416	0.2021	0.3362
A	212.5946	0.6640	0.3737	0.6338	0.7759
A	200.2102	2.9258	3.2373	0.2914	0.4513
A	189.7370	1.9771	4.5407	0.2059	0.3415
A	131.2936	2.9763	0.5176	0.6992	0.8230
A	119.5661	0.0746	0.0826	0.6921	0.8180
A	108.0431	0.0178	0.0649	0.7495	0.8568
A	99.6207	1.6654	0.3574	0.5671	0.7238
A	85.7623	0.2972	0.8642	0.7386	0.8497

A	81.9346	0.0311	0.1769	0.7288	0.8432
A	58.6770	3.6332	0.9010	0.7428	0.8524
A	54.0457	1.6769	2.0589	0.7490	0.8565
A	24.2960	1.3780	0.3380	0.7485	0.8562

Processing aupcphexdienoat6xprod6psd1pbedcms.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-1017.5148216

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
151.55061	161.574	132.975	127.159	161.608	43.821	33.383

30

O	2.888812	0.434308	-0.164773
C	1.639263	-0.226188	-0.139435
C	1.610530	-1.561428	-0.234065
C	2.868367	-2.372157	-0.292467
C	3.969179	-1.645794	0.472323
C	4.053803	-0.199982	0.080300
C	0.512884	0.755929	-0.055844
Au	-1.363375	-0.208253	-0.001051
P	-3.457857	-1.243770	0.076545
O	5.082213	0.438944	0.000663
H	-3.493719	-2.652209	0.090182
H	-4.361478	-0.988743	-0.973788
H	-4.286487	-0.969976	1.182550
C	0.650211	1.704556	1.158197
C	0.548785	1.788434	-1.207655
H	0.641463	-2.049807	-0.259207
H	2.709572	-3.363026	0.144176
H	3.176825	-2.538289	-1.335393
H	3.739696	-1.661038	1.547456
H	4.955344	-2.094070	0.335592
C	-0.344777	2.937632	-0.718582
H	1.579324	2.155006	-1.333690
H	0.228957	1.378178	-2.171893
C	-0.277066	2.884181	0.829073
H	0.411604	1.227366	2.115250
H	1.689317	2.064183	1.222095
H	-1.275777	2.711500	1.247799
H	0.093332	3.820541	1.261082
H	-1.376197	2.788593	-1.059624

H -0.012592 3.903186 -1.115920

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3229.7390	11.1358	229.1641	0.2456	0.3943	12.3995
A	3164.8346	12.4272	264.3211	0.4249	0.5964	
A	3125.0698	155.8001	310.7376	0.5790	0.7334	
A	3121.7543	21.7296	282.8571	0.4176	0.5892	
A	3110.1661	16.2882	225.0524	0.6885	0.8155	
A	3107.0636	5.4953	378.6953	0.3845	0.5554	
A	3100.5817	64.2665	18.4703	0.5591	0.7172	
A	3072.7621	95.4802	568.9652	0.0779	0.1445	
A	3067.7452	13.8974	162.6601	0.1838	0.3106	
A	3060.0692	42.0312	100.4706	0.7471	0.8552	
A	3042.5344	42.0948	541.7334	0.1325	0.2340	
A	3028.2533	123.8859	740.4934	0.2014	0.3353	
A	3022.9567	83.5035	371.8303	0.2597	0.4124	
A	2525.9566	9.5778	318.8310	0.7239	0.8398	
A	2523.8031	9.0288	313.4281	0.7446	0.8536	
A	2508.2253	67.0407	1114.3703	0.0429	0.0823	
A	1816.0635	734.1915	43.4530	0.3511	0.5197	
A	1744.6651	95.8023	202.6637	0.1750	0.2978	
A	1494.7937	1.7864	14.1020	0.4933	0.6607	
A	1476.3874	9.7118	20.9510	0.7494	0.8568	
A	1475.4968	9.7063	16.7821	0.7430	0.8525	
A	1465.4432	0.8371	27.5549	0.7310	0.8446	
A	1465.2532	7.4533	50.1305	0.5815	0.7354	
A	1440.3889	25.4848	16.5851	0.7350	0.8473	
A	1377.4504	115.2440	4.8627	0.6981	0.8222	
A	1346.7932	15.5280	21.0132	0.2213	0.3625	
A	1341.3096	7.4884	28.2418	0.0583	0.1102	
A	1332.6450	0.1937	1.0082	0.6367	0.7781	
A	1319.2774	5.6613	30.5335	0.4537	0.6242	
A	1313.7207	80.2364	50.5987	0.6179	0.7638	
A	1298.8394	1.1614	3.3524	0.7218	0.8384	
A	1256.1715	60.0116	28.5667	0.1479	0.2576	
A	1249.4423	6.1183	15.7855	0.7499	0.8571	
A	1247.4347	156.9080	10.8027	0.7459	0.8545	
A	1227.4108	141.7172	29.5801	0.3465	0.5147	
A	1204.9815	18.7998	108.2807	0.3842	0.5551	
A	1202.8202	1.9777	4.0304	0.6985	0.8225	
A	1171.9587	54.4743	5.8015	0.5806	0.7346	
A	1161.9453	260.5064	30.6011	0.7499	0.8571	
A	1122.0742	8.9429	46.9676	0.7499	0.8571	
A	1120.9006	6.9927	40.7483	0.7491	0.8566	
A	1104.8080	0.1514	11.4394	0.7487	0.8563	
A	1070.0468	76.5477	16.0882	0.5444	0.7050	

A	1067.5268	185.4327	14.4594	0.7081	0.8291
A	1045.7675	8.8690	7.2372	0.4866	0.6547
A	1044.6026	0.0583	0.8827	0.7275	0.8422
A	995.4697	12.1005	14.2564	0.2280	0.3714
A	989.8740	327.8710	35.8546	0.7484	0.8561
A	984.9460	9.7878	100.0686	0.6036	0.7528
A	973.5719	3.4561	2.3404	0.7500	0.8571
A	955.3835	27.1769	4.6998	0.3332	0.4999
A	949.1170	26.0788	23.4538	0.5847	0.7379
A	916.1632	5.4636	67.1669	0.1736	0.2959
A	904.4179	1.5639	22.9134	0.5552	0.7140
A	835.6259	3.1164	2.9079	0.7269	0.8419
A	811.7326	17.2818	5.2455	0.6496	0.7876
A	803.9671	1.9805	22.6938	0.1022	0.1854
A	769.9216	22.4623	7.9164	0.7456	0.8543
A	742.7045	22.1223	26.2686	0.4097	0.5812
A	668.6282	2.7203	3.4268	0.4064	0.5780
A	657.5464	7.9462	17.1318	0.1185	0.2119
A	624.2334	0.2023	1.5100	0.7099	0.8303
A	587.5387	18.8492	22.9692	0.1382	0.2428
A	535.3864	8.7962	9.8070	0.3661	0.5360
A	495.7701	4.9353	6.1090	0.1826	0.3087
A	473.3871	6.3480	20.5740	0.4812	0.6497
A	463.5627	0.0605	0.8915	0.6855	0.8134
A	455.6559	0.4445	0.9833	0.7463	0.8547
A	343.7929	2.1957	7.7347	0.2584	0.4107
A	317.1559	1.7854	3.3727	0.4718	0.6411
A	286.9513	0.1524	16.7223	0.1312	0.2319
A	277.1883	1.8398	4.4379	0.2302	0.3742
A	214.3854	1.9746	1.5675	0.7487	0.8563
A	201.7555	6.4301	3.4871	0.3423	0.5100
A	189.7812	3.3652	2.8471	0.2276	0.3708
A	132.9010	4.4921	1.1449	0.6742	0.8054
A	119.0047	0.1172	0.8139	0.6775	0.8077
A	114.4930	0.1361	0.1125	0.4867	0.6548
A	97.8550	2.7608	0.3496	0.7303	0.8442
A	90.0375	0.1509	1.4261	0.7472	0.8553
A	76.0844	0.0185	0.0177	0.7473	0.8554
A	63.5626	7.9720	0.6080	0.7087	0.8295
A	48.5258	3.2604	1.2691	0.7499	0.8571
A	25.1802	2.8903	1.2608	0.7491	0.8565

7-endo-trig prod for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid carboxylate:

Processing aupcphexdienoat7prod6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-1017.8777704

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
150.79509	160.806	133.057	125.989	160.846	43.821	33.372

30

C	-1.427044	0.500170	-0.107438
C	-0.450806	-0.649500	-0.115282
C	-0.780695	-1.953190	-0.148049
C	-2.144569	-2.585996	-0.095949
C	-3.186420	-1.782064	0.675400
C	-3.671325	-0.594299	-0.110176
O	-2.744267	0.200616	-0.673108
Au	1.570956	-0.193880	-0.022128
P	3.909134	0.251142	0.097733
O	-4.841248	-0.382954	-0.333546
C	-1.625900	1.184451	1.251570
C	-1.001076	1.690976	-0.974354
H	0.033977	-2.679288	-0.192836
H	4.696229	0.080732	-1.060243
H	4.698588	-0.488912	1.002491
H	4.334529	1.547590	0.455114
H	-2.515551	-2.794579	-1.112281
H	-2.044090	-3.568919	0.383316
H	-4.071740	-2.384425	0.900868
H	-2.755657	-1.456520	1.632087
H	-0.628342	1.343541	1.684961
C	-2.311743	2.516657	0.924221
H	-2.183993	0.567505	1.966087
H	0.053623	1.910814	-0.757990
H	-1.077798	1.444672	-2.039838
C	-1.900995	2.848950	-0.529611
H	-1.381587	3.811123	-0.606708
H	-2.788000	2.909177	-1.168857
H	-3.400791	2.407728	0.993361
H	-2.024355	3.300911	1.633826

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3124.1368	14.9347	85.3265	0.2460	0.3949	9.8835
A	3122.4175	7.0117	104.1287	0.5042	0.6704	
A	3119.9656	50.0850	58.5187	0.6860	0.8137	
A	3106.5327	17.5594	76.0492	0.6812	0.8104	

A	3102.1198	6.3990	94.0993	0.5565	0.7151
A	3093.5859	18.4087	32.9075	0.1873	0.3155
A	3065.2155	21.9098	113.9376	0.4076	0.5791
A	3060.8155	57.4968	240.3306	0.0472	0.0902
A	3050.7374	31.3951	65.0381	0.4624	0.6324
A	3049.5458	8.7972	85.0529	0.2130	0.3512
A	3040.5621	47.6854	94.7913	0.1360	0.2395
A	3034.4984	14.0145	16.7258	0.2536	0.4047
A	3008.9595	38.5336	248.9555	0.1422	0.2490
A	2502.3529	16.2025	136.3247	0.7389	0.8499
A	2499.8708	17.7022	151.7575	0.6810	0.8102
A	2487.3110	105.1923	657.1040	0.0942	0.1721
A	1841.8713	480.3273	11.6260	0.4564	0.6267
A	1685.0393	1.3253	45.5251	0.1420	0.2486
A	1486.6843	7.0443	2.6643	0.6076	0.7559
A	1461.7106	6.2652	7.3790	0.7268	0.8418
A	1454.4266	8.1436	12.0334	0.6362	0.7777
A	1450.9599	16.5936	16.4742	0.5875	0.7401
A	1442.7723	29.3053	3.4090	0.7172	0.8353
A	1436.8081	0.3557	6.6910	0.7500	0.8571
A	1373.2175	131.8459	8.7956	0.2369	0.3830
A	1365.7615	13.1149	19.7681	0.1444	0.2524
A	1343.2451	2.1272	1.4170	0.7289	0.8432
A	1339.5830	39.5402	6.3701	0.4163	0.5879
A	1323.3039	0.7095	0.4209	0.7432	0.8527
A	1313.6110	17.0489	11.6643	0.5090	0.6746
A	1296.2453	55.5051	2.9151	0.6181	0.7640
A	1291.2835	11.3857	2.5603	0.7068	0.8282
A	1242.0101	1.1899	3.8606	0.7100	0.8304
A	1233.8550	19.8103	14.7932	0.4950	0.6622
A	1225.1974	64.1255	2.9606	0.7389	0.8499
A	1208.5846	47.8002	7.3103	0.5716	0.7274
A	1202.9873	51.8938	5.0472	0.7469	0.8551
A	1161.9648	5.0833	1.5650	0.4083	0.5798
A	1146.5973	22.6698	3.5292	0.7439	0.8531
A	1134.7560	4.0670	17.1810	0.7343	0.8468
A	1131.4396	4.5157	17.5101	0.7462	0.8547
A	1119.3421	0.6205	2.4827	0.1057	0.1912
A	1072.7815	8.6509	4.8209	0.7491	0.8565
A	1060.7380	45.5705	8.0350	0.5656	0.7225
A	1037.8904	28.8291	8.7757	0.3569	0.5260
A	1025.0476	1.7079	2.7796	0.7307	0.8444
A	1022.9656	218.6534	20.1164	0.7037	0.8261
A	1014.8990	4.8926	16.8447	0.6959	0.8207
A	991.4118	28.0257	8.6002	0.5893	0.7416
A	969.3436	6.9849	0.9802	0.6953	0.8203
A	946.3867	7.9556	9.1330	0.1297	0.2296

A	907.0550	2.5550	5.2153	0.0409	0.0786
A	893.9002	1.4225	5.9175	0.3043	0.4666
A	880.0929	8.7117	5.6054	0.7492	0.8566
A	834.2936	8.2760	9.2772	0.1331	0.2349
A	821.1564	11.9305	5.6360	0.2877	0.4468
A	797.7451	2.3170	0.8455	0.6744	0.8055
A	770.2838	5.1657	5.6100	0.1191	0.2128
A	714.9711	10.4202	0.8326	0.4870	0.6550
A	689.2778	4.4920	16.9297	0.0448	0.0858
A	647.1776	0.0679	1.0632	0.1275	0.2261
A	593.5774	0.9141	0.8365	0.1917	0.3217
A	564.3727	7.1616	3.3969	0.3726	0.5429
A	551.7463	2.7456	0.4662	0.2953	0.4559
A	496.8896	2.9360	3.3271	0.1972	0.3294
A	438.9898	0.3958	0.7702	0.4074	0.5790
A	430.5871	0.4602	0.5562	0.6999	0.8235
A	394.2411	0.4531	1.0338	0.6976	0.8219
A	386.9226	2.8481	4.4166	0.1319	0.2331
A	341.3813	1.4740	3.1024	0.3144	0.4784
A	305.7506	7.8169	1.1081	0.6134	0.7603
A	257.3249	0.6491	5.3816	0.2226	0.3642
A	251.3812	2.2366	5.6933	0.1194	0.2133
A	201.8376	3.3155	0.9983	0.5043	0.6705
A	178.6534	0.9156	1.3052	0.6650	0.7988
A	165.3074	3.6872	2.3767	0.2661	0.4203
A	149.0240	1.2453	0.4064	0.7013	0.8244
A	118.8761	0.2598	0.3762	0.7008	0.8241
A	116.9791	1.0195	0.1762	0.7415	0.8516
A	78.5606	1.3604	0.5484	0.7217	0.8384
A	56.1590	5.2357	1.8426	0.7469	0.8551
A	55.1421	3.2912	1.0056	0.7498	0.8570
A	43.7772	0.1877	0.2188	0.7460	0.8545
A	25.9165	0.8762	0.2769	0.7088	0.8296

Processing aupcphexdienoat7prod6psd1pbedcms.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-1017.5128926

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
152.12998	162.035	131.744	125.691	162.073	43.821	33.372

30

C	-1.413689	0.521183	-0.073400
C	-0.455198	-0.650610	-0.081392
C	-0.811221	-1.952542	-0.075904
C	-2.174574	-2.582374	0.028836
C	-3.233725	-1.717406	0.709849
C	-3.667097	-0.588484	-0.178254
O	-2.748397	0.260263	-0.644313
Au	1.561399	-0.212068	-0.027985
P	3.848783	0.223055	0.051630
O	-4.815295	-0.458015	-0.567537
C	-1.586487	1.217695	1.287411
C	-0.955542	1.698940	-0.949382
H	-0.007172	-2.688465	-0.122106
H	4.607530	-0.044030	-1.104374
H	4.616202	-0.460104	1.014673
H	4.249425	1.548115	0.310079
H	-2.534174	-2.899782	-0.961800
H	-2.071958	-3.507387	0.609289
H	-4.127127	-2.303648	0.936523
H	-2.835534	-1.329947	1.653954
H	-0.585494	1.310013	1.724474
C	-2.177267	2.602494	0.971801
H	-2.190384	0.637380	1.990567
H	0.102623	1.880062	-0.729798
H	-1.039705	1.460079	-2.014605
C	-1.812777	2.889997	-0.505228
H	-1.272135	3.834767	-0.623648
H	-2.718678	2.959040	-1.115140
H	-3.263862	2.598446	1.105543
H	-1.776841	3.361683	1.651525

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3164.0236	8.8809	187.6035	0.5663	0.7231	12.9691
A	3154.6102	22.2109	244.1820	0.2613	0.4143	
A	3151.1122	92.0536	165.7836	0.5162	0.6809	
A	3144.2840	46.5307	186.8477	0.6951	0.8201	
A	3134.3938	9.4805	355.7550	0.5922	0.7439	
A	3121.2804	11.0886	66.0119	0.6036	0.7528	
A	3101.6998	19.4459	324.8088	0.0547	0.1038	
A	3094.4032	53.7664	830.8871	0.0334	0.0647	
A	3088.8909	4.9988	252.6599	0.7422	0.8520	
A	3084.8713	66.5087	67.0262	0.3222	0.4874	
A	3080.5204	52.3492	104.0722	0.7074	0.8286	
A	3074.3052	29.8569	191.4169	0.1548	0.2680	

A	3038.1529	48.8915	616.4613	0.1502	0.2612
A	2531.5915	8.0805	325.4703	0.7461	0.8546
A	2529.9121	8.7670	331.6343	0.7297	0.8437
A	2514.7632	60.5275	1114.8669	0.0435	0.0833
A	1782.0825	747.7980	30.3563	0.3240	0.4894
A	1681.1213	4.6730	177.7982	0.1282	0.2273
A	1495.8273	5.4717	6.8066	0.7204	0.8374
A	1476.5574	25.5539	14.6850	0.7255	0.8409
A	1473.4147	8.8121	26.2593	0.7477	0.8557
A	1463.3661	58.1619	38.5272	0.5028	0.6691
A	1460.1482	10.3826	19.0174	0.6578	0.7936
A	1456.9762	0.9107	27.4713	0.7309	0.8446
A	1391.1771	270.7288	13.9301	0.3077	0.4706
A	1375.6837	19.8582	55.7444	0.1634	0.2809
A	1357.3533	5.0754	3.2147	0.5729	0.7285
A	1353.8195	68.9837	28.3045	0.5552	0.7140
A	1334.7636	1.8658	0.8959	0.3285	0.4945
A	1327.5189	39.7774	13.5040	0.3519	0.5206
A	1310.1345	37.4803	15.4675	0.7496	0.8569
A	1303.0745	30.7964	7.4028	0.7430	0.8526
A	1255.3910	8.2002	13.3461	0.6021	0.7516
A	1239.9742	14.9420	21.5763	0.5680	0.7245
A	1237.7425	123.7578	9.9062	0.6920	0.8179
A	1219.9877	5.4466	14.1020	0.7214	0.8381
A	1203.2509	121.5338	14.1743	0.5706	0.7266
A	1170.4613	34.7108	5.8931	0.4959	0.6630
A	1155.3235	37.5040	8.6980	0.6811	0.8103
A	1123.9475	3.8037	14.8642	0.6701	0.8025
A	1121.0791	9.0840	39.8446	0.7289	0.8432
A	1119.4458	7.3820	34.3301	0.7255	0.8409
A	1079.7989	15.3058	10.6090	0.7486	0.8562
A	1060.2822	63.5142	18.6559	0.5837	0.7372
A	1041.4451	38.4093	13.3228	0.3953	0.5666
A	1034.8445	12.0587	8.2544	0.7205	0.8375
A	1016.4909	73.0663	30.1327	0.7288	0.8431
A	999.5936	0.9590	2.5946	0.3805	0.5512
A	990.4393	270.5839	77.9649	0.7169	0.8351
A	976.6510	14.4004	3.6133	0.6571	0.7931
A	953.2580	15.9682	10.7992	0.1269	0.2253
A	914.8630	4.2526	15.7312	0.0259	0.0504
A	896.9063	4.3911	11.2117	0.4288	0.6002
A	889.8000	19.6631	10.5154	0.7497	0.8570
A	840.8047	10.6016	12.9117	0.2479	0.3973
A	834.1605	18.1872	9.4466	0.1556	0.2693
A	803.3252	4.9376	1.4925	0.6859	0.8137
A	772.3934	20.4193	9.4886	0.1676	0.2871
A	735.6123	17.7010	0.9620	0.7322	0.8454

A	694.8695	10.0000	27.8813	0.0253	0.0493
A	651.0525	0.5432	4.4846	0.0798	0.1477
A	605.6313	3.8665	2.1772	0.4580	0.6282
A	561.4640	9.3337	3.1692	0.7485	0.8562
A	557.1612	14.6428	11.6384	0.2398	0.3868
A	503.0993	6.8344	4.9710	0.2590	0.4114
A	469.9654	0.2400	0.5313	0.4841	0.6524
A	467.8307	0.4065	1.3162	0.6150	0.7616
A	392.1626	4.8513	6.9566	0.2119	0.3497
A	377.9848	1.6769	3.1954	0.4597	0.6298
A	342.4022	2.8273	5.3769	0.2245	0.3667
A	305.5752	13.4923	3.0032	0.7131	0.8325
A	295.6254	0.1281	14.0288	0.0969	0.1767
A	256.0754	5.9908	3.4668	0.2588	0.4112
A	198.6820	7.9796	2.0566	0.6996	0.8233
A	175.7141	1.9030	2.3804	0.5038	0.6701
A	166.1208	3.9340	1.1875	0.5443	0.7049
A	152.0655	3.2064	0.7276	0.7291	0.8433
A	121.7950	1.2415	2.0254	0.7305	0.8442
A	99.4709	1.1169	0.8534	0.7488	0.8564
A	75.6802	1.1257	0.8139	0.7454	0.8541
A	63.7924	4.2588	0.5300	0.7421	0.8520
A	61.4680	6.9789	0.9662	0.7370	0.8486
A	51.2012	3.9838	0.8019	0.6938	0.8192
A	30.4717	1.3385	0.5240	0.7499	0.8571

SM^+ 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid:

Processing aupcphexdienic5sm6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-1018.2642755

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
156.77835	167.965	145.975	134.713	168.027	43.828	33.959

31

C	0.830496	3.954221	0.598064
C	-0.024028	2.732544	0.245841
C	0.994565	1.676879	-0.136622
C	2.354022	2.336298	-0.305648
C	2.022428	3.829379	-0.346326
C	0.786916	0.398544	-0.315893

C	0.743283	-0.944520	-0.488019
C	1.221450	-1.942546	0.550270
C	2.555877	-2.564232	0.152404
C	3.698343	-1.586822	0.168199
O	4.845812	-2.179769	-0.174286
Au	-1.431280	-0.416049	-0.105640
P	-3.763397	-0.392183	0.226895
O	3.611916	-0.412591	0.452229
H	-4.355004	0.868713	0.407513
H	-4.543929	-0.926707	-0.810885
H	-4.246420	-1.095914	1.341848
H	0.655528	-1.325200	-1.515156
H	1.309725	-1.442153	1.521728
H	0.488855	-2.752578	0.656842
H	2.811733	-3.387774	0.831140
H	2.511362	-3.020831	-0.846506
H	5.555506	-1.518025	-0.137334
H	2.957095	2.086216	0.577924
H	2.901160	1.958356	-1.174266
H	-0.649118	2.948121	-0.633931
H	-0.689930	2.400906	1.052597
H	2.874274	4.451082	-0.054393
H	1.730376	4.126920	-1.362997
H	0.280203	4.893782	0.490036
H	1.168673	3.886125	1.640843

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3801.9472	136.4707	113.3190	0.2318	0.3763	4.9726
A	3127.6569	7.2500	89.2554	0.7243	0.8401	
A	3123.8707	17.0912	89.3955	0.7473	0.8554	
A	3120.1411	11.2155	247.1431	0.2367	0.3829	
A	3115.6280	3.1370	23.1400	0.7091	0.8298	
A	3099.8296	0.2391	120.5682	0.4971	0.6641	
A	3085.0571	15.2721	43.2354	0.3716	0.5419	
A	3067.6800	0.4907	89.8210	0.3725	0.5428	
A	3053.2860	7.3993	58.8094	0.2167	0.3562	
A	3049.7419	21.4676	36.6535	0.7056	0.8274	
A	3049.2787	8.4805	81.9707	0.0710	0.1326	
A	3048.0763	5.0648	166.5944	0.0699	0.1307	
A	3041.5248	18.7624	252.0459	0.0567	0.1073	
A	3023.9294	11.9116	97.9914	0.0474	0.0905	
A	2540.1218	0.5955	133.8807	0.7206	0.8376	
A	2536.4510	0.4962	116.8659	0.6938	0.8192	
A	2514.7563	10.2520	411.4575	0.0500	0.0952	

A	1962.6761	62.4779	53.6170	0.4893	0.6571
A	1854.9436	332.8690	8.3179	0.0612	0.1153
A	1475.5881	1.5394	1.1575	0.5960	0.7468
A	1461.1028	10.1971	12.6669	0.7500	0.8571
A	1447.8240	65.1373	2.7299	0.7406	0.8510
A	1442.4380	61.6898	6.2941	0.5711	0.7270
A	1433.8522	6.3015	6.6272	0.7427	0.8524
A	1427.3498	29.4731	9.3799	0.7120	0.8318
A	1423.5960	39.3847	5.0103	0.2325	0.3773
A	1414.2377	14.3787	15.7631	0.5983	0.7487
A	1341.4472	2.1916	1.4087	0.6987	0.8226
A	1334.6096	4.2697	5.9909	0.7472	0.8553
A	1318.8988	0.0898	1.2561	0.7309	0.8445
A	1312.6435	18.4818	7.5569	0.5697	0.7259
A	1305.8846	14.8763	5.3627	0.6280	0.7715
A	1282.2034	0.8561	3.8614	0.5106	0.6760
A	1244.7653	5.8765	9.2027	0.5670	0.7237
A	1243.1341	14.3679	9.3569	0.6449	0.7841
A	1223.9712	15.8527	16.4593	0.1717	0.2930
A	1221.1269	3.9091	6.8878	0.5961	0.7469
A	1193.0186	97.7035	5.8024	0.1126	0.2025
A	1174.1117	185.4231	0.7440	0.5744	0.7297
A	1147.2556	6.4495	1.1242	0.3773	0.5478
A	1140.0105	4.5093	0.8583	0.7497	0.8570
A	1135.0013	3.2596	5.0752	0.6243	0.7687
A	1120.5966	2.5159	15.5724	0.7497	0.8569
A	1117.2817	3.3616	14.9166	0.7498	0.8570
A	1063.5142	10.3413	10.7264	0.2785	0.4357
A	1055.3628	0.6829	4.6242	0.7487	0.8563
A	1035.8038	2.0863	6.4213	0.7184	0.8362
A	1019.6996	2.9437	3.6616	0.4124	0.5840
A	991.9763	174.6613	16.1025	0.6359	0.7775
A	962.3717	5.4484	3.7012	0.6735	0.8049
A	956.5478	14.2115	7.7041	0.2438	0.3920
A	923.6643	0.7965	8.8941	0.0780	0.1447
A	900.7400	1.4037	1.4704	0.4425	0.6135
A	890.1318	19.0642	3.1808	0.7283	0.8428
A	876.1721	18.8649	7.4792	0.2744	0.4307
A	867.8618	1.0604	0.8612	0.6895	0.8162
A	837.9940	5.5614	8.3242	0.2285	0.3720
A	816.0123	22.8582	9.6453	0.0889	0.1632
A	694.0807	5.6402	12.1002	0.0602	0.1136
A	673.1643	95.1768	0.7015	0.6000	0.7500
A	629.1531	19.3462	3.1301	0.5358	0.6978
A	573.0369	4.3875	1.6268	0.6617	0.7964
A	556.7130	37.7025	1.9849	0.2639	0.4176
A	548.2864	19.7316	1.2584	0.6750	0.8059

A	536.6403	13.4438	0.7192	0.6710	0.8031
A	497.7097	13.1536	0.5616	0.7296	0.8437
A	474.5478	0.6439	0.5711	0.7209	0.8378
A	464.5066	1.3037	1.2042	0.3137	0.4776
A	456.2488	2.8186	6.4317	0.1809	0.3064
A	422.8455	12.1743	6.0133	0.7325	0.8456
A	374.8941	2.6829	4.7224	0.3323	0.4988
A	286.0329	1.6131	10.6375	0.2508	0.4010
A	269.4925	0.4333	0.7304	0.1756	0.2987
A	250.8778	1.9652	2.0401	0.2209	0.3619
A	218.8194	1.1714	2.3921	0.1766	0.3002
A	164.0012	1.7425	2.8366	0.3000	0.4615
A	150.8916	1.9067	1.7664	0.6873	0.8147
A	106.4806	1.4359	1.0500	0.5291	0.6920
A	101.4911	3.4056	0.8816	0.7460	0.8545
A	85.5975	2.5012	0.6826	0.5890	0.7413
A	77.7040	3.0430	0.3210	0.5350	0.6970
A	57.3431	1.7902	0.5773	0.6860	0.8137
A	54.1366	0.6409	0.5787	0.6923	0.8182
A	48.3104	2.9848	2.2690	0.6668	0.8001
A	43.3705	2.0589	0.5256	0.7320	0.8452
A	30.0086	0.3540	0.8407	0.7057	0.8275
A	25.2666	0.5574	0.2926	0.7456	0.8543

Processing aupcphexdienic5sm6psd1pbedcms.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-1017.9611714

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
158.40804	169.338	141.489	133.624	169.389	43.828	33.909

31

C	1.040179	3.882877	0.578252
C	0.082942	2.731589	0.243902
C	1.003991	1.607514	-0.191632
C	2.407600	2.161109	-0.398424
C	2.200410	3.679777	-0.397314
C	0.695240	0.344785	-0.374248
C	0.660753	-0.985463	-0.630829
C	1.117294	-2.067663	0.326618
C	2.504438	-2.584503	-0.053571
C	3.619341	-1.647795	0.323089

O	4.742200	-1.903638	-0.362357
Au	-1.446246	-0.358235	-0.112679
P	-3.713994	-0.302219	0.336041
O	3.555161	-0.779859	1.169259
H	-4.276711	0.980042	0.449499
H	-4.545144	-0.908929	-0.620155
H	-4.127605	-0.917135	1.529057
H	0.524028	-1.299689	-1.670995
H	1.127115	-1.690626	1.352258
H	0.416779	-2.907129	0.278590
H	2.703055	-3.522886	0.481244
H	2.573657	-2.821617	-1.120415
H	5.438978	-1.307252	-0.036358
H	3.027624	1.856587	0.454007
H	2.881614	1.773657	-1.304748
H	-0.562213	3.008665	-0.600260
H	-0.567783	2.438678	1.073613
H	3.106471	4.221743	-0.109425
H	1.909845	4.019933	-1.399356
H	0.561770	4.862383	0.484368
H	1.399816	3.781999	1.609843

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3749.1608	167.0070	189.6505	0.2093	0.3462	7.7776
A	3167.6095	5.2258	101.9763	0.5727	0.7283	
A	3146.3567	37.1100	239.3966	0.7370	0.8486	
A	3142.2313	29.8524	229.0843	0.7490	0.8565	
A	3138.6601	2.3285	189.7046	0.7431	0.8526	
A	3135.9853	36.6402	384.9329	0.2591	0.4115	
A	3132.9768	17.9524	182.5043	0.2749	0.4312	
A	3130.4122	1.1443	436.8156	0.2493	0.3992	
A	3103.9307	13.9508	372.4246	0.0593	0.1120	
A	3081.1760	8.4863	328.5393	0.1244	0.2212	
A	3078.2441	14.1067	245.8792	0.0835	0.1541	
A	3076.1551	45.6783	78.3891	0.7277	0.8424	
A	3072.0092	38.4805	578.0531	0.0817	0.1511	
A	3065.4142	15.6591	242.8522	0.0951	0.1736	
A	2562.8264	0.3367	320.2965	0.7375	0.8489	
A	2559.1200	0.3733	308.5224	0.6920	0.8180	
A	2538.2892	9.7080	853.6921	0.0188	0.0369	
A	1972.1534	37.5824	96.2902	0.5491	0.7090	
A	1823.6544	459.0587	14.9463	0.1863	0.3141	
A	1488.8107	0.4048	2.2131	0.7396	0.8503	
A	1474.2494	8.8955	27.8273	0.7494	0.8568	

A	1463.8807	41.9286	10.6916	0.7238	0.8398
A	1454.4272	18.0244	32.0188	0.6730	0.8046
A	1451.1661	17.0039	17.0916	0.6293	0.7725
A	1446.3286	32.5478	13.3275	0.2434	0.3915
A	1432.5751	79.2052	22.8849	0.3973	0.5687
A	1426.3309	47.9742	23.5013	0.7279	0.8425
A	1352.6120	3.9129	10.3134	0.7290	0.8432
A	1345.7307	3.1549	12.3828	0.7379	0.8492
A	1331.4645	2.8723	7.7768	0.7262	0.8414
A	1327.5435	4.6076	14.4750	0.5248	0.6884
A	1317.3770	17.7928	8.6823	0.4785	0.6473
A	1296.6769	1.5003	8.5466	0.5756	0.7307
A	1251.8094	3.5162	24.7304	0.7493	0.8567
A	1248.0498	19.2274	14.2159	0.5768	0.7316
A	1236.1160	12.8995	49.6559	0.1751	0.2980
A	1231.9847	5.6472	13.0536	0.6002	0.7502
A	1209.9593	111.1759	16.8904	0.2179	0.3579
A	1175.3838	216.0205	0.7212	0.3123	0.4759
A	1165.0727	48.9936	7.9922	0.4300	0.6014
A	1153.3266	0.8079	6.1073	0.3149	0.4789
A	1145.6050	2.8154	4.7726	0.7315	0.8450
A	1118.5020	9.4189	39.9119	0.7490	0.8565
A	1113.4398	9.7940	38.1461	0.7497	0.8569
A	1070.5813	30.1283	27.6785	0.2910	0.4508
A	1061.9063	0.5724	13.0380	0.7260	0.8412
A	1041.4015	2.3914	14.2299	0.7393	0.8501
A	1034.8390	6.5495	6.2940	0.5035	0.6697
A	975.7625	241.0404	26.1780	0.7446	0.8536
A	971.0024	9.7641	21.0858	0.4918	0.6594
A	970.2220	7.5664	3.5476	0.4903	0.6580
A	928.2079	4.6722	16.9559	0.1024	0.1858
A	917.0281	0.8070	3.0522	0.7499	0.8571
A	900.6455	27.4653	20.4253	0.5936	0.7450
A	887.7949	33.4335	14.5297	0.2721	0.4278
A	876.7327	4.1912	2.2726	0.7353	0.8475
A	848.1683	4.2814	15.3450	0.1947	0.3260
A	824.2824	35.0414	16.2049	0.0659	0.1236
A	713.2563	3.0441	22.7377	0.0631	0.1188
A	669.8624	102.8094	0.6277	0.2174	0.3572
A	631.3795	54.9786	3.7313	0.6696	0.8021
A	580.1650	9.3124	5.6547	0.7464	0.8548
A	563.8350	53.6569	20.6986	0.4992	0.6660
A	556.5641	22.3254	4.5618	0.7486	0.8562
A	540.9090	27.8295	3.6379	0.4501	0.6208
A	527.2571	23.4790	1.9364	0.6976	0.8219
A	511.8321	2.1312	1.2330	0.5254	0.6888
A	484.7983	0.5621	1.3817	0.7498	0.8570

A	463.3477	4.8844	14.6010	0.2837	0.4420
A	422.9321	13.4116	17.9786	0.7441	0.8533
A	375.4143	5.4147	12.7850	0.3163	0.4806
A	311.7320	7.9330	14.4328	0.2551	0.4065
A	266.5972	5.7238	3.6490	0.2961	0.4570
A	260.0849	1.9899	1.8686	0.6652	0.7989
A	218.5218	1.8061	3.4609	0.4154	0.5870
A	174.3974	4.1604	4.8497	0.4395	0.6106
A	170.7467	1.9546	4.5514	0.7452	0.8540
A	109.1480	0.8943	0.3426	0.7432	0.8527
A	104.0574	0.4587	1.7974	0.7430	0.8525
A	92.9323	1.7855	0.9887	0.6300	0.7730
A	88.9242	1.4315	1.3536	0.6656	0.7992
A	71.4892	3.5865	0.5907	0.7497	0.8569
A	65.6322	1.3457	0.9161	0.7491	0.8565
A	53.4597	2.6966	1.4862	0.7408	0.8511
A	52.2821	4.1821	1.9151	0.7231	0.8393
A	47.7810	1.9889	0.2924	0.7464	0.8548
A	35.3361	0.5154	1.7290	0.7496	0.8569

5-exo-trig prod for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid:

Processing aupcphexdienic5prod6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-1018.2657303

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
156.70126	167.822	144.106	134.307	167.879	43.828	33.788

31

C	3.864339	-1.403316	0.743847
C	3.959442	-0.792683	-0.626333
O	3.435634	0.243991	-0.973923
C	1.437498	-0.943334	1.226007
C	2.860353	-0.690827	1.642331
O	4.722145	-1.532740	-1.437929
C	0.664298	-0.005828	0.698261
Au	-1.364302	-0.431730	0.053117
P	-3.499615	-1.240470	-0.541500
C	0.495203	1.299695	0.323968
H	-4.542832	-0.300864	-0.589775
H	-4.044742	-2.220451	0.304106

H	-3.616643	-1.856071	-1.798437
C	0.044166	2.416182	1.238895
C	0.758041	1.870519	-1.035836
H	1.058841	-1.958211	1.358139
H	3.063997	0.387011	1.641545
H	2.992415	-1.050003	2.671024
H	4.870497	-1.369287	1.182839
H	3.634210	-2.471487	0.633094
H	4.786774	-1.078044	-2.293253
C	-0.044334	3.169240	-1.053610
H	1.842569	2.082626	-1.035099
H	0.594694	1.166209	-1.856709
C	0.125962	3.683602	0.376052
H	-0.981763	2.232092	1.584035
H	0.665802	2.430055	2.144457
H	-0.617162	4.432628	0.663249
H	1.114917	4.146957	0.485556
H	0.304396	3.874911	-1.812670
H	-1.103951	2.956123	-1.262536

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3804.2157	120.9989	97.8261	0.2169	0.3565	4.1417
A	3147.5906	1.7039	70.4605	0.2178	0.3577	
A	3131.0936	10.2178	101.5669	0.7369	0.8485	
A	3127.0679	10.8031	181.3059	0.2411	0.3885	
A	3125.3550	5.6267	34.4757	0.4482	0.6190	
A	3106.9261	4.2037	34.6085	0.6897	0.8164	
A	3097.1354	0.5140	145.2522	0.5838	0.7372	
A	3092.1451	4.3676	38.2255	0.5126	0.6777	
A	3057.7947	18.1580	110.0595	0.1755	0.2986	
A	3049.8060	6.3060	164.1257	0.1081	0.1951	
A	3046.1317	10.6858	35.2182	0.5001	0.6668	
A	3045.1884	11.4529	247.1740	0.0534	0.1013	
A	3028.1890	20.3251	65.7362	0.1306	0.2311	
A	3001.4619	17.4413	231.9558	0.1367	0.2405	
A	2541.1956	0.6408	130.0591	0.7308	0.8445	
A	2538.2207	0.8174	122.4631	0.7469	0.8551	
A	2516.7268	13.7447	448.8494	0.0559	0.1059	
A	1879.0056	22.7806	63.7367	0.6896	0.8163	
A	1850.4314	316.6806	4.4825	0.0706	0.1319	
A	1476.2904	8.0724	2.8080	0.4583	0.6285	
A	1462.7565	9.7414	10.9760	0.7494	0.8567	
A	1445.3943	86.0567	8.0107	0.6451	0.7843	
A	1439.3226	56.1840	7.7300	0.6982	0.8223	

A	1427.6785	48.8767	28.6956	0.1926	0.3231
A	1418.5120	39.8179	24.2906	0.5749	0.7301
A	1412.9371	14.9691	7.7265	0.5938	0.7452
A	1402.5230	34.8590	9.3543	0.6710	0.8031
A	1340.7987	1.7738	2.8054	0.6441	0.7835
A	1329.2393	7.0318	4.8601	0.7342	0.8467
A	1320.7450	0.4812	2.1635	0.7482	0.8560
A	1310.3799	6.8605	13.3410	0.3855	0.5565
A	1302.8030	28.7550	3.6617	0.5535	0.7126
A	1280.9307	4.5974	3.3232	0.7488	0.8564
A	1247.3688	2.8726	7.3634	0.6834	0.8119
A	1232.5438	15.5155	3.8933	0.7251	0.8407
A	1229.2086	17.8083	19.8623	0.2577	0.4099
A	1203.9486	1.4964	2.9149	0.7092	0.8298
A	1197.6121	110.8182	1.8593	0.2698	0.4250
A	1169.9110	78.3827	0.8946	0.5223	0.6862
A	1168.1177	66.6817	3.8263	0.6521	0.7894
A	1143.0265	13.2669	9.7972	0.3955	0.5668
A	1128.6374	26.8201	1.9149	0.3971	0.5685
A	1121.7927	2.0189	15.4073	0.7494	0.8568
A	1119.3585	2.7576	16.1606	0.7498	0.8570
A	1069.7529	16.2609	9.0053	0.2236	0.3655
A	1057.1405	8.3364	3.3607	0.6272	0.7709
A	1036.8086	2.2188	6.4294	0.7410	0.8513
A	999.2994	189.0050	16.6006	0.6382	0.7792
A	984.9133	8.1597	2.7490	0.7224	0.8388
A	962.1078	7.9645	1.8945	0.6464	0.7852
A	957.3979	25.2312	6.0499	0.3335	0.5002
A	922.4968	1.3950	9.9095	0.0449	0.0859
A	892.3347	8.0990	3.3542	0.1357	0.2390
A	891.9769	7.7748	1.0596	0.6141	0.7609
A	867.9084	10.7244	2.4975	0.7390	0.8499
A	855.8021	0.9129	6.1985	0.3406	0.5081
A	826.0363	7.4131	7.2873	0.2084	0.3450
A	808.5181	19.8009	8.0524	0.0839	0.1547
A	694.7451	2.2114	5.4328	0.0340	0.0657
A	674.9854	105.3134	0.7406	0.6146	0.7613
A	625.4742	21.1856	3.1703	0.5281	0.6912
A	578.8977	19.9170	2.5387	0.7324	0.8455
A	562.6027	64.2173	6.3960	0.4384	0.6096
A	555.2986	5.1598	2.0050	0.1975	0.3299
A	521.4186	12.1970	0.5090	0.4513	0.6219
A	517.0656	11.1802	5.0786	0.1804	0.3057
A	486.7585	13.0182	3.1941	0.5257	0.6891
A	476.9577	5.2442	0.3885	0.3216	0.4867
A	469.9122	4.9370	0.4512	0.0753	0.1400
A	424.5951	5.7965	2.1502	0.7497	0.8570

A	359.5243	3.1331	1.6381	0.5569	0.7154
A	283.5214	1.9673	12.2343	0.2052	0.3405
A	268.3956	3.7454	3.2909	0.6115	0.7590
A	261.1139	1.1103	0.4947	0.7484	0.8561
A	204.8279	1.4040	2.7586	0.1719	0.2934
A	190.1827	0.3437	2.3911	0.5323	0.6948
A	143.0305	0.7097	0.1627	0.6010	0.7508
A	112.5644	4.5230	2.1717	0.6415	0.7816
A	98.2638	4.6650	1.5272	0.5523	0.7116
A	89.3838	0.3011	1.2430	0.7086	0.8295
A	70.3090	1.9772	0.5321	0.7119	0.8317
A	67.3596	0.8099	0.4237	0.7431	0.8526
A	59.4816	4.7545	0.2119	0.5997	0.7498
A	52.8898	6.0905	2.1728	0.7499	0.8571
A	44.4117	0.2054	2.0295	0.7440	0.8532
A	42.0304	1.4911	1.6861	0.5473	0.7075
A	28.1104	0.2453	1.9627	0.7447	0.8537

Processing aupcphexdienic5prod6psd1pbetols.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-1017.9138387

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
160.06595	170.279	133.847	128.653	170.314	43.828	33.820

31

C	2.687024	-2.735128	0.645106
C	3.503209	-1.730084	-0.067237
O	2.873530	-0.788575	-0.616621
C	1.302481	-1.013537	-0.378629
C	1.354171	-2.001277	0.791219
O	4.788049	-1.813869	-0.143196
C	0.546246	0.228989	-0.174287
Au	-1.474406	-0.203889	-0.068046
P	-3.756179	-0.649811	0.029592
C	1.013126	1.486715	-0.081422
H	-4.580374	0.340397	0.597114
H	-4.172663	-1.775895	0.764879
H	-4.431848	-0.877398	-1.184470
C	0.126405	2.697592	0.154710
C	2.454632	1.986681	-0.168370
H	1.052477	-1.505306	-1.324943

H	1.318208	-1.446877	1.733343
H	0.499765	-2.679044	0.758754
H	3.159766	-3.051772	1.577850
H	2.622961	-3.617447	-0.008195
H	5.167803	-1.086516	-0.671715
C	2.352622	3.517825	-0.121412
H	3.026793	1.621572	0.695863
H	2.969364	1.631331	-1.065252
C	1.074378	3.778890	0.675200
H	-0.304248	3.020689	-0.804398
H	-0.709681	2.475135	0.825482
H	0.683617	4.792472	0.544309
H	1.262389	3.630992	1.746683
H	3.240178	3.987620	0.313958
H	2.237853	3.914021	-1.138261

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3711.2906	257.8193	124.3024	0.2501	0.4001	7.8368
A	3190.2677	1.1542	62.1293	0.5556	0.7144	
A	3172.7149	4.7474	158.5713	0.3457	0.5138	
A	3140.9867	43.7059	174.5329	0.6367	0.7780	
A	3135.8704	27.6520	150.8159	0.7247	0.8404	
A	3129.7437	30.5736	305.6989	0.1865	0.3144	
A	3124.9820	28.9945	53.6469	0.5207	0.6848	
A	3124.3367	7.3932	54.4935	0.2654	0.4195	
A	3116.5377	1.0142	193.4965	0.1074	0.1940	
A	3077.7975	10.4210	223.7540	0.1415	0.2480	
A	3073.8399	42.4766	124.9682	0.2616	0.4147	
A	3067.1201	36.6768	202.1456	0.1354	0.2385	
A	3056.5340	24.9706	196.5786	0.0789	0.1462	
A	3047.4733	15.8015	182.3294	0.1183	0.2116	
A	2535.5372	3.3910	237.9270	0.7421	0.8519	
A	2533.2483	4.4398	242.3783	0.6349	0.7767	
A	2517.4918	36.6258	742.4994	0.0556	0.1053	
A	1727.9567	41.2539	134.8300	0.2649	0.4189	
A	1677.0404	865.0838	6.4532	0.3044	0.4668	
A	1577.6925	119.7952	21.8602	0.1272	0.2257	
A	1503.0615	0.7817	1.8245	0.6906	0.8170	
A	1486.7400	6.9879	6.9681	0.7256	0.8410	
A	1485.7435	7.8963	20.9898	0.7499	0.8570	
A	1468.0272	9.0744	8.2945	0.6882	0.8153	
A	1462.9303	7.8283	9.8905	0.7500	0.8571	
A	1425.6981	49.4704	18.7128	0.5743	0.7296	
A	1381.6594	73.7177	21.2755	0.6498	0.7877	
A	1351.7421	2.0276	1.5949	0.4206	0.5921	
A	1339.8005	0.8122	3.0056	0.5350	0.6971	

A	1331.5917	7.5493	8.5866	0.4936	0.6609
A	1321.1022	26.0734	14.0415	0.5841	0.7375
A	1309.8154	28.4237	5.7525	0.2537	0.4047
A	1302.8059	1.0715	7.3060	0.6604	0.7954
A	1274.8802	50.4862	3.7688	0.7168	0.8350
A	1260.5074	3.9872	14.5608	0.6770	0.8074
A	1242.9739	5.1293	4.9743	0.7339	0.8465
A	1234.1212	37.4826	9.0023	0.4889	0.6567
A	1213.5702	79.9639	5.0810	0.7496	0.8569
A	1199.6681	18.2741	2.1794	0.5656	0.7225
A	1192.8496	10.1028	17.1113	0.1547	0.2679
A	1180.6791	7.6981	3.0108	0.2133	0.3516
A	1151.9014	3.4304	3.8258	0.1846	0.3117
A	1127.0305	7.4115	22.4268	0.7372	0.8487
A	1124.4615	5.7501	29.3854	0.7300	0.8439
A	1113.4961	47.8443	32.6843	0.5829	0.7365
A	1074.6566	15.5063	16.3513	0.7490	0.8565
A	1053.7704	5.0330	12.6947	0.4319	0.6033
A	1032.4585	2.4156	11.8186	0.4016	0.5731
A	1021.3316	15.6115	21.7309	0.4089	0.5804
A	998.2373	229.7401	41.7988	0.7239	0.8399
A	990.3927	1.4486	9.8577	0.5129	0.6780
A	965.2390	0.5588	11.2603	0.2116	0.3493
A	938.7012	3.5538	16.3775	0.0932	0.1705
A	927.4577	0.2127	4.5336	0.1675	0.2869
A	920.0107	62.5698	6.4621	0.3000	0.4615
A	878.5738	4.6668	3.0672	0.2755	0.4320
A	863.7474	14.9123	6.4465	0.5714	0.7272
A	845.4956	32.1825	1.5634	0.5406	0.7018
A	815.2602	4.0724	18.1384	0.2560	0.4077
A	733.4989	72.1313	3.4272	0.3162	0.4804
A	720.0373	99.7270	19.4529	0.1762	0.2996
A	681.2881	107.4883	3.1397	0.2752	0.4316
A	632.1534	12.4776	2.4008	0.7499	0.8571
A	600.8313	13.8851	2.9494	0.5982	0.7486
A	575.6787	0.8800	0.6912	0.3343	0.5011
A	529.9728	218.0376	33.9883	0.3855	0.5565
A	500.4755	98.2523	12.3799	0.5437	0.7044
A	496.9041	35.6772	20.3187	0.1760	0.2993
A	478.2996	0.6881	1.3986	0.1680	0.2877
A	468.2933	7.6731	5.8603	0.2303	0.3744
A	416.1149	70.2858	39.9435	0.3066	0.4693
A	358.1331	33.6655	7.2688	0.7374	0.8488
A	300.7626	2.5034	12.8371	0.1645	0.2825
A	288.5678	12.0335	10.2608	0.5688	0.7251
A	271.8529	1.3518	4.1718	0.4695	0.6390
A	238.0500	8.7650	11.4128	0.1882	0.3168

A	186.3225	12.3613	7.5678	0.4971	0.6641
A	168.8044	3.7465	5.0801	0.4618	0.6318
A	133.0310	0.0697	1.0915	0.3728	0.5431
A	124.2060	2.8429	0.3600	0.4157	0.5872
A	110.7737	2.6375	0.8089	0.6597	0.7950
A	98.1616	1.2686	0.6103	0.7017	0.8247
A	79.8057	0.8869	1.1854	0.5465	0.7067
A	76.0050	0.4045	0.1741	0.3902	0.5613
A	55.0994	3.8583	1.8143	0.7496	0.8569
A	53.3610	4.9332	0.3509	0.7138	0.8330
A	40.6260	2.4866	1.2769	0.7250	0.8406

6-endo-dig prod for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid:

Processing aupcphexdienic6prod6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-1018.2520914

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
158.11540	168.358	134.279	128.244	168.395	43.828	33.773

31

C	3.193383	-1.781428	0.013738
O	2.965522	-0.544318	-0.100528
C	1.577264	0.041495	-0.139946
C	0.529429	-0.975478	-0.339355
C	0.812543	-2.209863	0.524914
C	2.159889	-2.823856	0.150216
C	1.660947	1.370572	-0.043890
Au	-1.471619	-0.322092	-0.078259
P	-3.767869	0.232718	0.155898
O	4.434044	-2.165368	0.022751
C	2.937387	2.175989	0.058390
C	0.487351	2.318502	-0.022557
H	0.549482	-1.284317	-1.401218
H	-4.574750	0.151434	-0.993857
H	-4.102751	1.525011	0.601138
H	-4.531071	-0.540266	1.049963
H	0.810660	-1.940936	1.589615
H	0.035211	-2.968263	0.393759
H	2.534789	-3.578777	0.852628
H	2.105235	-3.328514	-0.827779

H	5.045505	-1.414473	-0.089404
C	1.089470	3.655812	0.419723
H	0.071224	2.404074	-1.038512
H	-0.326086	1.962223	0.623437
H	3.712321	1.835177	-0.636727
C	2.491513	3.620758	-0.178910
H	3.349692	2.068890	1.073629
H	0.495262	4.515342	0.095198
H	1.151236	3.693413	1.516279
H	3.175141	4.352642	0.261728
H	2.443236	3.824329	-1.257633

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3749.1627	197.7864	109.7215	0.3603	0.5298	3.4903
A	3123.4920	18.8552	110.3980	0.7449	0.8538	
A	3122.5577	3.3155	67.4837	0.5133	0.6784	
A	3119.6735	20.7042	170.6082	0.2828	0.4409	
A	3103.5567	12.7765	78.7446	0.3041	0.4664	
A	3098.4034	2.6033	179.9125	0.3782	0.5489	
A	3074.1146	16.9329	80.7227	0.3739	0.5443	
A	3053.3129	12.7911	35.7638	0.2242	0.3662	
A	3047.1674	27.6400	45.3037	0.5827	0.7363	
A	3038.8905	22.0626	129.7522	0.1419	0.2486	
A	3028.9098	7.2989	174.8056	0.1078	0.1945	
A	3023.5783	7.8896	167.0980	0.0722	0.1346	
A	3017.1728	15.3970	118.4685	0.0271	0.0527	
A	2979.3543	9.2289	109.2738	0.1673	0.2866	
A	2523.8427	5.0174	135.2981	0.7426	0.8523	
A	2520.7096	6.3826	131.9097	0.6228	0.7676	
A	2503.8537	35.7943	421.0948	0.0554	0.1049	
A	1771.7072	47.4269	210.7750	0.2012	0.3350	
A	1649.3052	660.6763	96.4045	0.2279	0.3712	
A	1551.4380	228.5701	31.7373	0.2591	0.4116	
A	1477.6113	2.3747	1.9998	0.4904	0.6581	
A	1463.3148	9.9326	12.9888	0.7418	0.8518	
A	1459.0412	4.9752	8.7347	0.5561	0.7148	
A	1437.5628	8.6253	6.8208	0.6294	0.7726	
A	1428.5119	11.1533	6.6081	0.5697	0.7259	
A	1401.7630	60.0667	24.0010	0.4637	0.6336	
A	1342.4812	5.4773	1.1547	0.7496	0.8569	
A	1337.7814	0.8457	4.7690	0.6382	0.7792	
A	1330.6353	16.0539	2.1798	0.7498	0.8570	
A	1324.5776	0.4270	0.7139	0.6318	0.7744	
A	1317.9229	2.1813	5.3325	0.5934	0.7448	
A	1296.3223	9.0741	7.8005	0.3169	0.4813	
A	1289.6458	0.6501	4.9915	0.6722	0.8040	

A	1248.6566	10.2702	11.1147	0.4333	0.6046
A	1244.2905	10.5807	17.4157	0.2199	0.3605
A	1225.1490	3.9546	4.2197	0.6853	0.8133
A	1220.6018	85.7361	7.4493	0.7281	0.8427
A	1200.4633	31.9141	37.7297	0.4663	0.6360
A	1185.1725	10.4101	4.1802	0.7112	0.8312
A	1165.5797	0.6244	3.0453	0.2451	0.3937
A	1145.5976	0.9266	1.3615	0.7356	0.8477
A	1128.0253	4.1588	15.2478	0.7464	0.8548
A	1127.3111	4.1805	14.9840	0.7390	0.8499
A	1104.4601	21.6424	14.4131	0.7483	0.8560
A	1093.4649	5.0372	61.3601	0.2546	0.4058
A	1045.4374	4.5889	27.2986	0.7500	0.8571
A	1035.8089	33.9809	40.3009	0.5453	0.7058
A	1015.2937	2.9714	5.7663	0.5087	0.6744
A	1009.2391	173.3053	5.5159	0.6746	0.8057
A	1005.7500	22.9106	17.8680	0.3500	0.5185
A	978.0651	1.7921	7.2810	0.3884	0.5595
A	962.8155	4.9508	22.0523	0.2579	0.4100
A	930.2211	0.1183	16.1404	0.1094	0.1972
A	908.9743	1.0152	1.3860	0.5456	0.7060
A	890.3538	10.8332	0.5217	0.5659	0.7228
A	876.9449	60.0483	50.8267	0.3503	0.5188
A	870.7984	8.6092	13.6098	0.3519	0.5206
A	847.8307	38.9947	27.7374	0.2752	0.4317
A	774.4914	81.0566	20.4598	0.6269	0.7707
A	745.8515	26.1206	26.0997	0.4801	0.6487
A	679.1184	97.5652	3.8370	0.6449	0.7841
A	658.8333	45.6344	13.4396	0.6648	0.7986
A	613.8503	3.4456	2.7239	0.6336	0.7757
A	583.4310	12.9830	6.4087	0.6540	0.7908
A	572.2046	12.7489	7.2601	0.1772	0.3010
A	554.7524	2.3042	5.3065	0.3008	0.4625
A	500.2568	1.8432	1.8013	0.5463	0.7066
A	489.9261	7.7321	5.9927	0.5921	0.7438
A	458.9794	0.2211	0.1731	0.7136	0.8329
A	441.3657	0.4608	0.4183	0.4315	0.6029
A	397.7384	2.4931	1.1348	0.4330	0.6043
A	358.5198	2.0608	16.8469	0.3270	0.4928
A	319.7031	2.8070	3.1962	0.4435	0.6145
A	304.5057	1.2324	2.1893	0.4785	0.6473
A	271.2574	0.0798	8.4692	0.1761	0.2995
A	259.5913	0.1733	0.3514	0.3288	0.4949
A	192.9815	0.1395	1.0547	0.1680	0.2876
A	167.5294	0.0285	2.6460	0.3376	0.5048
A	159.2991	0.0517	1.4625	0.4294	0.6008
A	140.8509	0.5825	1.7225	0.6126	0.7597

A	101.5295	0.9986	0.1642	0.7477	0.8556
A	88.5487	0.7185	0.1480	0.4763	0.6453
A	78.9354	0.0803	0.0221	0.7141	0.8332
A	74.8020	1.3798	0.8521	0.5713	0.7272
A	60.5130	4.4620	0.7628	0.6557	0.7921
A	52.0992	3.6919	1.9229	0.6890	0.8159
A	28.1906	0.6978	0.3581	0.2950	0.4556

Processing aupcphexdienic6prod6psd1pbetols.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-1017.9178832

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
159.80847	169.928	133.886	127.296	169.969	43.828	33.751

31

C	3.163496	-1.795346	0.006789
O	2.935420	-0.556046	-0.118859
C	1.566812	0.029648	-0.132476
C	0.501457	-0.977700	-0.315925
C	0.786774	-2.207264	0.560211
C	2.131430	-2.831428	0.188251
C	1.655492	1.359998	-0.030335
Au	-1.472998	-0.319806	-0.083248
P	-3.710241	0.258930	0.147069
O	4.405446	-2.170972	-0.019613
C	2.945223	2.152773	0.053192
C	0.488784	2.319996	0.013160
H	0.538556	-1.302142	-1.371799
H	-4.516653	0.231046	-1.006400
H	-4.009584	1.545878	0.633368
H	-4.488183	-0.526644	1.018489
H	0.791316	-1.931430	1.620498
H	0.010549	-2.964825	0.432332
H	2.507723	-3.559944	0.915392
H	2.067734	-3.364642	-0.772119
H	5.004694	-1.414445	-0.162450
C	1.113826	3.660421	0.423525
H	0.042710	2.398493	-0.987677
H	-0.304504	1.981360	0.688979
H	3.704693	1.803213	-0.652328
C	2.512571	3.603160	-0.187150

H	3.370634	2.049025	1.061215
H	0.526056	4.518304	0.084857
H	1.186331	3.719014	1.516877
H	3.207648	4.326596	0.248498
H	2.458649	3.802492	-1.264812

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3713.9113	222.3732	158.3805	0.3826	0.5535	3.8458
A	3160.2185	5.0016	106.3145	0.5420	0.7030	
A	3149.3071	32.2998	183.9055	0.7464	0.8548	
A	3143.3789	30.9082	255.0358	0.3235	0.4888	
A	3134.7556	17.6051	163.2466	0.2256	0.3681	
A	3132.7612	3.0175	298.0860	0.3672	0.5372	
A	3108.1529	17.1088	133.1000	0.3473	0.5156	
A	3096.8550	15.2118	77.3024	0.1906	0.3202	
A	3078.8606	34.7746	69.6512	0.5736	0.7290	
A	3073.3562	28.2987	243.3908	0.1343	0.2368	
A	3064.5409	14.2569	265.3994	0.1219	0.2174	
A	3060.1248	7.2440	301.7965	0.0638	0.1199	
A	3056.4924	23.4738	145.7214	0.0383	0.0738	
A	2996.8672	13.1217	192.9123	0.1816	0.3074	
A	2534.4212	3.2384	199.7299	0.7443	0.8534	
A	2532.7908	3.2903	211.4603	0.7454	0.8541	
A	2517.0641	34.0199	655.0982	0.0434	0.0831	
A	1773.1923	54.4786	385.2851	0.2161	0.3554	
A	1639.1281	801.0067	128.9403	0.2251	0.3675	
A	1561.2248	286.5191	52.7843	0.2429	0.3909	
A	1501.5086	0.7148	3.2691	0.5469	0.7071	
A	1485.5235	9.7409	19.7150	0.7426	0.8523	
A	1484.1062	3.9213	16.1990	0.5620	0.7196	
A	1461.2552	9.9301	11.5445	0.6136	0.7605	
A	1449.2655	15.4461	13.8333	0.5284	0.6915	
A	1418.4963	78.4549	42.4359	0.4540	0.6245	
A	1357.5819	4.8571	1.3963	0.7439	0.8531	
A	1353.1801	0.8799	9.0669	0.6279	0.7714	
A	1347.8509	13.2294	3.5942	0.5499	0.7096	
A	1342.2587	4.0220	2.8653	0.7014	0.8245	
A	1334.4558	1.5965	6.8933	0.5250	0.6885	
A	1312.9986	14.0131	12.0368	0.4288	0.6002	
A	1306.2762	0.8182	6.8462	0.6659	0.7994	
A	1266.9745	18.2035	25.5219	0.2702	0.4254	
A	1261.7944	7.7218	22.4603	0.3252	0.4908	
A	1240.8175	6.4534	8.5076	0.6292	0.7724	
A	1237.4657	120.7348	25.6882	0.6115	0.7589	

A	1213.0935	13.1596	58.2555	0.4366	0.6079
A	1196.8525	8.8604	7.7758	0.7443	0.8534
A	1187.6245	1.6114	2.6711	0.1537	0.2665
A	1159.9810	1.7618	2.1000	0.6869	0.8144
A	1128.2832	7.2928	22.9354	0.7418	0.8518
A	1125.3441	7.4698	23.5431	0.7125	0.8321
A	1112.7792	24.0771	27.0135	0.5911	0.7430
A	1111.1154	7.4674	86.8723	0.2949	0.4555
A	1058.2481	16.9123	55.4353	0.7493	0.8567
A	1050.1528	43.5210	33.4429	0.5833	0.7368
A	1031.5111	13.1204	6.5436	0.4273	0.5988
A	1019.1956	5.0655	20.4544	0.2079	0.3442
A	1002.3127	201.8316	30.2708	0.7085	0.8294
A	987.5312	0.8250	10.0322	0.5605	0.7184
A	971.0935	5.2389	31.7813	0.2790	0.4362
A	936.2685	1.6432	21.9512	0.1422	0.2490
A	923.8330	1.8202	3.2506	0.5237	0.6874
A	903.6322	14.7525	3.6307	0.2148	0.3536
A	888.6669	112.6783	117.6504	0.3769	0.5475
A	881.1134	6.4786	17.0333	0.3822	0.5530
A	856.9875	35.4059	31.1593	0.2933	0.4536
A	792.8199	90.9388	26.5529	0.6939	0.8193
A	760.9021	18.6126	33.7827	0.5075	0.6733
A	683.2727	35.1015	14.8616	0.7494	0.8567
A	659.6561	106.9997	7.1361	0.4368	0.6080
A	632.9486	3.7202	5.0923	0.5346	0.6967
A	594.2598	12.6479	8.9615	0.5806	0.7347
A	580.4064	24.6678	8.3199	0.1733	0.2954
A	566.4652	3.1252	6.2075	0.2885	0.4478
A	515.3435	2.8961	2.2991	0.5778	0.7324
A	498.8831	12.2489	7.3382	0.6143	0.7611
A	484.4283	0.2240	0.4982	0.7500	0.8571
A	477.6692	0.5502	1.7777	0.6309	0.7737
A	406.6083	2.8695	1.9620	0.4432	0.6142
A	365.5375	3.4965	24.1940	0.3572	0.5264
A	330.2589	2.4278	4.1435	0.2572	0.4092
A	308.5747	1.7992	2.7986	0.5933	0.7447
A	301.4197	0.7833	10.9294	0.1209	0.2157
A	259.3051	0.2516	0.6861	0.3213	0.4863
A	195.3507	0.1991	0.9925	0.1974	0.3297
A	172.1059	0.0040	2.9138	0.4137	0.5853
A	165.9228	0.1971	1.5557	0.4042	0.5757
A	142.3034	0.7531	2.6373	0.6035	0.7528
A	95.9222	0.2894	0.3516	0.6791	0.8089
A	87.5847	2.1621	0.4884	0.7261	0.8413
A	74.6542	3.6796	1.2580	0.5495	0.7093
A	66.1240	0.2524	0.1905	0.5466	0.7068

A	56.3220	2.5227	1.1806	0.6971	0.8215
A	42.3326	4.0203	1.7336	0.7264	0.8415
A	35.4402	2.0504	0.4695	0.3272	0.4931

6-exo-dig prod for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid:

Processing aupcphexdienic6xprod6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-1018.2328191

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
157.97721	168.264	134.862	128.115	168.299	43.828	33.445

31

O	2.625059	-0.055199	-0.673935
C	1.340418	-0.440775	0.025384
C	1.336852	-1.695101	0.475763
C	2.535316	-2.592685	0.442107
C	3.814431	-1.761669	0.524141
C	3.719107	-0.633801	-0.418249
C	0.408739	0.698324	0.109616
Au	-1.587477	-0.030340	-0.036874
P	-3.860018	-0.711857	-0.209846
O	4.789835	-0.204170	-0.999164
H	3.902480	-1.303592	1.524766
H	4.735701	-2.320373	0.338249
H	2.511540	-3.290525	1.284089
H	2.536106	-3.214122	-0.465717
H	-4.141110	-2.089899	-0.269684
H	-4.589427	-0.267245	-1.328367
H	-4.737595	-0.329814	0.821935
C	0.687435	1.808054	-0.927455
C	0.629761	1.465025	1.437808
H	0.403590	-2.058192	0.898005
H	4.608197	0.567244	-1.570053
H	0.715667	0.798940	2.304968
C	1.874213	2.318996	1.179099
H	-0.235478	2.118972	1.614629
H	0.969617	1.414452	-1.911134
H	-0.235252	2.378438	-1.084120
C	1.759854	2.735140	-0.300381
H	2.724619	2.655340	-0.819338

H	1.458304	3.784386	-0.390803
H	1.945197	3.176395	1.856458
H	2.782928	1.720205	1.354671

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3722.1258	196.1056	62.2162	0.2933	0.4536	6.2380
A	3206.1276	5.8733	56.3641	0.1958	0.3274	
A	3137.0448	0.5983	148.8974	0.3645	0.5343	
A	3119.3251	0.5012	109.9016	0.4191	0.5907	
A	3112.4913	39.9719	99.1033	0.4882	0.6561	
A	3105.4177	17.9396	146.7031	0.3747	0.5451	
A	3100.6697	10.7970	78.5095	0.4019	0.5733	
A	3091.4662	11.4921	39.1110	0.7473	0.8553	
A	3058.0755	17.5548	97.0121	0.0527	0.1002	
A	3037.7352	6.8840	105.2616	0.0736	0.1370	
A	3037.5716	75.7697	74.5211	0.2003	0.3338	
A	3035.5762	12.8330	148.8463	0.2215	0.3627	
A	3009.8681	5.8888	128.0907	0.0786	0.1458	
A	2997.4912	48.0718	65.7217	0.1768	0.3005	
A	2523.0185	6.6005	144.3606	0.6672	0.8004	
A	2518.1235	6.0833	128.9408	0.7349	0.8472	
A	2501.7783	47.0777	515.6969	0.0732	0.1364	
A	1753.0165	105.5865	113.3386	0.2610	0.4139	
A	1644.3450	694.9284	17.3920	0.1250	0.2222	
A	1571.7421	99.9206	34.0659	0.1317	0.2327	
A	1484.4957	7.0744	4.6205	0.5693	0.7255	
A	1464.2191	13.5550	3.7425	0.7481	0.8559	
A	1457.6682	7.8636	8.1845	0.7210	0.8379	
A	1453.5312	6.5411	21.2137	0.5733	0.7288	
A	1448.9392	6.3488	8.2554	0.6761	0.8067	
A	1406.6354	40.0508	8.6499	0.6612	0.7961	
A	1349.9450	1.9053	10.3302	0.3237	0.4891	
A	1324.5365	3.0007	15.1508	0.4308	0.6021	
A	1322.4917	3.8009	2.7500	0.6984	0.8224	
A	1314.3545	4.6703	4.6239	0.3078	0.4707	
A	1302.3782	3.9116	6.8117	0.3382	0.5054	
A	1283.9414	2.9663	7.3229	0.5866	0.7395	
A	1269.2227	1.7870	4.6924	0.6891	0.8159	
A	1247.0001	8.2545	10.4856	0.3787	0.5493	
A	1224.9837	15.0430	1.4118	0.7486	0.8562	
A	1217.5075	76.1988	13.4644	0.4876	0.6556	
A	1207.6387	14.5581	6.1217	0.2627	0.4161	
A	1196.4187	5.3171	6.2165	0.1394	0.2447	
A	1183.5463	4.4405	23.2988	0.3046	0.4670	
A	1167.3313	10.5121	1.5123	0.7288	0.8431	
A	1129.1321	3.1931	16.0716	0.7495	0.8568	

A	1125.7756	3.4002	16.3667	0.7469	0.8551
A	1099.7390	2.8980	4.7136	0.4459	0.6168
A	1083.2343	42.1118	9.6000	0.5851	0.7382
A	1053.1124	2.8582	24.2022	0.3968	0.5682
A	1042.0804	60.2681	3.5512	0.5702	0.7263
A	1031.4409	4.9946	4.3828	0.7194	0.8368
A	1028.8491	10.5267	3.0591	0.1177	0.2106
A	1011.9344	228.9287	16.4651	0.7432	0.8527
A	965.1948	18.8981	17.0963	0.0596	0.1124
A	941.7275	2.8335	9.6429	0.5540	0.7130
A	936.4755	21.0525	25.3650	0.4139	0.5855
A	919.2421	5.3662	6.2522	0.4120	0.5836
A	903.6641	8.2156	25.2456	0.5470	0.7072
A	897.6850	3.7151	38.2062	0.1392	0.2444
A	843.3148	24.8106	40.0868	0.2309	0.3752
A	827.7465	136.8490	8.8294	0.7500	0.8571
A	820.0941	19.8156	2.1467	0.7254	0.8408
A	780.0988	5.9857	19.2903	0.1004	0.1825
A	747.2763	41.3469	28.0336	0.2264	0.3692
A	740.1298	61.3800	5.2176	0.4417	0.6127
A	700.4874	111.4113	4.1547	0.2736	0.4297
A	654.8583	10.3711	1.0924	0.1802	0.3054
A	625.4823	30.9696	4.3742	0.5836	0.7371
A	591.9074	11.6318	8.6119	0.1815	0.3072
A	549.4505	4.1862	1.7004	0.4687	0.6383
A	478.4802	29.0296	3.8824	0.2644	0.4182
A	455.8113	1.9752	0.5471	0.7475	0.8555
A	450.9406	7.9754	2.0067	0.5173	0.6818
A	446.2754	8.4040	2.5405	0.6291	0.7724
A	436.6526	7.5848	3.0042	0.7236	0.8397
A	344.8137	1.9574	2.5329	0.5413	0.7024
A	325.5228	6.2007	11.9808	0.2320	0.3766
A	267.7389	1.4933	8.5088	0.2864	0.4453
A	255.0349	1.2755	4.1680	0.1605	0.2766
A	219.5974	1.8177	6.2670	0.2330	0.3780
A	190.4282	0.1024	2.8044	0.2956	0.4563
A	167.2142	0.1745	2.1911	0.4121	0.5837
A	155.3735	0.1611	1.4275	0.6892	0.8160
A	136.5448	0.5364	0.6110	0.7047	0.8268
A	120.0316	2.7318	0.1397	0.2940	0.4544
A	108.5563	0.3002	0.4865	0.3314	0.4978
A	88.6857	0.0685	0.0435	0.7225	0.8389
A	71.0934	0.3908	0.6514	0.7204	0.8375
A	60.7740	4.1327	0.7256	0.7412	0.8514
A	50.2569	4.9513	2.7795	0.7255	0.8409
A	16.9111	1.3231	0.8156	0.7420	0.8519

Processing aupcphexdienic6xprod6psd1pbetols.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-1017.8988083

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
159.80536	169.936	131.967	127.502	169.968	43.828	33.437

31

O	2.741147	0.046540	-0.380321
C	1.343815	-0.425820	-0.068537
C	1.237306	-1.749164	0.045714
C	2.404340	-2.687420	-0.007244
C	3.667211	-1.992132	0.496614
C	3.761109	-0.657633	-0.118540
C	0.404944	0.710051	0.024728
Au	-1.569006	-0.038118	-0.014792
P	-3.791480	-0.715114	-0.051976
O	4.923296	-0.167411	-0.393759
H	3.592746	-1.810184	1.581057
H	4.587741	-2.549736	0.314025
H	2.212443	-3.564365	0.615867
H	2.551002	-3.058580	-1.030992
H	-4.062933	-2.096894	-0.038570
H	-4.572370	-0.319299	-1.154827
H	-4.615376	-0.288890	1.007239
C	0.635956	1.763519	-1.093291
C	0.645845	1.551085	1.308543
H	0.237900	-2.148555	0.181120
H	4.856718	0.730861	-0.771819
H	0.851309	0.931649	2.188468
C	1.780461	2.530521	0.968784
H	-0.265277	2.120236	1.526204
H	0.966005	1.306146	-2.032434
H	-0.314339	2.259225	-1.313197
C	1.640979	2.807709	-0.543009
H	2.608376	2.738993	-1.052174
H	1.271283	3.821852	-0.724629
H	1.716022	3.445497	1.566099
H	2.755059	2.082744	1.196843

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3698.8927	240.8236	104.5336	0.2879	0.4471	6.9841
A	3250.4038	8.0228	136.4427	0.2117	0.3494	
A	3180.8409	1.5212	197.9458	0.3646	0.5343	
A	3152.5726	0.6331	168.3059	0.4233	0.5948	
A	3142.0430	80.5819	166.2340	0.5992	0.7494	
A	3132.7472	19.7118	134.0710	0.7279	0.8425	
A	3123.8649	8.0105	180.4988	0.4579	0.6281	
A	3113.0123	14.9400	59.3596	0.3375	0.5046	
A	3091.0886	45.8681	430.8132	0.0244	0.0477	
A	3081.1352	56.1225	67.3844	0.3729	0.5432	
A	3075.2676	27.9356	89.4042	0.1155	0.2070	
A	3070.9008	31.4349	83.8260	0.5119	0.6772	
A	3068.9354	11.2970	199.7593	0.2419	0.3896	
A	3050.7515	11.1009	231.5460	0.0812	0.1501	
A	2533.7490	3.8807	225.9773	0.6904	0.8168	
A	2530.0231	4.1010	213.0852	0.7021	0.8250	
A	2514.7167	40.9391	728.7835	0.0563	0.1065	
A	1768.5101	100.6407	132.2112	0.2185	0.3586	
A	1633.3519	861.0579	20.5321	0.1434	0.2509	
A	1579.7164	136.9179	44.1990	0.1126	0.2025	
A	1507.8016	8.1041	7.5634	0.4827	0.6511	
A	1487.0866	10.4506	8.7185	0.7300	0.8439	
A	1479.3957	11.1321	11.9290	0.6563	0.7925	
A	1473.6497	3.5039	13.6652	0.7452	0.8540	
A	1467.2748	6.6185	31.6919	0.5872	0.7399	
A	1429.7345	44.3457	12.8209	0.7072	0.8285	
A	1371.7674	1.1749	7.1718	0.2877	0.4468	
A	1348.6650	1.1857	16.2421	0.4680	0.6376	
A	1338.5814	3.3225	10.5876	0.4727	0.6419	
A	1331.1132	4.0059	3.8451	0.5660	0.7229	
A	1319.3412	3.3967	10.4287	0.3367	0.5038	
A	1300.8179	0.4941	13.1047	0.5731	0.7286	
A	1286.7819	8.4589	6.6393	0.5503	0.7100	
A	1267.4840	18.8199	10.0792	0.5549	0.7137	
A	1245.9858	16.1401	6.0803	0.6018	0.7514	
A	1241.1491	47.9180	12.6634	0.5476	0.7076	
A	1233.9609	54.7551	9.1094	0.1408	0.2468	
A	1214.8146	3.0940	8.4790	0.4804	0.6490	
A	1202.0629	5.3754	21.3393	0.3520	0.5207	
A	1187.5586	15.4811	2.0260	0.7492	0.8566	
A	1130.3427	5.4951	26.8489	0.7498	0.8570	
A	1121.7983	6.8980	24.5064	0.7497	0.8570	
A	1108.9784	27.6156	15.7660	0.7349	0.8472	
A	1095.2129	11.2211	9.9424	0.6485	0.7868	
A	1071.0602	4.8765	31.4732	0.5057	0.6717	

A	1055.4672	74.2836	5.6322	0.4279	0.5994
A	1045.1813	9.8782	3.9478	0.7413	0.8514
A	1040.4717	35.0160	2.5091	0.2755	0.4320
A	998.5810	227.2324	31.8879	0.7442	0.8533
A	981.1968	13.2565	39.6167	0.1654	0.2839
A	955.6216	9.5215	8.1789	0.6512	0.7887
A	948.7092	34.6135	17.2482	0.6220	0.7670
A	930.8989	7.4431	18.0616	0.3279	0.4939
A	910.2302	17.7774	39.3164	0.4328	0.6041
A	907.7383	1.4735	34.3186	0.1128	0.2028
A	849.9163	55.8566	12.3456	0.3026	0.4646
A	841.1029	14.5028	24.1952	0.1369	0.2409
A	827.5040	143.1226	10.6586	0.7499	0.8571
A	781.7382	9.4244	20.4753	0.0854	0.1574
A	760.5640	44.1241	20.8304	0.2397	0.3867
A	742.7979	102.9785	11.5188	0.6642	0.7982
A	703.8349	128.0019	5.4657	0.3474	0.5157
A	675.6917	15.5134	1.4689	0.4198	0.5914
A	630.6584	48.7913	8.4236	0.3528	0.5216
A	610.0039	8.8241	6.6280	0.1759	0.2991
A	565.6708	5.7418	1.7166	0.7107	0.8309
A	491.1268	0.1954	0.2801	0.7233	0.8394
A	476.3806	34.1134	10.3630	0.2364	0.3824
A	469.4101	17.2812	6.9002	0.3143	0.4782
A	454.3819	5.5610	3.7139	0.7452	0.8540
A	444.5047	37.2448	20.2543	0.5970	0.7477
A	329.3039	2.9164	10.2975	0.1929	0.3234
A	321.1899	1.4714	3.7938	0.7019	0.8249
A	299.6562	0.1531	12.9836	0.1926	0.3229
A	238.2904	0.7596	0.9048	0.2975	0.4586
A	225.7493	2.3882	8.5773	0.4105	0.5821
A	182.3423	0.9443	6.1994	0.2845	0.4430
A	174.7900	0.4224	0.4471	0.6424	0.7822
A	161.2053	1.2372	0.5163	0.6876	0.8149
A	143.2262	0.9939	0.5981	0.7474	0.8554
A	117.4148	1.1358	0.2410	0.7378	0.8491
A	110.1225	0.5482	0.9815	0.7388	0.8498
A	88.4460	0.4117	0.4446	0.7131	0.8325
A	73.7669	4.1187	0.5402	0.7363	0.8481
A	68.4118	5.8724	1.7214	0.7136	0.8329
A	56.1995	1.6102	0.4186	0.7291	0.8434
A	41.0378	0.6484	1.0098	0.7249	0.8405

7-endo-trig prod for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid:

Processing aupcphexdienic7prod-b6psdm6.log

PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-1018.2476281

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
158.22971	168.699	136.116	129.568	168.740	43.828	33.466

31

C	1.856357	2.903799	-0.507466
C	0.991213	1.722009	-0.953676
C	1.313545	0.591923	0.011178
C	1.539184	1.299494	1.336498
C	2.144968	2.669426	0.993708
O	2.850077	0.294845	-0.532818
C	3.608853	-0.633112	-0.171434
O	4.797288	-0.691439	-0.701211
C	0.458114	-0.613359	-0.020492
Au	-1.598774	-0.200066	-0.027839
P	-3.943311	0.144214	-0.025198
C	0.807491	-1.911446	0.005052
C	2.151260	-2.577260	0.110858
C	3.255058	-1.726070	0.752059
H	-4.664658	-0.270941	1.109008
H	-4.688133	-0.483878	-1.039964
H	-4.413969	1.464130	-0.151073
H	-0.002848	-2.640127	-0.043838
H	2.042058	-3.474437	0.731783
H	2.486474	-2.948528	-0.869836
H	2.887247	-1.301239	1.694068
H	4.152033	-2.316188	0.956033
H	2.124226	0.707124	2.049494
H	0.541075	1.402393	1.783204
H	1.119404	1.417857	-1.998387
H	-0.074310	1.946461	-0.815718
H	3.223181	2.679406	1.189168
H	1.713780	3.452680	1.624185
H	2.789590	2.936496	-1.080163
H	1.349262	3.855729	-0.689590
H	4.933207	0.035378	-1.336580

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3748.9680	197.9805	84.0286	0.2282	0.3716	3.1514
A	3148.9925	0.0944	90.8332	0.4511	0.6217	

A	3143.7679	2.6457	71.6268	0.2145	0.3533
A	3132.7360	22.8966	82.6129	0.6170	0.7632
A	3119.8959	3.1435	72.6092	0.6796	0.8092
A	3115.1775	3.6369	68.9633	0.4606	0.6307
A	3106.9556	12.4206	24.3689	0.3268	0.4926
A	3089.8463	1.5221	126.4282	0.4120	0.5836
A	3073.4128	31.0189	206.2839	0.0489	0.0933
A	3070.0056	1.3156	62.0816	0.1573	0.2718
A	3064.6852	15.2955	72.7232	0.3278	0.4937
A	3057.7266	23.2554	132.4923	0.0638	0.1199
A	3053.8529	5.7836	3.6807	0.3545	0.5235
A	3022.8716	15.0326	233.1630	0.1400	0.2456
A	2525.7695	5.4487	137.1007	0.7065	0.8280
A	2521.8496	5.8235	140.5667	0.6760	0.8067
A	2505.0386	37.1654	477.6493	0.0665	0.1248
A	1703.5308	22.5297	54.0030	0.1108	0.1994
A	1681.8315	649.1911	3.4111	0.2519	0.4025
A	1540.8723	198.6817	3.5768	0.1228	0.2187
A	1492.6571	10.0304	3.9529	0.5152	0.6800
A	1469.0354	8.9665	8.7633	0.7462	0.8547
A	1448.2847	15.1438	26.2630	0.6208	0.7661
A	1443.3927	1.8090	6.2777	0.7499	0.8571
A	1433.1924	29.7166	2.3483	0.7187	0.8363
A	1426.2893	12.6405	5.9488	0.7433	0.8528
A	1378.3606	38.4531	20.5501	0.1635	0.2810
A	1352.7366	3.8337	1.7624	0.4499	0.6206
A	1347.7307	3.4765	4.4596	0.2584	0.4107
A	1326.8044	0.9043	0.8305	0.6487	0.7869
A	1307.6035	1.4815	2.4749	0.4876	0.6556
A	1302.4116	5.4604	5.8671	0.7190	0.8365
A	1293.0905	8.6037	2.0375	0.7373	0.8488
A	1249.6978	4.4804	4.5484	0.5844	0.7377
A	1241.5627	16.9759	2.8898	0.7500	0.8571
A	1235.7668	19.0336	5.6332	0.7434	0.8528
A	1225.8947	117.9233	1.7882	0.7334	0.8462
A	1202.3157	4.1250	3.9027	0.6926	0.8184
A	1170.8695	27.6160	7.0089	0.2443	0.3927
A	1165.9930	5.6930	2.9272	0.5667	0.7234
A	1154.3562	47.1057	4.5651	0.6455	0.7845
A	1131.4647	6.0003	8.1094	0.1911	0.3209
A	1127.4906	3.1472	18.5757	0.6852	0.8132
A	1126.0005	3.5314	16.9606	0.7449	0.8538
A	1072.1555	4.8150	4.1055	0.7454	0.8541
A	1052.1126	13.5893	11.9953	0.4944	0.6617
A	1019.6103	1.4446	2.3401	0.3094	0.4726
A	1014.0099	12.6186	2.8509	0.4848	0.6530
A	1010.2380	179.4998	18.0325	0.7176	0.8356

A	982.5342	3.0791	9.1002	0.2497	0.3996
A	968.8679	6.8555	1.0048	0.6981	0.8222
A	940.5442	34.6487	4.1378	0.3411	0.5087
A	921.5467	48.1175	12.4631	0.4256	0.5971
A	899.7494	1.4407	6.4875	0.0417	0.0800
A	870.2193	3.7365	8.0456	0.7499	0.8571
A	848.3204	26.6041	2.6492	0.4398	0.6109
A	828.7485	22.9681	2.4006	0.4578	0.6281
A	804.9187	16.3775	12.1260	0.0906	0.1662
A	776.1998	10.4225	2.3570	0.0577	0.1092
A	758.3985	70.5130	1.2647	0.4461	0.6170
A	721.1323	44.4571	1.7422	0.0103	0.0204
A	680.2787	67.2002	1.5588	0.6328	0.7751
A	652.0195	8.3515	0.9637	0.4161	0.5877
A	616.5012	79.5530	8.8258	0.1270	0.2254
A	580.4871	8.5477	1.2066	0.3228	0.4881
A	549.2295	2.3615	2.2848	0.0793	0.1470
A	478.8542	29.2278	4.5946	0.1364	0.2401
A	467.4582	0.8241	0.2939	0.5706	0.7266
A	450.4071	0.9523	0.2430	0.1003	0.1824
A	412.0216	40.9555	7.9576	0.1341	0.2365
A	368.3036	11.2969	2.2280	0.4059	0.5774
A	335.6921	2.1161	1.7774	0.7426	0.8523
A	302.1753	4.7367	1.7824	0.2626	0.4160
A	274.8568	1.8410	10.8829	0.1987	0.3316
A	241.1954	5.0595	2.9454	0.1871	0.3153
A	216.0080	56.6133	8.3795	0.4517	0.6223
A	172.8373	11.6229	3.4783	0.4697	0.6391
A	166.6525	2.3824	1.1766	0.3160	0.4802
A	144.8816	3.6685	1.7368	0.5275	0.6906
A	120.3400	7.2958	3.4188	0.3135	0.4773
A	113.8896	37.6982	9.8104	0.2460	0.3948
A	100.3164	1.3057	1.4442	0.5431	0.7039
A	65.8819	2.4883	0.4808	0.7083	0.8292
A	62.8840	2.4139	0.3069	0.4678	0.6374
A	57.6626	3.6183	1.1000	0.5652	0.7222
A	55.1139	2.8232	1.9602	0.7062	0.8278
A	27.2486	2.0264	0.7599	0.6816	0.8107

Processing aupcphexdienic7prod-b6psd1pbetols.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy

-1017.9102590

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
160.35483	170.462	132.667	127.023	170.497	43.828	33.425

31

C	2.079399	2.672935	0.980375
C	1.819331	2.900529	-0.528671
C	0.981454	1.702596	-0.990397
C	1.320734	0.568954	-0.023396
C	1.490595	1.290404	1.312489
O	2.815183	0.296569	-0.509892
C	3.587116	-0.613479	-0.112616
C	3.218058	-1.746167	0.752359
C	2.149518	-2.584024	0.034117
C	0.797075	-1.931877	-0.066747
C	0.439501	-0.633113	-0.064378
Au	-1.587846	-0.211357	-0.032997
P	-3.874990	0.179916	0.028722
O	4.804699	-0.594900	-0.565211
H	-4.580871	-0.265262	1.162268
H	-4.657213	-0.382066	-0.997638
H	-4.302099	1.519944	-0.027378
H	-0.007654	-2.663064	-0.127549
H	2.042159	-3.511488	0.606389
H	2.518591	-2.889967	-0.955576
H	2.809649	-1.363455	1.694038
H	4.115395	-2.330494	0.962603
H	2.074730	0.717071	2.038088
H	0.480669	1.377640	1.727591
H	1.133711	1.410806	-2.033647
H	-0.086880	1.903940	-0.862020
H	3.151335	2.703439	1.198769
H	1.614058	3.446067	1.597768
H	2.763167	2.947060	-1.080337
H	1.296737	3.841362	-0.721441
H	4.943461	0.163023	-1.163956

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3713.1358	226.8465	123.6515	0.2287	0.3723	3.6556
A	3188.1051	0.5758	160.0018	0.4252	0.5967	
A	3182.4911	3.8960	133.7956	0.2410	0.3884	
A	3162.1158	38.9084	83.7137	0.7374	0.8489	
A	3155.5157	12.5450	89.7758	0.7419	0.8519	
A	3148.6378	3.3534	220.2070	0.4720	0.6413	
A	3135.4567	7.0650	36.6880	0.7500	0.8571	
A	3121.0129	1.3316	194.7586	0.4381	0.6092	

A	3105.0366	17.3054	577.0052	0.0271	0.0528
A	3101.8994	1.5304	87.3583	0.2477	0.3970
A	3098.6551	48.9078	42.2895	0.4220	0.5935
A	3095.8907	10.0346	47.3551	0.1183	0.2116
A	3092.2745	20.2149	68.8297	0.7475	0.8555
A	3062.8642	14.7529	401.1506	0.1353	0.2383
A	2536.7229	3.0411	204.2229	0.7497	0.8569
A	2535.6910	3.0074	226.5126	0.7477	0.8556
A	2519.5760	36.3602	720.5599	0.0504	0.0960
A	1702.0098	5.1404	99.9269	0.1101	0.1984
A	1664.5627	786.6470	12.3993	0.1213	0.2163
A	1558.4156	238.4004	5.3524	0.0814	0.1505
A	1513.5668	8.5334	5.3987	0.6224	0.7673
A	1489.8099	9.3578	13.4066	0.7329	0.8458
A	1476.3818	19.7177	32.7393	0.6702	0.8025
A	1469.8562	1.7693	15.5882	0.6620	0.7966
A	1463.5541	26.3968	8.6320	0.6823	0.8112
A	1456.1551	16.5166	10.0080	0.7291	0.8433
A	1383.7488	35.2920	36.3413	0.1821	0.3082
A	1367.4806	8.8403	1.4863	0.7491	0.8566
A	1364.6103	1.0674	8.0746	0.2603	0.4131
A	1344.4555	2.7456	0.8279	0.6816	0.8107
A	1324.3087	1.1444	3.7234	0.6607	0.7957
A	1321.4919	8.2373	11.6510	0.7169	0.8351
A	1307.3799	9.7886	2.5681	0.7275	0.8422
A	1264.6886	4.8124	11.9133	0.6514	0.7889
A	1257.1828	45.2000	5.9567	0.7456	0.8543
A	1251.9546	32.1878	3.9306	0.6985	0.8225
A	1247.5788	101.8834	4.1912	0.5812	0.7352
A	1222.2359	9.0563	7.7007	0.7015	0.8246
A	1188.4092	51.1409	14.0923	0.3874	0.5585
A	1172.9384	16.8833	1.4318	0.5564	0.7150
A	1166.2954	32.7878	4.9533	0.7396	0.8503
A	1136.9301	1.5552	7.2530	0.1699	0.2905
A	1126.4217	4.6858	27.1820	0.7191	0.8366
A	1125.4554	5.4524	27.9988	0.7493	0.8567
A	1082.6142	6.1335	6.0153	0.7498	0.8570
A	1060.9722	18.6727	18.2567	0.4955	0.6626
A	1035.1039	0.8178	3.3921	0.4244	0.5959
A	1028.7335	1.7687	6.2827	0.4928	0.6602
A	1001.0856	193.3816	26.5391	0.7499	0.8571
A	998.3888	26.7674	19.2799	0.4257	0.5971
A	982.0624	12.7219	1.1684	0.7225	0.8389
A	958.1284	68.7706	5.9454	0.5238	0.6875
A	941.2165	49.6363	12.6658	0.4200	0.5916
A	913.2571	1.1193	9.8877	0.0345	0.0667
A	884.6732	7.8452	13.8750	0.7286	0.8430

A	864.5684	29.5342	1.8830	0.2808	0.4385
A	840.4753	13.2090	3.8776	0.2929	0.4531
A	820.8466	29.8670	12.3015	0.0495	0.0943
A	791.7871	8.9636	2.2694	0.0637	0.1197
A	758.7452	69.4802	1.4868	0.4178	0.5893
A	742.1321	87.4709	1.4416	0.2159	0.3551
A	690.9433	82.9258	5.5545	0.2710	0.4264
A	661.8370	14.6875	1.8047	0.3402	0.5076
A	631.8248	70.8262	11.4812	0.1074	0.1940
A	596.8602	14.1069	1.7899	0.2556	0.4071
A	558.3172	11.0718	2.0773	0.1122	0.2017
A	502.5715	34.2476	10.2957	0.1199	0.2141
A	491.0694	11.0368	0.9039	0.2705	0.4258
A	479.6009	4.9243	1.4173	0.0897	0.1646
A	432.8378	50.9109	11.2224	0.2321	0.3767
A	390.2045	6.0624	4.9622	0.5293	0.6922
A	357.4985	3.8713	3.5509	0.7062	0.8278
A	322.0647	6.6169	6.1151	0.1427	0.2498
A	303.8541	3.6697	12.9717	0.1826	0.3088
A	277.2628	22.1998	9.7203	0.5288	0.6918
A	253.3998	3.7233	2.1402	0.3295	0.4957
A	190.2110	2.6458	2.7415	0.5392	0.7006
A	167.6933	2.2842	0.6211	0.5268	0.6901
A	163.8334	1.6370	2.4379	0.4699	0.6393
A	144.5438	1.0500	1.5987	0.2584	0.4107
A	124.2803	0.8017	1.0076	0.6682	0.8011
A	101.6195	1.6302	0.5830	0.7431	0.8526
A	76.6488	1.3952	0.6186	0.6934	0.8190
A	74.3733	0.8754	0.3932	0.7460	0.8546
A	72.7095	1.1736	0.7550	0.7016	0.8247
A	46.7008	5.0189	0.5525	0.7495	0.8568
A	29.3237	6.1568	1.4810	0.7493	0.8567

Less stable conformer of 7-endo-trig prod for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid:

Processing aupcphexdienic7prod6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-1018.2449703

ZPE E298 S298 Squasihar Equasihar Strans Srot

158.72063 168.975 133.446 127.846 169.009 43.828 33.276
31

C	0.428238	2.479738	1.274142
C	1.667737	1.581805	1.198881
C	1.440852	0.778326	-0.082699
C	0.875986	1.811384	-1.055783
C	0.010303	2.742247	-0.189927
C	0.660948	-0.482527	0.065605
Au	-1.425559	-0.322719	-0.045429
P	-3.793402	-0.285090	-0.157665
C	1.138738	-1.717332	0.309098
C	2.540028	-2.227405	0.506080
C	3.598338	-1.168531	0.845391
C	3.750375	-0.275682	-0.314756
O	4.864293	-0.362914	-0.977893
O	2.872667	0.511247	-0.748994
H	3.274214	-0.579766	1.711375
H	4.565523	-1.625725	1.068366
H	2.531790	-2.943677	1.336921
H	2.866826	-2.809976	-0.368962
H	-4.420967	0.946975	-0.419254
H	-4.406772	-1.087638	-1.136858
H	-4.510992	-0.691315	0.982329
H	0.408361	-2.523880	0.389094
H	4.858060	0.221999	-1.758395
H	0.337025	1.340307	-1.884500
H	1.718071	2.371756	-1.479300
H	1.787583	0.956703	2.089824
H	2.570793	2.195824	1.069913
H	0.165837	3.786447	-0.479193
H	-1.057505	2.537024	-0.331133
H	-0.370678	1.957747	1.814480
H	0.638055	3.399549	1.828047

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3742.1045	219.8256	88.4981	0.2389	0.3857	3.9464
A	3152.5995	0.0537	82.5208	0.4886	0.6564	
A	3142.3475	2.8866	64.0216	0.2125	0.3505	
A	3128.9723	37.8303	77.2639	0.5328	0.6952	
A	3123.5975	3.1957	76.7353	0.6226	0.7674	
A	3118.0911	5.3819	87.5320	0.2917	0.4517	
A	3108.5367	6.3124	35.3923	0.7299	0.8438	
A	3087.0085	0.8782	134.3243	0.3084	0.4714	
A	3076.9169	1.9652	64.4666	0.3416	0.5092	

A	3063.3087	16.5546	305.2784	0.0486	0.0926
A	3060.0415	24.1260	29.0324	0.4612	0.6312
A	3056.2938	9.7056	28.7655	0.7494	0.8568
A	3036.9453	15.0484	81.3219	0.1304	0.2307
A	3023.0207	15.0681	236.6651	0.1412	0.2474
A	2524.0441	5.4542	127.3486	0.7391	0.8500
A	2522.3513	5.3002	132.9123	0.7425	0.8522
A	2505.4873	38.5598	471.9944	0.0621	0.1170
A	1688.1287	44.4640	48.8687	0.1138	0.2043
A	1667.9003	637.0615	3.0105	0.4165	0.5881
A	1553.5383	205.5658	3.8893	0.1476	0.2572
A	1484.7717	12.4410	5.4170	0.7449	0.8538
A	1462.2063	16.9668	3.2575	0.7353	0.8475
A	1456.9303	2.7174	3.2209	0.7468	0.8551
A	1447.0669	10.2061	24.1573	0.6417	0.7818
A	1444.1981	7.0887	6.8034	0.6797	0.8093
A	1435.1377	30.2777	7.2292	0.6733	0.8048
A	1375.5145	33.3601	19.9743	0.2537	0.4047
A	1350.9902	11.6322	1.6901	0.7471	0.8552
A	1345.9523	0.6108	3.9950	0.2865	0.4454
A	1327.7120	3.4792	0.8846	0.7288	0.8431
A	1313.7076	9.7668	3.3775	0.7342	0.8468
A	1306.9147	6.3488	3.2707	0.4811	0.6497
A	1295.7815	1.4888	1.6171	0.7500	0.8571
A	1275.3146	14.0624	3.5457	0.7406	0.8509
A	1243.7312	11.1379	3.9653	0.7315	0.8449
A	1230.6236	30.5087	5.1079	0.7452	0.8540
A	1225.0753	87.2171	4.2802	0.6972	0.8216
A	1224.5002	17.8480	1.9406	0.0959	0.1750
A	1197.4224	6.8802	4.4462	0.5129	0.6781
A	1170.0333	5.0880	3.1268	0.4342	0.6055
A	1155.5077	30.8823	1.7346	0.7172	0.8353
A	1129.5470	3.1527	16.0746	0.7457	0.8544
A	1126.8532	3.5588	16.3084	0.7500	0.8571
A	1095.1545	0.9674	4.5146	0.2436	0.3918
A	1077.8988	2.3430	6.6072	0.6707	0.8029
A	1048.2787	6.4633	2.4538	0.2474	0.3967
A	1034.4454	4.2342	2.3328	0.1388	0.2438
A	1013.0811	93.0239	8.8764	0.7473	0.8554
A	1011.4403	81.4403	10.1977	0.6441	0.7835
A	988.8041	7.6838	2.4240	0.3708	0.5410
A	982.5226	6.0386	9.2211	0.2348	0.3803
A	947.2165	25.9090	1.4412	0.3886	0.5597
A	925.8901	63.9814	12.3512	0.7243	0.8401
A	908.4366	0.0510	9.8767	0.0208	0.0408
A	866.6639	4.2591	11.8723	0.3583	0.5276
A	848.7593	29.3998	3.4609	0.4822	0.6506

A	834.3369	32.7292	0.4847	0.7063	0.8278
A	802.3960	10.1832	1.6377	0.2681	0.4228
A	782.8758	12.9971	4.3437	0.0582	0.1100
A	755.2069	59.1881	2.2701	0.5179	0.6824
A	703.7637	3.7478	5.7085	0.0147	0.0289
A	685.0706	63.6342	2.1193	0.4414	0.6125
A	675.6028	188.7814	2.3678	0.5175	0.6821
A	632.7105	18.8466	1.6339	0.2409	0.3882
A	611.7066	13.6523	6.3201	0.0220	0.0430
A	561.2078	12.6290	1.2941	0.7430	0.8526
A	500.0645	3.5483	0.6862	0.4091	0.5807
A	463.3564	1.5209	0.8817	0.2095	0.3464
A	455.8067	3.0302	0.0395	0.7461	0.8546
A	441.3740	10.2026	0.8946	0.5989	0.7491
A	371.9319	1.5130	4.4298	0.2107	0.3481
A	322.2052	0.7908	1.8431	0.7485	0.8561
A	306.6909	10.7782	4.6523	0.1670	0.2863
A	273.6870	1.0724	9.1981	0.1834	0.3100
A	251.1765	1.3768	2.5149	0.1946	0.3258
A	247.5583	26.8698	6.9056	0.3175	0.4819
A	187.3584	4.1567	2.0811	0.3980	0.5694
A	171.7087	1.4931	0.5708	0.3060	0.4686
A	155.4980	1.7314	2.6781	0.2050	0.3403
A	149.3043	0.1833	0.6053	0.5742	0.7295
A	118.7515	0.6927	0.6537	0.7381	0.8493
A	105.7620	0.3605	0.2048	0.7373	0.8488
A	91.3810	1.6226	1.0191	0.7500	0.8571
A	69.0033	1.3597	0.2273	0.7086	0.8294
A	61.3636	4.0938	0.3678	0.6380	0.7790
A	55.4690	4.5111	1.4395	0.7478	0.8557
A	27.0464	1.6362	0.9294	0.7389	0.8499

Processing aupcphexdienic7prod6psd1pbetols.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-1017.9069905

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
160.91177	170.834	129.875	125.918	170.858	43.828	33.247

31

C	0.382302	2.448442	1.286733
C	1.634588	1.569020	1.213940
C	1.431385	0.770350	-0.081770

C	0.845000	1.806205	-1.051597
C	0.009914	2.764228	-0.179146
C	0.642605	-0.497107	0.058222
Au	-1.416590	-0.331094	-0.049746
P	-3.736655	-0.263445	-0.151205
C	1.130898	-1.731947	0.294101
C	2.535114	-2.235097	0.493631
C	3.594693	-1.177239	0.832113
C	3.731102	-0.256863	-0.308010
O	4.845699	-0.294353	-0.971221
O	2.839155	0.525038	-0.733322
H	3.285701	-0.606022	1.712980
H	4.563651	-1.637854	1.031434
H	2.527640	-2.945304	1.328524
H	2.859954	-2.817580	-0.379861
H	-4.338943	0.949696	-0.535299
H	-4.367575	-1.152712	-1.041700
H	-4.450226	-0.538195	1.030996
H	0.405416	-2.541491	0.364774
H	4.822846	0.315178	-1.733171
H	0.272683	1.325761	-1.849178
H	1.676528	2.347973	-1.513107
H	1.756108	0.937870	2.096906
H	2.526875	2.197030	1.099250
H	0.238026	3.802954	-0.436044
H	-1.061782	2.623324	-0.347088
H	-0.425692	1.893817	1.774692
H	0.564748	3.348245	1.880917

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3711.0833	245.8331	127.7247	0.2440	0.3922	4.3731
A	3194.3298	0.6460	100.2338	0.6484	0.7867	
A	3184.3601	3.8934	121.2301	0.2329	0.3778	
A	3164.6116	38.2988	110.2389	0.6737	0.8051	
A	3161.5078	15.1506	80.0917	0.5100	0.6755	
A	3152.3590	18.6852	240.0389	0.3327	0.4992	
A	3136.4691	6.1696	66.3976	0.6391	0.7798	
A	3128.7622	3.2913	153.6934	0.0864	0.1591	
A	3111.3357	2.8533	170.8591	0.7256	0.8410	
A	3101.7772	20.2858	549.4977	0.0560	0.1061	
A	3095.0944	36.6687	44.7420	0.5887	0.7411	
A	3090.9888	12.1187	73.2171	0.5269	0.6902	
A	3077.9514	17.6398	135.3419	0.1547	0.2680	
A	3062.8325	16.4470	387.9671	0.1385	0.2434	

A	2537.9438	2.8306	225.6888	0.7349	0.8472
A	2536.3027	3.1046	213.5429	0.7144	0.8334
A	2520.5244	34.5555	712.7668	0.0504	0.0960
A	1690.5337	17.0568	88.4752	0.1147	0.2059
A	1655.8974	800.3908	9.9650	0.1783	0.3026
A	1566.3988	245.2766	7.1551	0.0718	0.1339
A	1505.5178	9.4626	6.3443	0.7343	0.8468
A	1493.8771	29.1410	12.8522	0.7268	0.8418
A	1484.2116	21.6720	4.0501	0.7497	0.8569
A	1475.1515	2.3296	24.2236	0.6973	0.8217
A	1471.6868	19.4401	24.1454	0.5202	0.6844
A	1464.6726	15.5181	15.6801	0.7365	0.8483
A	1389.1879	29.8186	34.8270	0.2964	0.4573
A	1374.0426	16.4308	2.1903	0.6272	0.7709
A	1366.7239	2.8635	9.3453	0.2976	0.4587
A	1344.7264	6.8078	1.1242	0.7448	0.8537
A	1330.6272	1.7883	4.9017	0.7242	0.8401
A	1325.2826	17.9885	5.5526	0.4709	0.6403
A	1317.8902	1.1417	3.5491	0.7494	0.8567
A	1291.5786	16.1566	8.2463	0.7433	0.8528
A	1258.7287	30.7882	5.4393	0.7090	0.8297
A	1249.5862	11.3775	5.9483	0.7247	0.8404
A	1247.4834	105.3887	4.5598	0.2678	0.4224
A	1245.6828	24.1102	6.5225	0.7115	0.8314
A	1212.1806	10.0265	5.7053	0.6103	0.7580
A	1179.5256	44.2510	2.3409	0.7488	0.8563
A	1170.6658	8.0944	6.8504	0.4060	0.5775
A	1129.6986	5.7325	26.5373	0.7500	0.8571
A	1126.8306	4.6646	27.3221	0.7418	0.8518
A	1110.6689	2.7784	4.6249	0.2063	0.3420
A	1093.1759	4.3389	10.0625	0.6516	0.7890
A	1063.0583	7.8016	3.6386	0.2741	0.4303
A	1044.2934	5.7845	3.4989	0.2102	0.3473
A	1023.8338	1.0936	3.1595	0.6866	0.8142
A	1006.2723	4.8822	4.7632	0.6555	0.7919
A	1003.4494	194.9199	28.6629	0.7447	0.8537
A	996.6193	21.6741	18.0247	0.2556	0.4071
A	955.2705	57.9787	1.7515	0.4462	0.6170
A	940.4859	62.4282	14.7511	0.7371	0.8486
A	925.0953	0.1328	14.4407	0.0365	0.0704
A	880.1861	9.4539	16.5943	0.3969	0.5683
A	863.3974	24.7249	1.0715	0.4058	0.5774
A	845.8269	35.4066	0.7069	0.5865	0.7394
A	815.7660	17.6713	2.5866	0.2865	0.4454
A	784.9019	15.9359	4.4822	0.0774	0.1436
A	762.1131	58.9039	3.1362	0.5173	0.6819
A	720.3897	43.1323	12.4290	0.0356	0.0688

A	706.2007	133.2633	4.4614	0.7208	0.8378
A	695.0529	116.0297	0.5245	0.5714	0.7273
A	639.6006	17.0431	3.0058	0.1835	0.3101
A	622.3359	14.6468	7.7965	0.0390	0.0752
A	574.7028	13.7729	2.7201	0.6205	0.7659
A	518.6821	7.4158	1.2809	0.3328	0.4994
A	491.8099	1.8732	0.3861	0.3694	0.5396
A	489.5677	0.2333	0.8518	0.1613	0.2777
A	450.0743	11.3517	2.5401	0.5532	0.7123
A	375.2220	1.9470	4.7250	0.2568	0.4087
A	338.2883	1.9198	2.8979	0.6913	0.8175
A	324.8726	12.9722	8.3335	0.1547	0.2679
A	305.0095	2.9286	12.2958	0.1416	0.2481
A	269.3614	13.9493	5.7692	0.4089	0.5805
A	265.3785	2.2188	2.3279	0.1809	0.3063
A	211.2619	1.9942	1.8538	0.6244	0.7688
A	186.7343	3.6884	2.2063	0.1431	0.2504
A	174.2716	0.6560	0.3229	0.5645	0.7217
A	156.4670	0.4619	1.3825	0.4666	0.6363
A	126.7928	0.7655	2.3283	0.7494	0.8568
A	102.6706	1.5997	0.4506	0.7353	0.8475
A	101.7181	0.1840	0.0367	0.7039	0.8262
A	97.9410	0.0797	0.1009	0.7499	0.8571
A	77.1589	3.9216	1.1088	0.7268	0.8418
A	54.0303	3.8845	0.9073	0.7340	0.8466
A	32.7866	6.5445	1.2589	0.7400	0.8506

5-exo-trig TS for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid:

Processing aupcphexdienic5ts6psd1pbetols.log
PG=C01

WARNING: Imaginary frequencies

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	1

HF Energy
-1017.9130185

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
159.15743	169.244	133.878	127.865	169.282	43.828	33.878

31

C	0.943522	1.491948	-0.057775
C	0.508816	0.219282	-0.099161

C	1.258264	-1.010184	-0.101020
C	1.738201	-1.592426	1.216446
C	3.009965	-2.384896	0.928993
C	3.612097	-1.653840	-0.215086
O	4.853133	-1.866176	-0.539830
Au	-1.512829	-0.254063	-0.064963
P	-3.784097	-0.737627	-0.059678
O	2.884627	-0.864356	-0.845507
H	-4.156135	-2.092445	0.022806
H	-4.561618	-0.190892	0.978200
H	-4.529903	-0.334441	-1.183092
C	0.043514	2.698468	0.102411
C	2.380557	1.989198	-0.150986
H	0.922114	-1.755584	-0.824600
H	1.935332	-0.778669	1.920205
H	0.953089	-2.222294	1.642855
H	3.703762	-2.454833	1.770432
H	2.808453	-3.409948	0.588108
H	5.101284	-1.343553	-1.324184
C	2.275974	3.521451	-0.134239
H	2.946568	1.633730	0.722182
H	2.896205	1.609547	-1.036966
H	3.148881	4.000330	0.319707
H	2.192141	3.898979	-1.160907
C	0.973825	3.797381	0.619799
H	-0.353795	2.988755	-0.881003
H	-0.815740	2.489284	0.748909
H	0.582637	4.805018	0.451253
H	1.131206	3.678401	1.699725

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3730.0619	244.0084	6.1870
A	3176.3889	0.1053	
A	3170.9701	4.7777	
A	3155.1624	7.9970	
A	3143.8809	32.3066	
A	3138.9290	24.5499	
A	3133.2375	31.5538	
A	3120.9727	21.4135	
A	3110.6342	1.6787	
A	3082.9056	6.2226	
A	3076.2106	40.4797	
A	3068.9155	35.2701	
A	3051.6071	5.8927	
A	3047.9421	27.3063	
A	2539.5211	2.6013	

A	2538.2031	2.3506
A	2521.6841	34.7779
A	1728.2357	67.8288
A	1701.9159	953.4523
A	1546.3628	161.4072
A	1501.0014	1.2122
A	1484.5091	8.5073
A	1468.9978	19.6841
A	1461.8034	6.3951
A	1457.4064	7.0311
A	1434.2165	51.4476
A	1402.8460	98.6847
A	1350.4104	2.1121
A	1337.4263	0.0657
A	1330.5177	0.7950
A	1321.6721	2.0301
A	1311.7283	25.4073
A	1300.4403	1.2176
A	1260.3033	3.1981
A	1239.6594	89.6209
A	1236.6541	4.4908
A	1228.2336	44.4358
A	1208.8787	51.0508
A	1205.1460	91.7450
A	1195.5209	5.8662
A	1169.7746	11.8354
A	1151.5776	4.2348
A	1128.1270	8.2412
A	1122.8591	5.5175
A	1112.5089	94.2730
A	1075.2109	30.2775
A	1051.2908	11.7250
A	1031.0502	4.1909
A	1018.0111	10.0721
A	1000.1772	255.5304
A	984.4155	7.0572
A	948.9937	3.1585
A	935.6964	2.1972
A	924.0071	0.6040
A	907.0754	26.8964
A	875.8629	4.4637
A	858.6770	33.3776
A	841.3620	25.8787
A	785.9887	16.5603
A	722.3593	72.9726
A	694.0436	62.6477
A	666.3423	108.5141

A	621.1737	3.8728
A	585.8746	13.5536
A	557.6715	20.4681
A	518.1484	24.8029
A	498.7465	9.2739
A	491.5557	4.7658
A	480.7773	16.6280
A	446.4229	76.0876
A	385.4888	55.0049
A	306.3205	0.5076
A	305.4401	56.3296
A	262.1206	8.1182
A	233.1275	17.7289
A	187.5622	34.8623
A	-184.6136	560.9826
A	169.4378	14.0536
A	145.4402	5.2310
A	120.2304	3.8211
A	109.5729	3.0365
A	93.4995	1.1375
A	71.9570	5.1392
A	71.3011	0.4835
A	62.1159	4.4116
A	50.5484	6.0400
A	31.1856	3.6973

6-endo-dig TS for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid:

Processing aupcphexdienic6ts6psdm6.log
PG=C01

WARNING: Imaginary frequencies

Method	BasisSet	Imaginary Freqs
RM06	GenECP	1

HF Energy
-1018.2477285

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
157.22546	167.441	134.225	128.501	167.481	43.828	33.831

31

C	1.584536	1.425601	-0.083684
C	1.400170	0.126382	-0.193846
C	0.537288	-0.999637	-0.326895
Au	-1.486157	-0.346825	-0.086952

P	-3.780929	0.185395	0.128852
C	0.889994	-2.126747	0.648842
C	2.230186	-2.755955	0.281744
C	3.290171	-1.750061	0.003859
O	3.103953	-0.543289	-0.214411
O	4.507918	-2.237390	-0.018641
C	2.888706	2.192184	-0.056529
C	0.436827	2.411392	0.052095
H	0.543555	-1.371313	-1.366178
H	-4.119538	1.413104	0.725778
H	-4.571346	-0.695103	0.888403
H	-4.537867	0.257269	-1.054003
H	0.925136	-1.734622	1.673675
H	0.124501	-2.908938	0.637350
H	2.610525	-3.442865	1.046968
H	2.143093	-3.358611	-0.635759
H	5.148751	-1.538582	-0.239447
C	2.465708	3.659764	-0.159999
H	3.388039	1.999542	0.904009
H	3.577052	1.868719	-0.842818
H	3.203360	4.340153	0.275830
H	2.343193	3.941479	-1.214846
C	1.114942	3.691874	0.545937
H	-0.008669	2.573972	-0.941125
H	-0.358352	2.038519	0.710349
H	0.526005	4.588329	0.329022
H	1.256741	3.643850	1.634449

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3767.1862	185.0400	1.0747
A	3126.4046	12.9379	
A	3122.4324	11.4454	
A	3120.0774	14.5655	
A	3118.6247	5.3872	
A	3106.5834	1.5319	
A	3083.7862	17.7872	
A	3054.9273	12.6335	
A	3049.6703	27.7366	
A	3042.9572	16.8864	
A	3038.2500	9.0765	
A	3036.2977	2.7221	
A	3022.6202	13.1992	
A	3007.4044	4.1959	
A	2529.0430	3.7559	
A	2527.4201	3.4773	
A	2508.8670	29.2035	

A	1835.9506	88.0519
A	1716.4868	753.6654
A	1501.0058	219.1234
A	1476.9032	2.0481
A	1462.2543	10.1516
A	1456.4491	4.9254
A	1436.4156	10.6241
A	1431.1722	9.9399
A	1410.2798	49.9444
A	1355.8214	7.2787
A	1341.0226	1.7899
A	1328.9144	34.7567
A	1322.6299	0.6064
A	1318.3690	0.7585
A	1304.8913	6.4028
A	1283.1784	2.0508
A	1249.0204	13.5726
A	1246.0899	9.3672
A	1224.3029	4.1853
A	1209.2312	151.5396
A	1191.3017	13.8434
A	1175.5902	2.5082
A	1166.6569	7.0668
A	1143.9301	1.6938
A	1126.3473	3.6597
A	1125.1580	4.2890
A	1113.1853	26.3899
A	1074.4096	2.3683
A	1046.0841	7.4353
A	1034.6499	11.0992
A	1020.6466	1.0965
A	1008.9977	129.8136
A	995.9886	126.4490
A	970.6343	1.7420
A	954.1806	6.7709
A	929.2216	0.2879
A	905.8784	1.1015
A	886.2457	13.7840
A	872.7072	1.6963
A	854.5736	16.5599
A	832.6786	30.5852
A	733.6996	23.1406
A	707.2223	46.6633
A	673.9216	90.3370
A	600.3661	96.5558
A	586.1815	9.7180
A	560.5246	15.4099

A	550.9894	8.9153
A	496.3072	14.5351
A	479.2392	12.7215
A	465.5360	0.2518
A	458.8316	20.5697
A	447.3280	86.9375
A	389.9576	3.1267
A	333.0244	4.5760
A	-286.6792	391.5149
A	277.6452	0.3022
A	276.1382	0.9479
A	238.1243	0.9837
A	189.8085	0.3236
A	158.9415	0.1563
A	149.8664	0.5266
A	125.6022	0.8317
A	94.1855	1.2889
A	81.9202	2.2495
A	80.9363	0.0213
A	71.2888	0.4613
A	61.1827	3.1424
A	50.8861	2.7296
A	39.1459	1.3481

Processing aupcphexdienic6ts6psd1pbedcms.log
PG=C01

WARNING: Imaginary frequencies

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	1

HF Energy
-1017.9351268

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
158.59317	168.635	131.748	127.977	168.663	43.828	33.824

31

C	1.560508	1.428855	-0.101311
C	1.345224	0.134763	-0.207368
C	0.514708	-0.999226	-0.338797
Au	-1.491478	-0.337992	-0.091002
P	-3.728792	0.177121	0.151740
C	0.866205	-2.126415	0.638760
C	2.203909	-2.763130	0.269431
C	3.282121	-1.769116	0.014176
O	3.116841	-0.562407	-0.209112

O	4.498404	-2.272483	0.014746
C	2.887881	2.163779	-0.076607
C	0.434652	2.444394	0.039316
H	0.515844	-1.366722	-1.376787
H	-4.055535	1.512257	0.450588
H	-4.425708	-0.504966	1.165166
H	-4.559138	-0.063744	-0.957517
H	0.908283	-1.738259	1.662030
H	0.100966	-2.906309	0.618582
H	2.560088	-3.459763	1.035143
H	2.114019	-3.345391	-0.658919
H	5.145647	-1.574954	-0.202982
C	2.502000	3.646613	-0.141634
H	3.398428	1.938193	0.867872
H	3.551562	1.847228	-0.884781
H	3.254599	4.291013	0.322606
H	2.395043	3.959074	-1.187981
C	1.143802	3.701245	0.554569
H	0.003493	2.633156	-0.952733
H	-0.372051	2.082347	0.684494
H	0.579393	4.613420	0.337982
H	1.275693	3.636483	1.642021

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3712.2787	273.1784	1.5797
A	3156.4945	11.1836	
A	3151.8296	22.5064	
A	3143.5446	41.9943	
A	3143.0431	3.8532	
A	3137.7529	38.4200	
A	3128.8915	20.4776	
A	3096.5105	22.6531	
A	3082.4173	15.0362	
A	3076.2215	49.2656	
A	3073.6659	6.4941	
A	3072.2931	37.3626	
A	3066.0553	16.1407	
A	3049.9300	5.6854	
A	2547.6184	3.6551	
A	2545.5416	3.7061	
A	2528.1251	34.0663	
A	1857.1071	223.3931	
A	1707.7200	1022.5749	
A	1490.5602	4.2352	
A	1486.7089	273.1871	
A	1475.7076	8.9084	

A	1471.3622	28.2596
A	1450.8923	16.2591
A	1450.2225	17.2331
A	1416.7211	73.4068
A	1372.5081	13.3933
A	1351.9906	3.3610
A	1340.4131	52.7922
A	1334.5316	0.6246
A	1329.9395	0.9889
A	1317.5127	11.6361
A	1296.4605	2.0910
A	1261.3799	29.0920
A	1259.6116	14.1792
A	1235.0539	6.6268
A	1218.7166	223.2038
A	1202.7978	34.2079
A	1187.4995	6.1713
A	1171.3916	11.0689
A	1152.0514	4.5316
A	1127.1783	49.4796
A	1122.0231	10.6004
A	1118.6457	6.4440
A	1076.5681	3.0881
A	1053.7077	9.2547
A	1044.7571	14.3820
A	1033.7633	3.8571
A	991.2548	179.5684
A	980.8756	2.2565
A	979.0600	166.0852
A	955.4092	88.3402
A	936.9326	5.6257
A	918.5090	1.7178
A	890.4403	26.8246
A	883.3104	4.6530
A	857.6157	12.4814
A	841.9305	53.9413
A	733.8817	28.2822
A	711.1160	41.8712
A	657.1748	136.0454
A	599.6769	59.8690
A	592.6527	95.5585
A	567.7974	17.3007
A	555.3953	35.2449
A	505.2710	31.8957
A	501.6578	2.8783
A	497.6354	1.0219
A	475.2169	44.7678

A	453.3742	158.5111
A	393.5637	6.7641
A	331.5769	10.2083
A	311.7366	0.9762
A	-290.9609	670.8882
A	279.7514	1.5261
A	234.4843	2.5156
A	191.9738	0.7707
A	160.5919	0.2132
A	147.2574	0.7298
A	117.8240	2.2471
A	107.0537	0.7531
A	97.4629	2.1017
A	93.5794	0.2819
A	82.9606	1.2058
A	62.7887	3.2863
A	56.1210	4.4878
A	54.9044	2.9049

Processing aupcphexdienic6ts6psd1pbetols.log
PG=C01

WARNING: Imaginary frequencies

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	1

HF Energy
-1017.9103162

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
158.97818	169.027	131.960	128.141	169.055	43.828	33.829

31

C	1.558652	1.432292	-0.100366
C	1.338114	0.140864	-0.208149
C	0.514108	-0.998025	-0.342000
Au	-1.491816	-0.339043	-0.089388
P	-3.731705	0.176272	0.150583
C	0.868108	-2.129766	0.629842
C	2.206244	-2.766157	0.257513
C	3.287256	-1.770122	0.013678
O	3.121732	-0.566652	-0.218036
O	4.503553	-2.272739	0.034224
C	2.886142	2.166795	-0.083630
C	0.433878	2.448912	0.049060
H	0.510392	-1.358799	-1.382398

H	-4.062291	1.510425	0.450699
H	-4.433189	-0.507364	1.159995
H	-4.558908	-0.062488	-0.961647
H	0.910231	-1.745833	1.654633
H	0.103217	-2.910110	0.609494
H	2.558470	-3.472298	1.016104
H	2.117784	-3.341567	-0.675252
H	5.149705	-1.574023	-0.170735
C	2.500553	3.649483	-0.148629
H	3.400384	1.941489	0.858796
H	3.545516	1.847606	-0.893912
H	3.255876	4.294281	0.309479
H	2.389080	3.961717	-1.194271
C	1.147630	3.706458	0.556655
H	-0.005373	2.635356	-0.939876
H	-0.366835	2.088734	0.702936
H	0.582859	4.618497	0.342319
H	1.285751	3.645427	1.643249

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3742.3059	192.6453	1.1743
A	3157.7624	6.3531	
A	3157.1125	13.8457	
A	3149.7890	23.1623	
A	3145.2235	2.0691	
A	3144.3361	24.1278	
A	3128.0996	18.5563	
A	3098.8238	13.1173	
A	3085.4683	17.6823	
A	3081.6683	24.7712	
A	3077.0085	25.9543	
A	3076.3122	4.0334	
A	3066.3246	13.1698	
A	3048.6636	3.3234	
A	2546.8309	1.5084	
A	2544.5469	1.5070	
A	2527.1798	24.7400	
A	1861.5632	172.4780	
A	1724.6083	875.0084	
A	1501.7714	0.8709	
A	1495.6419	220.5796	
A	1485.2416	8.9792	
A	1481.6677	25.0541	
A	1457.8549	12.8460	
A	1457.3322	13.6283	
A	1433.9388	62.0108	

A	1378.1559	9.1825
A	1355.7192	2.6377
A	1345.7405	48.4852
A	1338.3262	0.3196
A	1333.2543	0.5691
A	1323.2053	4.6317
A	1297.9468	2.3611
A	1264.5246	25.5151
A	1261.7417	7.5930
A	1238.2346	5.2488
A	1220.1064	193.5003
A	1206.2127	26.5643
A	1194.1216	4.3698
A	1169.6848	8.5169
A	1155.8603	4.9491
A	1129.7156	35.1138
A	1128.0095	5.8660
A	1123.7874	2.9103
A	1082.6874	4.3310
A	1058.2393	6.1073
A	1048.2626	14.8895
A	1036.7899	2.3954
A	1000.2325	112.7560
A	989.5127	212.1010
A	983.1033	2.3118
A	959.9348	28.1327
A	938.0006	3.2542
A	919.8869	1.4000
A	892.4143	19.4428
A	885.3483	2.6240
A	857.4661	8.9201
A	841.9311	43.5854
A	735.0060	23.7618
A	713.6213	38.6604
A	663.3538	101.7469
A	598.9537	74.9202
A	594.5778	64.8885
A	568.7115	9.8669
A	557.0447	34.5658
A	506.8103	27.5389
A	502.5154	6.1528
A	498.7754	0.5056
A	475.9768	50.1940
A	454.6949	105.9744
A	392.6821	6.0216
A	326.2774	6.5825
A	310.9332	0.9544

A	276.9385	1.1435
A	-264.3542	467.0559
A	234.1932	1.6988
A	194.0782	0.5706
A	159.4194	0.0690
A	143.8369	1.0965
A	111.1354	1.2513
A	105.9155	1.4067
A	99.5587	0.1247
A	93.5154	2.6619
A	78.6186	1.6903
A	63.9817	0.1736
A	56.8979	3.5949
A	53.6001	3.7129

6-exo-dig TS for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid:

Processing aupcphexdienic6xts6psdm6.log
PG=C01

WARNING: Imaginary frequencies

Method	BasisSet	Imaginary Freqs
RM06	GenECP	1

HF Energy
-1018.2314342

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
157.08090	167.445	136.499	128.785	167.490	43.828	33.495

31

C	0.427246	0.709992	-0.002922
Au	-1.580960	-0.058314	-0.003448
P	-3.859911	-0.699997	-0.004615
C	1.259808	-0.454705	-0.101844
C	1.273795	-1.778000	-0.052985
C	2.485970	-2.657284	-0.129295
C	3.718563	-1.985919	0.462920
C	3.846303	-0.610032	-0.065765
O	2.863543	0.082707	-0.397113
O	5.049210	-0.120892	-0.165516
H	3.617457	-1.886814	1.555412
H	4.645901	-2.535803	0.278335
H	2.294635	-3.592182	0.405254
H	2.672232	-2.941471	-1.175363
H	-4.161671	-2.073332	-0.052117

H	-4.660262	-0.229732	-1.061605
H	-4.639871	-0.308574	1.098607
C	0.621913	1.732734	-1.153064
C	0.664201	1.545893	1.277624
H	0.301735	-2.255179	0.044801
H	5.025815	0.797808	-0.491201
H	1.071642	1.261074	-2.035148
H	-0.348142	2.122760	-1.481359
C	1.483090	2.884683	-0.578455
H	0.909280	0.923921	2.147791
C	1.751228	2.553724	0.898463
H	-0.258552	2.088835	1.524682
H	2.414795	3.012742	-1.141610
H	0.941229	3.833326	-0.664616
H	1.727991	3.442909	1.537537
H	2.745572	2.105433	1.025193

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3747.3259	175.5113	4.7695
A	3198.3289	11.5811	
A	3133.0027	0.3815	
A	3119.6642	1.7130	
A	3116.1686	43.7959	
A	3105.8774	7.5626	
A	3094.0708	6.6628	
A	3092.8159	12.6298	
A	3058.9682	38.3996	
A	3050.8195	20.7802	
A	3044.8159	41.5514	
A	3040.7758	8.6458	
A	3033.7986	15.7637	
A	3029.1808	2.2762	
A	2522.8760	4.3460	
A	2522.1424	4.3408	
A	2503.5322	38.8794	
A	1803.8757	143.4156	
A	1690.0271	795.6344	
A	1538.6301	160.7257	
A	1485.6681	7.0162	
A	1466.6658	9.5758	
A	1455.9245	4.5609	
A	1453.2409	5.7763	
A	1449.2148	10.1147	
A	1414.2199	42.7327	
A	1358.4213	2.2822	
A	1333.4385	7.2421	

A	1328.1600	5.2611
A	1320.6919	7.3292
A	1306.7027	15.2757
A	1299.8791	6.2718
A	1273.2389	1.6508
A	1258.8319	5.3417
A	1234.9021	14.7964
A	1218.8910	100.7806
A	1205.5416	29.8712
A	1193.5548	3.0730
A	1187.4338	3.8731
A	1176.1212	7.4009
A	1124.7550	3.2105
A	1124.3211	3.5210
A	1104.5200	21.5087
A	1092.1272	6.1374
A	1062.4138	0.3269
A	1045.7741	17.4321
A	1036.5499	7.3847
A	1019.2100	13.8308
A	1006.3767	227.8483
A	961.6854	12.9925
A	951.1920	2.6385
A	926.1090	26.1275
A	908.2881	7.6104
A	901.3548	0.6493
A	873.7822	14.7979
A	836.5130	3.2966
A	817.5512	14.4973
A	779.0157	95.1671
A	754.5566	29.3583
A	745.5003	1.9299
A	719.7080	88.0577
A	669.5753	93.5520
A	635.8340	33.9126
A	584.3983	17.5822
A	579.1418	84.5297
A	544.3702	4.9084
A	464.9188	4.1983
A	454.5985	1.2415
A	448.4486	2.2794
A	422.9537	2.7263
A	-324.8731	662.1411
A	320.2798	12.0307
A	306.8373	1.4617
A	275.1362	0.5745
A	244.5725	1.6375

A	213.5860	6.9178
A	177.0361	5.6254
A	174.6569	1.5190
A	160.9122	0.3089
A	118.8380	2.0004
A	100.1028	1.9565
A	73.4423	0.8237
A	66.4106	0.5748
A	57.7550	3.7513
A	51.5687	4.3298
A	45.8187	1.5920
A	29.7528	0.9901

Processing aupcphexdienic6xts6psd1pbedcms.log
PG=C01

WARNING: Imaginary frequencies

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	1

HF Energy
-1017.9214391

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
158.34653	168.616	134.553	128.925	168.653	43.828	33.487

31

C	0.406386	0.753068	-0.011011
Au	-1.580194	-0.050606	0.004235
P	-3.786816	-0.722779	0.018455
C	1.183954	-0.433640	-0.110102
C	1.203508	-1.755330	-0.131597
C	2.408251	-2.645961	-0.213432
C	3.639041	-2.046441	0.453004
C	3.841456	-0.653377	-0.007051
O	2.902801	0.095570	-0.329516
O	5.073827	-0.217850	-0.051705
H	3.500811	-1.990219	1.542676
H	4.542053	-2.631414	0.265773
H	2.175189	-3.600206	0.264942
H	2.622273	-2.869698	-1.267303
H	-4.056232	-2.074684	-0.261668
H	-4.644800	-0.084438	-0.895575
H	-4.498254	-0.550151	1.219710
C	0.578146	1.764703	-1.168981
C	0.651336	1.610732	1.251792
H	0.228562	-2.234364	-0.093949

H	5.093527	0.717282	-0.334495
H	0.881284	1.275439	-2.099905
H	-0.382744	2.252606	-1.362336
C	1.601644	2.814729	-0.675111
H	0.916486	1.006615	2.125507
C	1.741343	2.619404	0.851693
H	-0.271977	2.148670	1.495453
H	2.567503	2.679049	-1.171109
H	1.257272	3.825013	-0.919873
H	1.631955	3.560849	1.400398
H	2.731215	2.220098	1.094935

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3703.5491	289.3448	5.0770
A	3221.5453	27.1538	
A	3171.9389	0.7504	
A	3152.8459	5.7177	
A	3146.8188	92.7836	
A	3138.9712	26.6049	
A	3129.6179	3.4961	
A	3118.6029	14.2090	
A	3093.2052	68.3807	
A	3082.3311	81.2262	
A	3078.4897	29.8141	
A	3076.5394	14.9684	
A	3074.6033	17.8594	
A	3066.6899	5.8739	
A	2546.0661	3.6167	
A	2544.5795	3.7148	
A	2527.2914	39.0612	
A	1824.3817	244.9839	
A	1688.3583	1136.0774	
A	1518.4017	294.0357	
A	1494.6964	2.3710	
A	1475.6726	10.2481	
A	1471.5982	10.0732	
A	1466.0926	3.2188	
A	1458.5261	4.8335	
A	1423.7927	59.4426	
A	1373.2350	3.4942	
A	1352.3230	32.7512	
A	1338.0034	4.2154	
A	1329.0908	3.4594	
A	1325.7932	18.4775	
A	1302.9696	2.6096	
A	1287.3058	0.8604	

A	1265.0644	19.4855
A	1251.4358	33.0912
A	1240.2501	177.3941
A	1213.0845	12.2936
A	1212.4164	3.7529
A	1197.3899	13.2040
A	1185.5665	14.5017
A	1120.6146	34.3132
A	1119.7105	13.5452
A	1118.1691	4.3103
A	1109.4494	2.6682
A	1072.9190	4.7983
A	1055.4036	28.3432
A	1047.3199	10.3749
A	1028.7025	40.1834
A	991.3315	244.0444
A	971.8974	13.5946
A	959.1937	2.3245
A	939.6297	39.4307
A	913.1305	10.6472
A	904.5035	4.6317
A	868.3207	37.1008
A	827.6060	7.8513
A	819.7166	30.0920
A	790.4522	8.1414
A	765.2152	214.2584
A	730.0709	26.9367
A	707.6222	122.0467
A	655.2859	127.8747
A	649.2542	51.5585
A	581.8125	73.0618
A	576.2617	85.3672
A	551.5989	16.0522
A	500.0046	0.2298
A	493.6586	0.5108
A	463.0930	8.3831
A	416.4071	0.7814
A	-350.8312	1200.6490
A	321.0192	15.6524
A	314.1365	6.1424
A	300.4825	2.6068
A	220.5455	3.6524
A	205.0581	4.6350
A	176.3033	7.9019
A	154.3869	0.6542
A	139.2091	1.4732
A	122.5418	1.6031

A	105.7522	1.1660
A	82.4806	0.2350
A	78.7208	2.6670
A	69.8137	4.8164
A	66.8045	5.8873
A	57.5218	0.0600
A	32.7411	0.2760

Processing aupcphexdienic6xts6psd1pbetols.log
PG=C01

WARNING: Imaginary frequencies

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	1

HF Energy
-1017.8953496

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
158.84825	169.007	132.353	128.531	169.036	43.828	33.487

31

C	1.715551	2.641763	0.835996
C	0.642248	1.617575	1.243549
C	0.404105	0.747765	-0.013392
C	0.570501	1.752666	-1.179144
C	1.596288	2.803553	-0.696415
Au	-1.577999	-0.056063	0.005245
P	-3.791250	-0.717268	0.026131
C	1.196118	-0.432142	-0.107562
C	1.216309	-1.753935	-0.140594
C	2.421478	-2.643499	-0.234561
C	3.652300	-2.049889	0.438789
C	3.842602	-0.645078	0.008179
O	5.070245	-0.198574	-0.022479
O	2.899448	0.103624	-0.301971
H	3.519144	-2.020299	1.530165
H	4.560153	-2.623112	0.237276
H	2.191896	-3.604601	0.231737
H	2.633894	-2.856261	-1.291120
H	-4.228836	-1.482631	1.122847
H	-4.243644	-1.506287	-1.047417
H	-4.750943	0.311573	0.021665
H	0.241933	-2.233322	-0.109149
H	5.082956	0.739137	-0.287483
H	0.865394	1.259104	-2.110196

H	-0.391014	2.240518	-1.369164
H	0.915439	1.024148	2.121875
H	-0.287588	2.143186	1.487724
H	2.565545	2.647261	-1.179001
H	1.267277	3.810846	-0.970073
H	1.575763	3.590596	1.363390
H	2.710760	2.275096	1.107170

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3730.1719	197.4647	4.6980
A	3226.9305	19.7326	
A	3170.7389	0.5610	
A	3152.7400	56.9836	
A	3152.6430	6.3299	
A	3142.9173	18.1184	
A	3134.3837	1.8535	
A	3123.8275	13.0002	
A	3098.8378	52.2381	
A	3086.3464	53.1223	
A	3084.8714	13.7692	
A	3080.1550	13.9827	
A	3076.6111	10.2949	
A	3066.5614	4.0787	
A	2546.1512	2.4043	
A	2538.7041	1.9222	
A	2523.0100	30.0827	
A	1824.9262	195.4534	
A	1698.7006	976.1746	
A	1530.0281	215.2438	
A	1509.1802	3.9807	
A	1486.6336	9.2466	
A	1482.5144	10.0145	
A	1474.6649	3.2570	
A	1470.2291	4.6879	
A	1438.3699	51.2019	
A	1376.8187	3.3582	
A	1353.0374	19.8325	
A	1343.3270	7.2310	
A	1333.0321	9.6416	
A	1329.7489	10.9343	
A	1305.7061	2.2035	
A	1293.7439	0.8805	
A	1267.9540	18.6912	
A	1254.2397	8.5299	
A	1235.3526	143.8753	
A	1218.1740	4.9149	

A	1215.1470	23.9698
A	1202.7507	6.5844
A	1193.4615	10.4135
A	1125.1730	5.2714
A	1124.7168	34.1792
A	1123.4491	1.6282
A	1109.4178	0.8970
A	1077.0885	2.4867
A	1057.0259	24.5848
A	1051.0339	11.1297
A	1032.0012	33.1161
A	990.2308	223.3439
A	973.9176	16.2551
A	962.2681	1.4521
A	940.9341	34.8799
A	912.6225	10.7236
A	906.7925	3.6366
A	870.8181	26.8574
A	825.9994	6.9609
A	823.0965	21.2681
A	797.1501	4.8403
A	772.3242	172.7616
A	733.9117	23.0518
A	711.3333	93.4646
A	661.8919	122.5773
A	655.5535	22.5793
A	586.0034	50.3953
A	578.4211	78.8604
A	555.3385	13.1459
A	488.9966	0.6322
A	482.7188	0.0077
A	464.0190	8.5513
A	417.9243	1.3027
A	320.8708	14.1241
A	-320.1878	896.9449
A	312.0543	4.5750
A	302.9233	2.4631
A	222.0591	3.4434
A	205.4396	4.9031
A	179.4731	8.4424
A	154.8255	0.2894
A	139.9308	0.8255
A	130.4807	1.9438
A	113.3403	1.7124
A	101.9702	0.2438
A	85.8337	0.1113
A	80.1995	0.5146

A	70.8964	4.6418
A	65.5921	6.1479
A	44.5677	0.5324

7-endo-trig TS for 4,5-Au-PH3 complex of 6,6-cyclopentano-hexa-4,5-dienoic acid:

Processing aupcphexdienic7ts6psdm6.log
PG=C01

WARNING: Imaginary frequencies

Method	BasisSet	Imaginary Freqs
RM06	GenECP	1

HF Energy
-1018.2476133

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
157.93378	168.035	133.501	127.025	168.075	43.828	33.475

31

O	2.881161	0.299314	-0.520547
C	1.290006	0.598345	0.014988
C	0.455936	-0.612376	-0.022208
C	0.806843	-1.909606	-0.004748
C	2.152637	-2.573384	0.086866
C	3.257256	-1.736693	0.744380
C	3.630710	-0.632267	-0.160397
O	4.832663	-0.690376	-0.664627
Au	-1.603610	-0.199822	-0.026631
P	-3.947556	0.139197	-0.023133
C	1.520442	1.309103	1.334184
C	0.998294	1.716574	-0.969251
C	2.139617	2.671034	0.985743
C	1.856754	2.901732	-0.517299
H	-4.666508	-0.276870	1.112113
H	-4.690081	-0.492034	-1.037484
H	-4.420090	1.458206	-0.150218
H	-0.003117	-2.638705	-0.053288
H	2.043703	-3.484253	0.687536
H	2.485980	-2.923411	-0.902254
H	2.886955	-1.320184	1.689405
H	4.146798	-2.337566	0.949822
H	2.096519	0.712486	2.050841
H	0.521973	1.423966	1.778002
H	1.149241	1.398979	-2.006723
H	-0.069813	1.945572	-0.859960
H	3.217482	2.669668	1.182519

H	1.715815	3.461722	1.611879
H	2.792346	2.938071	-1.085360
H	1.345903	3.851176	-0.701943
H	4.983827	0.044924	-1.286203

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3752.5964	194.7351	2.7911
A	3147.8053	0.1436	
A	3143.8929	2.6697	
A	3133.5469	22.0414	
A	3120.5856	3.3134	
A	3115.7586	2.8177	
A	3107.0454	11.8455	
A	3090.3239	1.8399	
A	3075.1353	30.4413	
A	3069.0738	1.5272	
A	3065.8394	16.2079	
A	3056.6988	24.8235	
A	3052.5390	3.9899	
A	3023.3592	14.6309	
A	2526.4414	5.0925	
A	2522.7381	5.4968	
A	2505.7036	36.3167	
A	1708.7560	40.9345	
A	1690.4285	650.4832	
A	1533.3451	197.2152	
A	1492.6049	10.2149	
A	1468.7127	9.0686	
A	1448.6420	15.6008	
A	1441.6666	3.5080	
A	1432.7261	33.3270	
A	1425.3298	11.3722	
A	1381.7735	45.0943	
A	1354.2628	3.9748	
A	1348.4101	3.3673	
A	1327.2755	0.7624	
A	1310.0550	1.6547	
A	1301.5866	5.5329	
A	1293.4983	9.2821	
A	1250.3472	5.6253	
A	1243.5035	13.3196	
A	1238.1763	13.9361	
A	1225.6285	131.1907	
A	1201.6169	4.4336	
A	1171.2910	17.7089	
A	1164.3264	13.9771	

A	1156.1702	55.7359
A	1134.1685	8.4916
A	1127.3435	3.0126
A	1125.8462	3.4956
A	1073.7896	5.2854
A	1054.0899	13.9506
A	1017.2921	0.7164
A	1014.1292	12.8516
A	1009.6525	183.3725
A	980.6039	2.8176
A	969.3774	6.5441
A	938.7090	26.5156
A	918.8162	49.6287
A	899.2368	1.9105
A	867.6466	3.8873
A	844.8963	26.2901
A	827.3003	34.5477
A	798.8360	11.1697
A	773.6811	7.8932
A	758.5515	69.5507
A	717.0381	41.9222
A	676.4669	67.4896
A	651.1866	4.3703
A	609.3441	84.7231
A	578.1341	9.3600
A	549.1094	1.8128
A	474.9743	23.5820
A	467.4903	3.0385
A	451.9645	0.9419
A	405.2923	33.7955
A	359.8603	13.8785
A	327.9899	1.3606
A	292.7431	3.1561
A	275.4091	1.3070
A	240.0112	2.9597
A	190.0507	14.1168
A	168.8013	5.9944
A	158.6920	5.1498
A	142.6517	2.2832
A	-120.1118	181.4058
A	117.9489	0.7529
A	97.1748	1.9435
A	64.7082	5.0435
A	63.0439	2.6145
A	59.5874	1.8388
A	54.6407	2.9133
A	28.7877	1.7077

SM+ for 5,6-Au-PH3 complex of hexa-4,5-dienoic acid:

Processing auphexdienic6sm6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-862.3215188

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
98.66091	107.426	126.576	117.902	107.474	43.392	32.358

21

C	-0.332792	0.482290	1.556813
C	-0.905153	0.825936	0.385801
Au	1.370553	0.026069	0.179026
P	3.384456	-0.577465	-0.880434
C	-1.603258	1.157340	-0.663578
C	-3.045160	1.589679	-0.533619
C	-4.006807	0.486433	-0.957998
C	-4.009898	-0.681222	-0.008222
O	-3.350475	-0.762661	1.004919
O	-4.847778	-1.637052	-0.420170
H	-0.587055	-0.483543	2.001396
H	0.073747	1.251530	2.217322
H	-1.165751	1.095771	-1.660651
H	4.010544	0.414027	-1.651992
H	3.325676	-1.655845	-1.777192
H	4.418718	-0.971877	-0.017045
H	-3.250931	1.880950	0.501787
H	-3.199185	2.473735	-1.162590
H	-5.032011	0.875409	-1.007985
H	-3.790549	0.111338	-1.967521
H	-4.839298	-2.354011	0.234780

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3800.9846	132.7255	101.7608	0.2162	0.3555	4.6067
A	3190.3536	9.3541	68.9682	0.7366	0.8483	
A	3161.6530	4.6683	64.2863	0.1502	0.2611	
A	3128.5317	2.0404	54.9393	0.7402	0.8507	
A	3102.6627	0.4443	146.1696	0.5348	0.6969	
A	3090.8395	9.5881	135.5873	0.1293	0.2289	

A	3065.4718	8.1008	137.8558	0.1028	0.1865
A	3052.1036	4.0422	170.9841	0.0799	0.1480
A	2543.1497	0.1953	121.6588	0.7487	0.8563
A	2541.9339	0.1758	124.5851	0.7447	0.8537
A	2518.4517	6.6383	379.4900	0.0354	0.0684
A	1976.7163	132.0761	51.4491	0.5656	0.7225
A	1853.1293	300.3609	6.6174	0.0708	0.1322
A	1450.1103	22.5493	11.9657	0.6514	0.7889
A	1440.3609	119.6161	0.8485	0.7322	0.8454
A	1427.7026	20.6461	8.7055	0.7500	0.8571
A	1419.7771	21.0463	13.7354	0.7481	0.8559
A	1358.1675	7.7847	5.3334	0.4971	0.6641
A	1309.5304	7.1154	5.3504	0.4655	0.6353
A	1301.4341	31.1819	3.8425	0.5764	0.7313
A	1231.0994	24.5363	5.5291	0.6300	0.7730
A	1199.9724	80.5765	2.2687	0.7500	0.8571
A	1174.3698	158.1211	0.4810	0.3642	0.5340
A	1118.4686	3.1255	16.8782	0.7432	0.8527
A	1116.9436	3.3337	16.7954	0.7461	0.8546
A	1098.2164	1.1291	21.9057	0.1559	0.2697
A	1055.9260	11.8613	9.7943	0.2177	0.3576
A	1022.3571	26.0073	50.9900	0.1579	0.2728
A	1015.8208	1.1632	0.2249	0.5517	0.7111
A	992.4524	170.7975	14.6873	0.6286	0.7720
A	946.4776	27.3758	3.8584	0.7294	0.8435
A	922.5000	71.7845	2.4082	0.6049	0.7538
A	892.4395	5.7321	6.8694	0.7085	0.8294
A	873.1131	9.5886	3.2503	0.3792	0.5499
A	814.6898	8.2052	14.4675	0.0476	0.0908
A	716.0624	16.5027	1.4646	0.1873	0.3156
A	672.5074	106.4042	0.5327	0.6789	0.8087
A	619.1387	30.9829	2.6525	0.6381	0.7791
A	557.7734	8.3780	2.3707	0.2859	0.4446
A	521.9066	22.2178	0.7860	0.7498	0.8570
A	490.6530	21.4792	1.6473	0.5847	0.7379
A	481.9629	2.3314	0.5182	0.5585	0.7167
A	472.1480	2.8836	0.9283	0.3297	0.4959
A	360.2355	11.8802	5.7443	0.5650	0.7221
A	347.6592	4.5136	2.1585	0.7396	0.8503
A	304.2380	3.9008	0.5632	0.6214	0.7665
A	289.4325	2.3425	9.9249	0.2034	0.3381
A	261.6255	1.5400	0.6854	0.7327	0.8457
A	175.4702	2.1378	1.4953	0.3948	0.5662
A	129.5313	0.4299	0.3336	0.1486	0.2587
A	96.7124	5.3268	1.6194	0.6708	0.8029
A	88.0691	9.5077	2.4767	0.4766	0.6455
A	59.3817	2.4360	0.6200	0.6993	0.8230

A	52.3970	2.9245	3.0452	0.7086	0.8294
A	44.2291	0.0484	0.6359	0.7311	0.8446
A	37.3664	0.6807	0.5652	0.6892	0.8160
A	27.8977	0.8760	2.2823	0.7141	0.8332

SM+ for 4,5-Au-PH3 complex of hexa-4,5-dienoic acid:

Processing auphexdienic5sm6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-862.3194829

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
98.43642	107.200	124.283	117.735	107.240	43.392	31.896

21

C	0.857348	2.431166	0.133644
C	0.840992	1.167328	-0.180498
C	1.039643	-0.129891	-0.498830
C	1.704282	-1.111142	0.446713
Au	-1.200532	-0.005436	-0.083705
P	-3.503917	-0.389818	0.232487
H	-3.966688	-1.657507	-0.154671
H	-3.980050	-0.293580	1.549491
H	-4.376022	0.464077	-0.460885
H	-0.013410	2.986413	0.469793
H	1.812395	2.953015	0.057729
H	1.027047	-0.394601	-1.563207
H	1.674556	-0.709508	1.466417
H	1.161022	-2.063681	0.446086
C	3.146614	-1.382444	0.026386
H	3.583876	-2.164549	0.659105
H	3.202792	-1.777539	-0.997928
C	4.033534	-0.168891	0.102290
O	5.302280	-0.482196	-0.166346
O	3.660514	0.953644	0.364376
H	5.838394	0.325835	-0.108980

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3797.5271	153.9249	128.1689	0.2346	0.3801	4.5631
A	3242.9581	12.1237	77.0503	0.7454	0.8541	
A	3136.3392	31.5970	248.1911	0.1610	0.2774	

A	3118.7271	1.5940	20.9290	0.6646	0.7985
A	3105.0954	0.0791	111.6853	0.4140	0.5856
A	3094.5619	2.2693	74.9119	0.4475	0.6183
A	3054.7293	6.8727	49.7122	0.0893	0.1640
A	3049.0930	2.9366	158.4726	0.0598	0.1129
A	2543.4039	0.1519	121.6947	0.7499	0.8571
A	2541.0984	0.1316	124.8940	0.7293	0.8435
A	2517.6594	6.6825	393.0001	0.0394	0.0759
A	1972.7174	86.5287	43.6769	0.7051	0.8271
A	1853.7729	312.1409	11.0511	0.0809	0.1496
A	1448.5705	74.0936	2.7667	0.7488	0.8564
A	1443.2833	70.9772	5.0618	0.6375	0.7787
A	1422.6687	57.6650	5.2033	0.3616	0.5312
A	1414.9901	4.9509	28.5209	0.6898	0.8164
A	1352.7881	7.7255	9.0761	0.2609	0.4139
A	1314.0019	15.6828	8.3013	0.6584	0.7940
A	1306.8627	21.7772	2.0012	0.6399	0.7805
A	1242.2418	10.2518	9.9725	0.3770	0.5475
A	1197.9561	82.3916	2.1415	0.6002	0.7502
A	1176.2929	202.8538	1.6818	0.3529	0.5217
A	1117.6648	3.4989	37.0414	0.1754	0.2985
A	1117.0473	3.3085	14.4724	0.7105	0.8307
A	1116.0880	3.2357	16.6967	0.7409	0.8512
A	1060.7386	6.7676	13.0070	0.1987	0.3316
A	1032.6425	1.9530	17.2057	0.1681	0.2879
A	989.8160	166.9114	14.3921	0.6641	0.7982
A	951.9832	4.7530	4.3561	0.4463	0.6171
A	931.1304	29.3749	1.8213	0.5506	0.7102
A	922.8032	15.4105	3.9769	0.6804	0.8098
A	898.7208	57.0585	1.0874	0.6219	0.7669
A	864.3365	8.7611	2.4454	0.7477	0.8557
A	809.5868	16.4782	17.7339	0.0689	0.1289
A	679.8529	92.3275	1.2605	0.6933	0.8189
A	632.2381	23.8049	2.9218	0.7060	0.8276
A	587.0510	47.2901	1.1809	0.7036	0.8260
A	537.4580	27.5385	4.6566	0.3431	0.5109
A	509.3375	6.0683	1.9342	0.5566	0.7151
A	489.1726	3.2795	0.3482	0.4574	0.6277
A	475.2134	4.1634	1.1175	0.1735	0.2957
A	472.7482	1.4584	0.5095	0.7352	0.8474
A	406.5239	12.3258	7.9177	0.5538	0.7129
A	339.5012	6.8516	0.4414	0.3614	0.5310
A	284.5354	1.7856	11.5477	0.2545	0.4058
A	257.1193	3.1263	1.3996	0.5439	0.7046
A	229.1300	1.2933	4.6421	0.2159	0.3551
A	186.5959	2.9601	1.8474	0.5166	0.6813
A	140.5690	3.1381	5.7732	0.6443	0.7837

A	106.3904	3.9104	1.4601	0.5902	0.7423
A	99.3986	5.5819	0.5346	0.7499	0.8571
A	75.7416	6.9584	0.3038	0.6987	0.8227
A	55.4084	0.0307	0.1177	0.7426	0.8523
A	50.3789	1.9341	1.8663	0.7193	0.8367
A	45.9749	2.5285	0.8699	0.6460	0.7849
A	37.0410	0.6887	0.3510	0.7197	0.8370

5-exo-trig prod for 4,5-Au-PH3 complex of hexa-4,5-dienoic acid:

Processing auphexdienic5prod6psdm6.log
PG=C01

WARNING: Imaginary frequencies

Method	BasisSet	Imaginary Freqs
RM06	GenECP	1

HF Energy
-862.3090589

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
100.05213	107.585	113.357	109.361	107.610	43.392	31.845

21

C	0.943967	2.127558	0.458845
C	0.679713	0.886262	0.037966
C	1.705556	-0.044559	-0.437517
C	1.975928	-1.277194	0.421956
C	3.463967	-1.575450	0.243694
C	4.001255	-0.237123	-0.083012
O	5.261592	0.024434	-0.033433
Au	-1.252331	0.114312	-0.010563
P	-3.505072	-0.641764	-0.046101
O	3.157611	0.629679	-0.429963
H	-4.042533	-1.045557	-1.281726
H	-3.845755	-1.750664	0.749809
H	-4.487847	0.275392	0.367883
H	0.158408	2.785044	0.821891
H	1.949773	2.550981	0.451322
H	1.612848	-0.277044	-1.507138
H	1.746306	-1.039346	1.467427
H	1.337169	-2.110689	0.119107
H	3.971061	-2.013186	1.108394
H	3.675263	-2.230921	-0.614725
H	5.459576	0.941944	-0.300664

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3737.1737	261.3569	95.8697	0.2496	0.3994	6.6783
A	3222.7877	2.6262	69.4928	0.7291	0.8433	
A	3149.0191	0.5868	33.7487	0.5718	0.7276	
A	3134.0511	3.5464	91.8845	0.3868	0.5578	
A	3121.9725	14.3819	156.0678	0.1776	0.3016	
A	3077.8092	5.1587	12.8453	0.2950	0.4555	
A	3067.4149	3.4056	98.6943	0.1683	0.2882	
A	3045.8643	6.6488	149.2986	0.1161	0.2080	
A	2523.6883	4.3872	134.1995	0.7150	0.8338	
A	2519.6187	5.6694	133.0095	0.7454	0.8541	
A	2503.1352	33.3910	437.7720	0.0527	0.1002	
A	1690.1165	428.5137	15.2502	0.1815	0.3073	
A	1685.5977	354.6518	23.0820	0.1133	0.2036	
A	1572.2514	97.7667	13.0881	0.1786	0.3031	
A	1458.4550	7.0534	4.2542	0.7076	0.8288	
A	1430.9812	35.1118	23.6629	0.4097	0.5813	
A	1411.1261	38.0380	10.9025	0.6159	0.7623	
A	1361.7406	37.9992	8.3458	0.7365	0.8483	
A	1301.8150	12.5728	7.0983	0.5803	0.7344	
A	1286.6000	36.8398	6.4980	0.3433	0.5112	
A	1250.3480	57.9733	2.0310	0.7017	0.8247	
A	1219.5264	22.3604	5.0525	0.5403	0.7016	
A	1193.8831	61.1250	3.1925	0.7296	0.8436	
A	1172.7400	4.8479	2.5680	0.2820	0.4399	
A	1126.3222	5.8483	16.7382	0.6731	0.8046	
A	1124.7116	4.8652	15.5835	0.6841	0.8124	
A	1118.8993	10.5089	49.8941	0.4543	0.6248	
A	1082.3603	1.3327	2.5895	0.6332	0.7754	
A	1033.1922	2.7666	4.9250	0.1435	0.2510	
A	1007.4741	96.5894	21.0597	0.6823	0.8112	
A	997.1420	99.8856	10.0016	0.6205	0.7658	
A	949.6775	2.2688	6.1049	0.2084	0.3450	
A	942.2728	36.0999	1.8782	0.4784	0.6472	
A	901.0609	89.9589	6.1369	0.2384	0.3849	
A	837.9502	38.6453	1.3319	0.6826	0.8114	
A	730.7145	69.6885	2.2035	0.5426	0.7035	
A	718.4068	93.6482	4.2728	0.5544	0.7134	
A	690.6121	114.9295	10.3159	0.2899	0.4495	
A	656.9556	22.8222	25.0543	0.1343	0.2368	
A	592.2362	8.4765	3.6067	0.1098	0.1979	
A	527.7313	178.7088	26.8883	0.3868	0.5578	
A	506.2258	14.2556	5.5334	0.2867	0.4457	
A	486.9724	62.6553	16.8679	0.2613	0.4144	

A	453.3294	0.6985	0.0605	0.6988	0.8227
A	438.6945	8.3473	5.6447	0.2252	0.3676
A	387.1248	42.0261	19.6267	0.5687	0.7251
A	284.1214	10.9995	4.7909	0.2750	0.4314
A	273.0666	1.1405	12.0325	0.1617	0.2784
A	261.7885	0.7553	2.5210	0.6597	0.7949
A	188.2935	12.0440	8.3816	0.3996	0.5710
A	157.6963	0.2259	0.8690	0.5498	0.7095
A	117.6861	2.0500	0.3073	0.5708	0.7268
A	93.5640	1.5797	2.0606	0.5533	0.7124
A	76.8636	4.0632	0.6729	0.7499	0.8571
A	50.5874	4.7105	1.0984	0.7493	0.8567
A	36.0371	1.8059	0.4051	0.7155	0.8341
A	-32.3757	0.0496	0.0739	0.7348	0.8471

5-endo-dig prod for 4,5-Au-PH3 complex of hexa-4,5-dienoic acid:

Processing auphexdienic6prod6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-862.3122667

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
100.23146	108.010	114.507	110.542	108.037	43.392	31.690

21

O	-3.124398	0.944059	-0.020281
C	-1.632698	1.061843	0.054368
C	-0.941013	-0.194309	0.381674
C	-1.577656	-1.363591	-0.373108
C	-3.056198	-1.488362	-0.006848
C	-3.722213	-0.173151	-0.035049
C	-1.273776	2.319256	-0.157746
Au	1.155248	-0.070223	0.078319
P	3.508261	-0.015341	-0.220268
O	-5.015099	-0.154751	-0.086805
H	-2.006256	3.103688	-0.318777
H	-0.220651	2.576765	-0.161690
H	-1.053114	-0.370242	1.466216
H	4.308044	-0.187366	0.923961
H	4.074888	1.157978	-0.750390
H	4.077178	-0.977463	-1.074127
H	-1.475533	-1.225195	-1.457644

H	-1.074345	-2.303735	-0.130671
H	-3.634449	-2.169966	-0.642898
H	-3.177378	-1.865756	1.021652
H	-5.369579	0.754410	-0.081900

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3735.9148	242.5647	128.2850	0.2939	0.4543	4.5407
A	3285.1986	0.5438	55.7164	0.7368	0.8485	
A	3179.0930	3.7124	124.2840	0.1446	0.2527	
A	3127.2188	2.6139	57.6199	0.4935	0.6608	
A	3101.1242	2.2498	162.0967	0.3652	0.5350	
A	3054.9719	11.2025	33.8576	0.2094	0.3463	
A	3027.1845	8.6460	142.0178	0.0986	0.1794	
A	3001.7611	4.7326	95.9660	0.1944	0.3255	
A	2528.8143	4.7798	123.1207	0.7475	0.8555	
A	2527.5542	4.4310	131.0502	0.7472	0.8553	
A	2509.4332	31.2962	420.8791	0.0477	0.0911	
A	1760.8298	78.7101	97.0286	0.1227	0.2186	
A	1640.9023	654.6562	31.0541	0.2032	0.3378	
A	1561.6143	198.0742	18.3580	0.2608	0.4137	
A	1460.1198	5.5236	8.7610	0.5630	0.7204	
A	1399.7006	61.0490	15.5684	0.5050	0.6711	
A	1386.1800	22.0417	18.0560	0.4464	0.6173	
A	1338.2843	4.1188	7.3649	0.4506	0.6212	
A	1327.1500	5.9198	1.4903	0.4730	0.6422	
A	1295.5909	8.9104	6.4089	0.4119	0.5835	
A	1241.2679	12.0971	15.0943	0.2267	0.3697	
A	1215.3891	96.6238	11.5162	0.6405	0.7808	
A	1167.4190	0.9705	1.6656	0.4169	0.5885	
A	1128.1974	4.0364	16.0932	0.7428	0.8524	
A	1127.2581	3.3688	16.1805	0.7489	0.8564	
A	1094.3420	48.0572	23.6638	0.6400	0.7805	
A	1088.5129	25.2861	55.2972	0.1995	0.3326	
A	1062.7788	74.6337	49.1003	0.5739	0.7293	
A	1011.2884	152.8985	8.9009	0.7015	0.8246	
A	1005.6212	50.4969	5.9015	0.2263	0.3691	
A	997.3338	0.8756	20.4946	0.2908	0.4506	
A	929.9379	41.3890	2.7041	0.6897	0.8163	
A	911.1580	30.5961	32.7980	0.3066	0.4693	
A	891.3547	38.3976	4.9049	0.5099	0.6754	
A	848.2931	105.5063	18.0007	0.4091	0.5806	
A	760.4395	8.7112	5.5397	0.3889	0.5600	
A	720.1098	29.0447	5.4626	0.6763	0.8069	
A	687.0222	118.5232	5.6970	0.2704	0.4256	
A	651.0778	83.2494	8.1321	0.2596	0.4122	
A	602.3950	11.0820	4.3452	0.2515	0.4019	

A	554.3583	7.4951	3.7454	0.5758	0.7308
A	513.7442	18.2551	5.0225	0.5636	0.7209
A	477.7625	4.5317	1.8191	0.7384	0.8495
A	461.4944	2.5688	0.7067	0.2553	0.4068
A	454.8303	1.1881	0.2427	0.6965	0.8211
A	447.9324	1.5523	7.3544	0.4623	0.6323
A	334.7997	0.6505	2.1226	0.7177	0.8356
A	297.4070	2.0501	3.6391	0.6953	0.8202
A	273.6818	0.0916	8.3843	0.2048	0.3400
A	194.0845	0.0690	1.4565	0.1944	0.3255
A	167.8638	0.0837	3.4000	0.3122	0.4758
A	148.5397	1.0000	1.2918	0.7088	0.8296
A	144.0442	0.6886	0.7556	0.3110	0.4745
A	85.4466	0.2247	0.0991	0.6962	0.8209
A	71.1246	5.1933	1.4879	0.5743	0.7296
A	58.6690	5.2459	1.3468	0.7448	0.8537
A	37.3040	2.1665	0.1822	0.3771	0.5476

SM for 4,5-Au-PH3 complex of hexa-4,5-dienoic acid carboxylate:

Processing auphexdienoat5sm16psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-861.9071454

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
90.26472	98.690	121.329	114.564	98.725	43.383	31.379

20

C	-1.882675	2.836334	0.469862
C	-0.848367	2.148273	0.042512
Au	-0.559473	-0.054917	-0.123181
P	-1.580527	-2.206184	0.204937
C	0.414935	1.868522	-0.406099
C	1.677671	1.780857	0.425665
C	2.715512	0.800119	-0.126873
C	2.541715	-0.721945	0.078005
O	1.359564	-1.244553	0.011095
O	3.569026	-1.369524	0.249900
H	-1.164859	-3.133040	-0.768478
H	-1.108982	-2.852064	1.361961
H	-2.951724	-2.527261	0.280957
H	-2.825918	2.368881	0.735726

H	-1.812626	3.920310	0.566642
H	0.574066	1.948015	-1.488655
H	2.121841	2.789150	0.429070
H	1.425838	1.553659	1.470107
H	2.811721	0.959859	-1.212863
H	3.695424	1.043339	0.296364

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3232.1897	0.2163	121.8022	0.7475	0.8555	8.9876
A	3127.6293	5.8176	461.0447	0.2210	0.3619	
A	3111.8997	13.4333	111.9038	0.3852	0.5562	
A	3091.9472	3.2889	62.3702	0.1924	0.3227	
A	3076.5674	7.7107	70.1031	0.7226	0.8390	
A	3020.2000	17.8745	120.7859	0.1061	0.1918	
A	3007.7626	23.7520	221.8516	0.1889	0.3178	
A	2524.1708	8.0585	108.4051	0.7148	0.8337	
A	2516.0817	12.7340	159.7914	0.4500	0.6207	
A	2489.9213	81.6254	518.9534	0.1471	0.2564	
A	1906.4375	26.6128	20.3051	0.7398	0.8504	
A	1758.4853	776.4806	41.8283	0.5184	0.6828	
A	1441.9645	10.0142	11.8709	0.6170	0.7631	
A	1437.2667	7.6039	14.2435	0.7340	0.8466	
A	1429.8560	5.1318	13.9223	0.7417	0.8517	
A	1380.8309	360.5586	13.5950	0.1987	0.3315	
A	1361.5240	1.4728	18.2949	0.2361	0.3821	
A	1322.3251	8.9095	7.3867	0.1708	0.2917	
A	1294.6726	5.3456	5.6697	0.5759	0.7309	
A	1220.6202	21.9592	9.4151	0.1806	0.3059	
A	1174.6017	0.9370	6.8635	0.2666	0.4210	
A	1126.5240	5.5217	15.7372	0.7447	0.8537	
A	1117.3100	16.7259	18.8424	0.6394	0.7801	
A	1105.2688	4.1604	35.1197	0.1577	0.2724	
A	1062.2292	1.5648	2.2691	0.4555	0.6259	
A	1029.2572	9.5124	29.4835	0.0996	0.1812	
A	998.0548	116.7587	5.5614	0.6122	0.7594	
A	988.8357	57.6557	1.0206	0.6876	0.8149	
A	962.4432	33.8345	30.8545	0.7177	0.8357	
A	917.5301	3.6674	5.6255	0.5248	0.6883	
A	891.8267	51.4841	1.6243	0.6007	0.7505	
A	863.2546	6.4171	13.8004	0.2354	0.3811	
A	836.2782	34.1769	5.0399	0.7470	0.8552	
A	694.4806	5.5372	10.3143	0.2167	0.3562	
A	624.5569	10.0907	8.3065	0.5244	0.6880	
A	575.5246	3.8077	5.6621	0.1195	0.2134	

A	522.2934	9.2969	9.7897	0.2278	0.3711
A	462.5688	5.0361	11.7060	0.7490	0.8565
A	444.7011	4.2218	19.4324	0.4153	0.5869
A	433.0874	1.8656	5.5981	0.6835	0.8120
A	407.6151	0.2377	1.6779	0.5411	0.7023
A	333.4256	0.6882	5.6249	0.6633	0.7976
A	312.4548	7.9087	3.3095	0.7490	0.8565
A	282.5798	42.7280	10.2048	0.2934	0.4537
A	261.8809	7.4924	0.9567	0.6170	0.7631
A	239.8728	15.4844	5.3010	0.5758	0.7308
A	181.9987	3.4239	10.3280	0.6103	0.7580
A	154.1492	8.7661	6.5701	0.7499	0.8571
A	103.5728	6.4219	0.6375	0.2932	0.4534
A	81.0598	0.1405	0.7736	0.7480	0.8558
A	77.1599	0.6201	1.8921	0.7484	0.8561
A	59.1677	7.8724	0.1877	0.5239	0.6876
A	42.8518	3.9163	2.7226	0.7499	0.8571
A	20.3250	3.3310	0.7708	0.7280	0.8426

Processing auphexdienoat5sm16psd1pbedcms.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-861.6008562

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
90.91166	99.442	122.369	117.260	99.478	43.383	32.291

20

C	-1.091893	3.046052	0.526344
C	-0.339132	2.124436	-0.027659
Au	-1.004332	-0.006543	-0.060624
P	-2.271157	-1.925765	0.210955
C	0.661202	1.461848	-0.653302
C	1.971590	1.080070	-0.015439
C	2.417949	-0.335839	-0.353986
C	3.849607	-0.686608	0.107165
O	4.583171	0.259949	0.489887
O	4.151713	-1.906331	0.034321
H	-2.704822	-2.550165	-0.969948
H	-1.650066	-2.979800	0.900742
H	-3.470848	-1.766222	0.923866
H	-2.021578	2.818070	1.038802
H	-0.777517	4.088058	0.472241

H	0.595404	1.364916	-1.741205
H	2.717340	1.789573	-0.398989
H	1.920684	1.229691	1.066741
H	1.725600	-1.067781	0.081443
H	2.380374	-0.491631	-1.441135

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3269.6870	5.5190	224.8340	0.7470	0.8552	26.7821
A	3168.5226	7.6058	738.9494	0.1723	0.2939	
A	3152.3805	4.2808	144.6856	0.2472	0.3965	
A	3139.5325	18.9852	192.6335	0.5858	0.7388	
A	3097.4806	31.8199	188.4227	0.7483	0.8560	
A	3069.3260	12.8485	519.9970	0.1607	0.2769	
A	3051.0777	32.6824	357.9848	0.0445	0.0853	
A	2564.2703	0.2023	299.3238	0.7487	0.8563	
A	2563.2432	0.2382	313.8473	0.7490	0.8565	
A	2541.3102	10.7741	850.8062	0.0145	0.0287	
A	1953.7734	106.2777	76.2500	0.7274	0.8422	
A	1672.5132	989.7866	28.2502	0.6338	0.7758	
A	1454.4429	25.0006	46.5407	0.6145	0.7612	
A	1450.0091	29.9876	16.3066	0.7377	0.8490	
A	1436.2964	13.5035	24.9010	0.7222	0.8387	
A	1414.9944	495.2517	118.8526	0.6189	0.7646	
A	1377.8080	2.5054	25.2035	0.1668	0.2860	
A	1324.9714	14.1306	12.3515	0.1038	0.1881	
A	1282.7875	3.5117	28.8394	0.5137	0.6787	
A	1224.4118	2.6374	26.1717	0.5277	0.6909	
A	1169.7696	5.2944	61.1962	0.1734	0.2956	
A	1117.8224	9.4654	130.2404	0.1312	0.2319	
A	1114.1753	8.5597	43.0341	0.7447	0.8537	
A	1113.6282	8.9852	43.9934	0.7374	0.8489	
A	1084.6815	1.0756	5.2450	0.6906	0.8170	
A	1056.6144	6.1340	67.7932	0.1139	0.2044	
A	1005.8357	15.8855	16.4403	0.2353	0.3810	
A	969.9024	228.4597	21.9261	0.7499	0.8571	
A	958.5172	11.3832	54.0235	0.2986	0.4599	
A	926.7493	41.5281	30.8098	0.3935	0.5648	
A	911.6858	76.9934	22.6568	0.4002	0.5716	
A	905.4931	56.8781	8.7452	0.6505	0.7882	
A	793.2422	34.5334	2.7916	0.5091	0.6747	
A	685.0341	25.3467	3.0330	0.4662	0.6360	
A	612.8098	33.9319	28.5343	0.2327	0.3776	
A	588.7978	5.0235	3.0157	0.2441	0.3925	
A	549.8277	22.5205	5.3255	0.5403	0.7015	
A	498.3539	1.2591	0.8196	0.7421	0.8520	
A	488.9136	2.1172	2.1758	0.6326	0.7750	

A	458.0702	3.5804	5.5531	0.1663	0.2851
A	390.8954	16.0479	41.5276	0.3361	0.5031
A	347.4695	10.2256	4.7863	0.2673	0.4218
A	297.9683	16.2386	23.5224	0.3348	0.5016
A	266.6874	35.7858	20.6436	0.6392	0.7799
A	249.2294	3.8687	9.3461	0.5861	0.7391
A	174.6054	1.8881	8.5906	0.6661	0.7996
A	146.4982	5.9807	3.8696	0.7237	0.8397
A	96.6830	6.9095	2.3762	0.6218	0.7668
A	89.5883	0.0878	0.8418	0.5714	0.7272
A	83.5818	0.2360	1.6355	0.7213	0.8381
A	77.7588	9.4864	4.9699	0.7356	0.8477
A	60.5829	0.9630	3.8679	0.7479	0.8558
A	48.2117	2.3506	2.8377	0.6746	0.8057
A	45.1057	17.1135	1.8417	0.7309	0.8445

5-exo-trig prod2 for 4,5-Au-PH3 complex of hexa-4,5-dienoic acid carboxylate:

Processing auphexdienoat5prod26psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-861.9544438

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
92.72362	100.427	115.581	110.506	100.459	43.383	31.640

20

C	-1.221765	1.855685	-0.499799
C	-0.813654	0.717583	0.076757
C	-1.769861	-0.180491	0.814798
C	-1.987289	-1.535539	0.123399
C	-3.145313	-1.223749	-0.809624
C	-3.899929	-0.139393	-0.072571
O	-5.024469	0.245642	-0.259526
Au	1.162706	0.127541	0.008506
P	3.468373	-0.493969	-0.081765
O	-3.102499	0.379880	0.888186
H	4.186400	-0.626778	1.124798
H	3.824639	-1.720949	-0.679051
H	4.362978	0.348891	-0.772798
H	-0.535459	2.500774	-1.044841
H	-2.256950	2.198183	-0.433823
H	-1.440555	-0.299250	1.854948

H	-1.082897	-1.883790	-0.384938
H	-2.282437	-2.291247	0.861839
H	-3.809944	-2.061040	-1.035783
H	-2.802557	-0.799775	-1.762866

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3205.7582	6.3484	10.7466
A	3140.6344	9.4845	
A	3122.1823	17.8521	
A	3110.6982	15.5517	
A	3063.7377	33.1192	
A	3062.7771	3.2706	
A	3051.5855	16.1947	
A	2502.7090	17.9787	
A	2500.9398	16.6942	
A	2487.4394	89.4433	
A	1893.4145	565.7813	
A	1665.0325	11.0522	
A	1464.3112	11.2074	
A	1429.7927	11.0758	
A	1410.3811	16.1874	
A	1363.8244	39.2590	
A	1331.3140	27.7249	
A	1300.9247	1.3396	
A	1285.4646	64.1110	
A	1215.2933	43.0942	
A	1193.3159	184.3255	
A	1156.5698	5.2501	
A	1133.7052	5.9005	
A	1130.9940	8.2738	
A	1130.1834	3.9585	
A	1069.7615	87.7417	
A	1053.4433	2.9150	
A	1016.8260	169.6406	
A	1002.7108	84.6267	
A	978.2818	34.1051	
A	930.2830	38.6061	
A	910.0515	11.4386	
A	876.1902	14.9883	
A	813.3404	3.0681	
A	788.1168	4.8583	
A	702.7990	2.0560	
A	663.6029	12.5554	
A	620.4476	2.9179	
A	543.4201	3.0985	
A	504.1926	1.5873	

A	476.9567	9.9934
A	425.2143	0.9480
A	412.5612	3.8215
A	332.8095	2.8439
A	283.7954	4.8802
A	255.2128	0.6737
A	246.3160	3.9276
A	161.9096	3.2105
A	127.4651	2.5124
A	88.7644	3.1081
A	73.1448	3.1137
A	64.0931	0.1039
A	50.2156	0.5397
A	36.2054	0.1743

Processing auphexdienoat5prod26psd1pbedcms.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-861.6480843

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
93.52771	101.154	115.358	110.164	101.186	43.383	31.643

20

C	1.208436	-1.882418	-0.513725
C	0.784098	-0.738367	0.050985
C	1.745643	0.167520	0.778200
C	1.973664	1.524326	0.086604
C	3.185321	1.245302	-0.791766
C	3.907320	0.152209	-0.044194
O	5.050147	-0.227804	-0.184219
Au	-1.175210	-0.132252	0.001539
P	-3.414572	0.527162	-0.048349
O	3.087556	-0.399265	0.864654
H	-4.046905	0.784364	1.183170
H	-3.735253	1.707770	-0.745691
H	-4.340334	-0.363471	-0.624800
H	0.527736	-2.541894	-1.048057
H	2.247702	-2.211524	-0.455556
H	1.421287	0.293049	1.815510
H	1.090569	1.846024	-0.468755
H	2.213851	2.287422	0.833952
H	3.846884	2.099064	-0.952123

H 2.906158 0.844812 -1.774124

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3227.1692	13.0896	232.5687	0.7460	0.8545	13.9206
A	3173.1317	12.6264	180.4808	0.5477	0.7077	
A	3165.7099	11.1925	178.9603	0.4459	0.6168	
A	3137.3490	33.8564	445.0182	0.1703	0.2911	
A	3120.9737	30.1010	305.1169	0.2247	0.3670	
A	3096.4411	29.1851	129.1162	0.3336	0.5003	
A	3092.0951	4.6674	306.7928	0.0634	0.1193	
A	2534.1525	7.0877	329.9258	0.7482	0.8560	
A	2532.7638	7.7119	337.2817	0.7424	0.8522	
A	2516.9863	49.7341	1024.1456	0.0335	0.0648	
A	1831.6207	815.8663	28.4750	0.4184	0.5900	
A	1660.3344	23.2102	104.9195	0.1303	0.2306	
A	1477.4569	13.1080	13.4872	0.7500	0.8571	
A	1436.6195	16.3089	16.2202	0.7499	0.8571	
A	1427.7983	14.2888	72.8060	0.4390	0.6101	
A	1387.4344	80.9908	14.9563	0.3681	0.5381	
A	1347.4403	33.5979	8.0343	0.4449	0.6158	
A	1318.7248	2.9577	10.4142	0.6718	0.8037	
A	1297.5822	97.3303	6.8299	0.7064	0.8280	
A	1226.8238	34.2387	24.2387	0.7214	0.8382	
A	1214.1386	317.0866	7.9947	0.5486	0.7085	
A	1169.0779	6.9416	11.4060	0.2726	0.4284	
A	1145.3909	6.4839	21.1011	0.1548	0.2681	
A	1119.2962	9.2712	44.3097	0.7500	0.8571	
A	1119.0292	9.6266	44.7826	0.7489	0.8564	
A	1067.5476	60.7252	17.7255	0.6641	0.7981	
A	1061.1076	30.0636	7.1999	0.3689	0.5390	
A	998.1477	64.7270	8.7741	0.6017	0.7513	
A	991.4986	128.0954	59.8981	0.7182	0.8360	
A	982.8988	239.4024	9.6991	0.5899	0.7421	
A	925.0974	91.2494	11.1399	0.6883	0.8154	
A	922.4229	6.2094	6.8889	0.5439	0.7046	
A	876.8325	11.0565	32.8951	0.0760	0.1412	
A	815.1693	12.1757	10.2199	0.0754	0.1403	
A	795.6681	11.5484	6.6969	0.4210	0.5926	
A	705.1410	6.7446	22.2295	0.0916	0.1678	
A	663.4586	20.9909	5.8925	0.4545	0.6250	
A	627.8234	5.9302	12.1809	0.1458	0.2545	
A	550.0816	5.3869	3.9858	0.7108	0.8309	
A	516.3314	5.3940	3.3292	0.7464	0.8548	
A	491.7652	17.7750	2.3561	0.1863	0.3141	
A	475.8566	0.7853	0.7081	0.5828	0.7364	
A	442.8281	12.5398	3.0377	0.2396	0.3866	

A	329.4643	5.2327	3.1996	0.0941	0.1720
A	295.1139	0.3507	10.2717	0.0966	0.1761
A	284.9537	10.7636	5.9963	0.3567	0.5258
A	243.9844	6.4728	3.4454	0.7097	0.8302
A	153.8199	3.4010	0.6325	0.7499	0.8571
A	117.9231	8.0189	2.5868	0.7446	0.8536
A	93.2940	2.4391	3.6347	0.7214	0.8382
A	78.9975	4.4533	0.6497	0.7414	0.8515
A	58.7776	1.0597	0.8656	0.7262	0.8414
A	47.0290	0.0280	0.1298	0.7403	0.8507
A	35.0085	0.3559	0.6760	0.7441	0.8533

5-exo-trig prod1 for 4,5-Au-PH3 complex of hexa-4,5-dienoic acid carboxylate:

Processing auphexdienoat5prod6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-861.9539096

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
92.65412	100.388	115.408	111.305	100.414	43.383	31.798

20

O	-3.100640	0.636795	0.407059
C	-1.802556	-0.008758	0.433738
C	-1.992997	-1.257309	-0.433980
C	-3.458616	-1.586641	-0.212167
C	-4.076199	-0.235432	0.078094
C	-0.706927	0.900939	-0.019870
Au	1.204937	0.128172	0.011985
P	3.445354	-0.700075	0.035053
O	-5.239921	0.069008	0.048515
C	-0.955719	2.151236	-0.429437
H	3.966252	-1.231895	1.232852
H	3.796611	-1.751697	-0.836603
H	4.490966	0.193621	-0.275360
H	-0.161858	2.809114	-0.777591
H	-1.966284	2.563025	-0.425392
H	-1.627331	-0.304263	1.482816
H	-1.804062	-0.991595	-1.482751
H	-1.298031	-2.056901	-0.157461
H	-3.971294	-2.066102	-1.049712
H	-3.612720	-2.218374	0.673730

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3210.4351	5.9036	106.8616	0.7199	0.8372	10.7290
A	3138.6438	7.5476	91.3022	0.4869	0.6549	
A	3118.4050	26.9654	10.6444	0.2783	0.4355	
A	3117.9172	3.0456	219.2260	0.2001	0.3334	
A	3052.4894	22.9357	40.3130	0.4019	0.5734	
A	3048.4822	6.6433	134.6347	0.0452	0.0864	
A	2990.7020	24.6750	96.2411	0.2311	0.3755	
A	2505.1179	16.2899	138.5689	0.7496	0.8569	
A	2501.2892	20.4461	155.2587	0.5990	0.7492	
A	2488.5503	88.4167	543.6085	0.0776	0.1441	
A	1894.3668	599.2847	13.5505	0.5050	0.6711	
A	1669.7012	12.0643	37.4288	0.1423	0.2492	
A	1462.8115	5.0535	3.5801	0.7269	0.8419	
A	1433.2574	8.4849	7.9701	0.7254	0.8409	
A	1411.8463	22.7916	27.3313	0.4518	0.6224	
A	1363.8440	3.2735	11.1188	0.4421	0.6131	
A	1339.4048	53.0193	10.0256	0.4519	0.6225	
A	1305.1389	86.1372	2.8528	0.3016	0.4634	
A	1285.4446	17.7657	0.7721	0.6015	0.7512	
A	1234.1675	74.7109	9.9619	0.5072	0.6730	
A	1209.1811	156.1426	4.9896	0.7369	0.8485	
A	1161.6102	16.3157	34.6379	0.2297	0.3736	
A	1148.0782	43.2294	6.9374	0.6816	0.8107	
A	1133.9468	4.2623	18.2353	0.7498	0.8570	
A	1130.7146	4.3586	18.3011	0.7482	0.8560	
A	1079.4803	29.6694	2.9265	0.7044	0.8266	
A	1055.7192	63.1808	6.6850	0.5236	0.6874	
A	1022.6243	56.5372	15.4155	0.7497	0.8570	
A	1011.8322	225.4915	12.4658	0.5301	0.6929	
A	999.5197	12.4765	7.1413	0.4317	0.6031	
A	935.4329	40.1324	2.3416	0.1637	0.2814	
A	928.2586	37.8637	2.0977	0.7214	0.8382	
A	868.0639	3.4859	9.9440	0.1074	0.1939	
A	820.4972	5.2947	9.5317	0.0956	0.1745	
A	738.1555	2.3527	5.7614	0.5268	0.6901	
A	686.9094	8.5406	13.3296	0.1500	0.2609	
A	651.6912	6.0331	2.2204	0.2918	0.4517	
A	612.0266	3.7510	1.6624	0.0721	0.1345	
A	526.4372	1.2731	1.8339	0.7353	0.8475	
A	519.2501	8.6382	0.5877	0.4521	0.6227	
A	478.4713	7.6196	6.4121	0.1458	0.2545	
A	432.7386	0.7663	0.4998	0.7326	0.8456	
A	418.4415	3.7125	2.1417	0.1362	0.2398	
A	299.2356	2.8218	3.2893	0.2881	0.4473	

A	279.7650	3.9663	0.9421	0.6778	0.8080
A	253.6710	0.1048	9.4243	0.1828	0.3091
A	208.0201	6.6726	2.1665	0.4668	0.6365
A	157.3444	1.1233	0.4858	0.7462	0.8547
A	123.0561	1.0148	0.5682	0.5439	0.7046
A	95.9224	1.6318	1.7603	0.7318	0.8452
A	90.4832	0.0126	0.0767	0.7496	0.8569
A	76.3315	4.2521	0.7180	0.7357	0.8478
A	50.3173	0.8225	1.4109	0.7499	0.8571
A	37.2597	0.8513	0.4736	0.7387	0.8497

Processing auphexdienoat5prod6psd1pbedcms.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-861.6485977

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
93.41804	101.130	117.248	110.647	101.165	43.383	31.789

20

O	3.092069	0.629403	-0.422706
C	1.780019	-0.015976	-0.426228
C	1.983373	-1.264138	0.444162
C	3.455492	-1.584634	0.228169
C	4.057803	-0.237527	-0.085412
C	0.688096	0.903221	0.030810
Au	-1.212029	0.131391	-0.009929
P	-3.387765	-0.712976	-0.046605
O	5.227107	0.083441	-0.071515
C	0.962771	2.155083	0.436983
H	-3.953381	-1.015960	-1.299893
H	-3.632939	-1.919239	0.637185
H	-4.403551	0.094920	0.498998
H	0.181019	2.827208	0.784486
H	1.978248	2.554299	0.435591
H	1.600302	-0.311973	-1.468915
H	1.793676	-1.011649	1.492981
H	1.306063	-2.070557	0.155179
H	3.962592	-2.044795	1.078648
H	3.615957	-2.226393	-0.647913

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole

A	3229.6671	13.2263	247.8344	0.7382	0.8494	13.9821
A	3170.2239	14.0704	159.0020	0.7225	0.8389	
A	3164.1786	8.5101	182.3972	0.2733	0.4293	
A	3140.9830	33.4510	424.4295	0.1828	0.3090	
A	3096.4720	24.9929	127.3556	0.1185	0.2119	
A	3083.5626	8.2521	281.5651	0.1062	0.1920	
A	3065.1000	25.3281	312.6993	0.2289	0.3725	
A	2534.3861	7.9286	336.3264	0.7233	0.8394	
A	2532.5611	7.7109	331.2968	0.7435	0.8529	
A	2516.9908	49.1813	1002.7798	0.0324	0.0627	
A	1831.5334	815.5250	29.8342	0.4389	0.6101	
A	1662.7981	26.2276	124.5085	0.1149	0.2062	
A	1477.6213	7.8991	11.8177	0.7242	0.8400	
A	1437.6121	14.3059	15.2890	0.7485	0.8562	
A	1430.6252	20.7265	82.1178	0.4457	0.6166	
A	1382.1940	17.7720	17.1339	0.3632	0.5328	
A	1356.0674	59.3436	17.0805	0.6569	0.7929	
A	1324.4334	128.0492	6.8513	0.3062	0.4688	
A	1299.2156	17.0283	1.5173	0.7227	0.8390	
A	1251.7346	144.4727	15.2504	0.5165	0.6811	
A	1218.9999	222.7783	10.6042	0.7400	0.8506	
A	1172.0927	19.2938	33.1547	0.1461	0.2550	
A	1160.1681	46.8308	13.6078	0.6200	0.7654	
A	1119.9662	9.4111	43.9400	0.7499	0.8571	
A	1119.0989	9.3284	44.8747	0.7486	0.8562	
A	1085.7246	9.3886	6.5152	0.7303	0.8441	
A	1049.4990	56.4258	21.2362	0.4319	0.6033	
A	1016.8665	66.9365	21.9604	0.7463	0.8547	
A	1001.8318	50.5572	6.5897	0.3778	0.5484	
A	990.8772	320.6145	56.5672	0.7339	0.8465	
A	944.1395	58.7931	4.8757	0.1628	0.2800	
A	925.9041	85.6362	17.1498	0.7498	0.8570	
A	873.3921	10.8441	16.7483	0.1341	0.2364	
A	826.8600	14.7516	20.7828	0.0915	0.1676	
A	748.0151	4.5302	5.4041	0.5614	0.7191	
A	691.2755	17.8840	24.0196	0.1222	0.2179	
A	654.9530	15.3640	5.8987	0.7346	0.8470	
A	619.8317	6.9791	2.7707	0.0972	0.1772	
A	537.0868	6.4181	5.4518	0.6798	0.8094	
A	529.1572	15.3446	2.0720	0.3042	0.4665	
A	492.5297	12.0242	6.1021	0.1814	0.3071	
A	473.9778	0.8121	0.4282	0.6731	0.8046	
A	450.5935	10.7099	5.5911	0.1734	0.2956	
A	308.7416	6.4640	5.3448	0.3963	0.5676	
A	295.0237	0.6445	12.8645	0.0898	0.1648	
A	280.4037	8.0571	3.4149	0.5760	0.7310	
A	208.9711	9.4625	2.9936	0.6688	0.8015	

A	155.0017	1.8314	1.0841	0.6936	0.8191
A	122.9429	1.9458	0.7195	0.7085	0.8294
A	91.7420	2.1065	3.4388	0.7363	0.8481
A	79.7295	6.0219	1.7198	0.7480	0.8558
A	51.0846	1.5450	1.1915	0.7240	0.8399
A	37.2370	0.0680	0.0870	0.7490	0.8565
A	25.1915	1.7247	0.2774	0.7500	0.8571

6-endo-dig prod for 4,5-Au-PH3 complex of hexa-4,5-dienoic acid carboxylate:

Processing auphexdienoat6prod6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-861.9512852

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
92.33705	100.060	115.919	110.417	100.091	43.383	31.630

20

C	3.817339	-0.150501	0.070318
O	3.092141	0.993573	0.065446
C	1.698057	1.070332	-0.059895
C	0.972599	-0.191898	-0.391382
C	1.614772	-1.359594	0.356626
C	3.079810	-1.458020	-0.038281
C	1.207055	2.300671	0.101883
Au	-1.105522	-0.079383	-0.086009
P	-3.467521	-0.011657	0.256143
O	5.017506	-0.070045	0.155711
H	1.872228	3.138773	0.288133
H	0.138738	2.476671	0.036451
H	1.102603	-0.375606	-1.473040
H	-4.321986	-0.279517	-0.833564
H	-4.054993	1.191382	0.699061
H	-4.040877	-0.889690	1.199139
H	1.525685	-1.206850	1.442376
H	1.100991	-2.301507	0.130537
H	3.648026	-2.188666	0.548049
H	3.163699	-1.773065	-1.089428

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3269.6799	8.4216	52.0257	0.6963	0.8210	10.4885
A	3165.4574	0.3707	134.2398	0.1909	0.3205	
A	3107.2936	15.9765	152.4317	0.4369	0.6081	
A	3088.0035	22.3321	71.9985	0.3875	0.5586	
A	3033.6532	19.6953	58.5330	0.2244	0.3666	
A	3025.9020	17.6665	116.5510	0.0664	0.1245	
A	2988.3198	12.1823	109.1933	0.2020	0.3360	
A	2502.6788	16.4184	134.3525	0.7432	0.8527	
A	2501.0495	16.5868	132.5058	0.7083	0.8293	
A	2487.0780	89.2542	545.3680	0.0717	0.1338	
A	1864.2726	569.6070	29.3279	0.2319	0.3765	
A	1721.8128	129.2495	68.3029	0.1673	0.2867	
A	1464.0183	7.4339	8.3721	0.6056	0.7543	
A	1427.5289	8.2957	7.7411	0.7049	0.8269	
A	1382.7741	1.4504	19.7018	0.4207	0.5922	
A	1354.5706	125.9756	0.9019	0.4385	0.6097	
A	1339.2828	1.0407	12.6174	0.4088	0.5804	
A	1311.6813	32.5762	13.9336	0.4750	0.6441	
A	1285.6940	197.9108	1.4638	0.7493	0.8567	
A	1245.5226	17.8126	26.6287	0.3844	0.5553	
A	1192.5011	392.6044	25.1597	0.4983	0.6652	
A	1165.7309	18.2332	9.6959	0.1244	0.2212	
A	1132.7210	3.7444	16.6909	0.7499	0.8571	
A	1130.9515	4.7344	16.6532	0.7121	0.8319	
A	1107.4248	2.3095	100.4916	0.2752	0.4316	
A	1080.3918	15.0809	44.0147	0.3912	0.5624	
A	1038.7001	15.1868	8.7267	0.1877	0.3161	
A	1020.1206	176.4472	9.4619	0.7441	0.8533	
A	1013.9937	27.7877	35.2462	0.4910	0.6586	
A	969.7707	9.7798	9.2227	0.4272	0.5987	
A	914.4204	9.4067	3.7350	0.2935	0.4537	
A	871.2924	6.6391	3.6394	0.7134	0.8327	
A	850.9799	53.1761	4.6310	0.7466	0.8549	
A	758.9134	1.6594	1.6040	0.4896	0.6574	
A	725.1244	2.2801	12.3567	0.1241	0.2208	
A	702.3710	2.7744	13.8152	0.1405	0.2464	
A	625.7057	0.4810	1.7333	0.4994	0.6662	
A	589.6189	14.8194	7.6287	0.1211	0.2160	
A	562.6882	10.1081	2.5169	0.3302	0.4965	
A	510.7680	6.0020	0.5983	0.5204	0.6845	
A	454.4346	5.3685	4.3070	0.2971	0.4581	
A	432.4115	1.8253	0.4084	0.7382	0.8494	
A	420.7090	0.6509	0.1847	0.5714	0.7272	
A	354.3624	1.9018	2.7621	0.7229	0.8391	
A	302.4840	0.7465	3.4898	0.6355	0.7771	
A	254.9958	0.7560	9.1928	0.2016	0.3355	

A	201.6911	3.1055	3.1108	0.2240	0.3661
A	171.4478	1.5255	3.7125	0.3243	0.4897
A	147.5645	2.4595	0.4125	0.1469	0.2561
A	103.3115	0.4688	0.9882	0.6450	0.7842
A	74.9337	0.0337	0.0894	0.7467	0.8550
A	61.9624	5.8075	1.4329	0.6439	0.7834
A	56.7059	1.7339	1.4626	0.7454	0.8542
A	23.2332	1.5168	0.3943	0.5920	0.7437

Processing auphexdienoat6prod6psd1pbedcms.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-861.6431559

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
93.16017	100.697	113.308	109.383	100.723	43.383	31.615

20

C	3.806882	-0.152362	0.055410
O	3.092190	0.990930	0.057266
C	1.688757	1.064683	-0.056169
C	0.953128	-0.194804	-0.372215
C	1.615120	-1.366602	0.360070
C	3.080246	-1.461464	-0.047540
C	1.210881	2.303683	0.102118
Au	-1.114081	-0.080441	-0.075846
P	-3.422084	-0.005550	0.226946
O	5.015231	-0.055799	0.133452
H	1.878518	3.143968	0.270380
H	0.142305	2.478733	0.055395
H	1.090228	-0.373604	-1.452975
H	-4.236287	-0.245437	-0.896742
H	-3.981168	1.203027	0.684818
H	-3.994611	-0.907104	1.145062
H	1.539548	-1.232813	1.446782
H	1.110086	-2.307407	0.121319
H	3.649050	-2.190823	0.537559
H	3.156519	-1.770256	-1.099709

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3296.1342	7.8559	127.2339	0.7500	0.8571	13.2665
A	3191.2355	0.7798	320.9549	0.1800	0.3050	

A	3137.4065	20.9367	317.6580	0.5291	0.6920
A	3130.6103	29.7676	254.9278	0.3315	0.4979
A	3070.5076	41.6404	54.6217	0.5527	0.7119
A	3064.7043	9.7877	430.3717	0.0754	0.1402
A	3005.1727	26.0019	342.4575	0.2532	0.4041
A	2533.3151	8.6982	308.1538	0.7465	0.8549
A	2532.2193	8.4000	320.8910	0.7487	0.8563
A	2516.3986	54.9249	997.6488	0.0329	0.0637
A	1807.3069	763.3055	109.2098	0.1651	0.2834
A	1710.8518	277.9139	206.4041	0.1812	0.3068
A	1478.5329	10.2833	21.6721	0.6056	0.7543
A	1431.2013	8.4477	16.3525	0.7409	0.8512
A	1401.8166	3.6725	55.1289	0.4646	0.6344
A	1367.4078	204.4923	3.9017	0.1879	0.3164
A	1350.9778	1.7561	23.7827	0.6049	0.7538
A	1316.4863	31.2667	18.2542	0.5357	0.6977
A	1297.9080	328.4417	1.8354	0.4859	0.6540
A	1252.4864	28.7023	34.2354	0.3595	0.5289
A	1178.1650	26.8487	12.5099	0.4796	0.6483
A	1162.7217	618.8423	66.2463	0.4930	0.6604
A	1124.9119	11.3146	39.0823	0.6811	0.8103
A	1121.6355	10.2014	42.3846	0.7492	0.8566
A	1111.6873	4.4610	149.2763	0.2572	0.4091
A	1084.4428	60.3503	69.1897	0.3955	0.5669
A	1039.9064	53.3469	10.5854	0.0472	0.0901
A	1023.2110	9.9218	34.3418	0.2982	0.4595
A	996.2188	248.2028	65.6131	0.7390	0.8499
A	971.0868	18.0237	21.3685	0.3684	0.5385
A	922.3555	19.1055	6.8610	0.4055	0.5770
A	879.8442	20.9190	7.5981	0.7389	0.8498
A	864.9817	114.7467	24.8870	0.7426	0.8523
A	765.8247	2.0035	3.6542	0.7344	0.8469
A	733.2992	7.4428	14.6314	0.1337	0.2359
A	704.3573	9.1387	30.2677	0.1351	0.2380
A	634.1895	3.2866	4.9896	0.2545	0.4057
A	595.6546	20.3430	11.8922	0.1594	0.2750
A	567.7672	23.7627	4.1825	0.2609	0.4139
A	517.2613	12.6697	0.5704	0.6148	0.7614
A	480.1169	0.5688	1.5462	0.3628	0.5324
A	476.9848	1.0699	0.4757	0.6559	0.7922
A	456.9638	8.3648	8.7314	0.3836	0.5545
A	358.0931	4.4325	5.1063	0.7358	0.8478
A	308.9806	3.3550	5.8650	0.7037	0.8261
A	297.1695	0.2582	15.1444	0.1277	0.2264
A	198.6981	5.3647	2.2564	0.2700	0.4253
A	175.5273	3.0083	3.6064	0.3820	0.5528
A	152.7571	3.4662	0.7875	0.2921	0.4521

A	115.6599	0.6864	2.0872	0.6493	0.7874
A	81.4510	0.1927	0.3026	0.7498	0.8570
A	74.6540	10.4196	1.8699	0.6319	0.7744
A	60.0182	3.2380	1.1586	0.7500	0.8571
A	37.2076	2.5749	1.8067	0.6605	0.7956

6-exo-dig prod for 4,5-Au-PH3 complex of hexa-4,5-dienoic acid carboxylate:

Processing auphexdienoat6xprod6psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-861.9584026

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
92.35384	100.155	118.330	111.445	100.187	43.383	31.990

20

O	2.897035	-0.921254	-0.131735
C	1.704529	-0.180515	-0.105034
C	1.739690	1.152703	-0.202182
C	3.038192	1.892201	-0.277752
C	4.102617	1.099919	0.469299
C	4.113283	-0.349399	0.066466
C	0.543989	-1.100941	-0.013829
Au	-1.353119	-0.232721	0.007351
P	-3.555707	0.687074	0.038613
O	5.104211	-1.023977	-0.050144
H	0.654999	-1.715457	0.891707
H	0.592785	-1.807638	-0.855136
H	0.795245	1.689376	-0.224922
H	-4.625770	-0.137592	0.444235
H	-3.821427	1.798727	0.865505
H	-4.111106	1.179147	-1.160947
H	3.343330	2.045478	-1.325489
H	2.945129	2.893325	0.159612
H	5.115195	1.488649	0.331889
H	3.879865	1.122828	1.546846

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3201.3749	14.5335	88.7586	0.2197	0.3603	9.7631
A	3131.0073	12.6033	119.5858	0.4247	0.5962	
A	3080.4696	22.4620	112.9466	0.4430	0.6140	

A	3074.3695	3.5827	81.2418	0.7500	0.8571
A	3033.6825	14.9978	77.7714	0.1503	0.2613
A	3029.5643	16.9136	167.8048	0.0512	0.0975
A	3004.7105	38.7888	213.2381	0.1380	0.2425
A	2501.3826	18.6773	122.4225	0.7458	0.8544
A	2497.5451	21.2741	152.1372	0.5516	0.7110
A	2484.5818	84.9474	479.8919	0.0756	0.1406
A	1875.5236	515.3961	18.9300	0.4682	0.6378
A	1755.9238	61.9855	41.9372	0.1408	0.2468
A	1461.9456	4.4760	16.3083	0.5711	0.7270
A	1432.8324	14.7652	6.8243	0.7484	0.8561
A	1427.7664	8.8819	17.5217	0.6981	0.8222
A	1363.0979	87.7280	1.6013	0.6364	0.7778
A	1334.8711	3.9037	8.6295	0.3367	0.5038
A	1302.6314	34.6537	51.5138	0.5598	0.7178
A	1246.0268	99.6714	22.6283	0.4143	0.5859
A	1236.2030	133.3091	19.0238	0.1235	0.2199
A	1188.3993	204.8587	22.6654	0.4690	0.6385
A	1159.4300	55.4223	4.6053	0.1911	0.3209
A	1141.8460	9.9447	0.8090	0.7257	0.8410
A	1133.5558	5.4953	16.9759	0.7414	0.8515
A	1131.9521	3.6076	18.3565	0.7500	0.8571
A	1117.2779	90.4529	68.9292	0.2089	0.3457
A	1070.9468	117.4696	3.5594	0.6313	0.7739
A	1036.9345	4.9280	5.3839	0.2323	0.3770
A	1019.4666	211.8127	21.3828	0.7197	0.8370
A	985.3020	19.9886	2.6678	0.2278	0.3710
A	945.9028	4.6066	4.0486	0.3945	0.5658
A	908.0787	6.6520	2.1281	0.2536	0.4045
A	806.5619	16.8057	2.8941	0.4974	0.6644
A	775.5005	11.9778	11.9981	0.0664	0.1245
A	705.7638	8.0478	4.9391	0.0994	0.1808
A	689.7806	0.1330	1.4217	0.2088	0.3454
A	640.4023	4.0618	11.7210	0.2400	0.3871
A	598.1291	3.8647	2.3213	0.1651	0.2834
A	540.9708	6.2126	2.3495	0.5594	0.7175
A	530.0034	1.4395	1.6133	0.6188	0.7645
A	461.0033	3.1994	8.0548	0.3592	0.5286
A	444.9731	2.7017	0.8675	0.3446	0.5125
A	424.3545	2.0411	0.3053	0.7496	0.8569
A	409.2034	1.6343	1.3829	0.1171	0.2097
A	255.1750	0.6048	6.9306	0.1583	0.2733
A	235.8732	1.0786	1.0258	0.6962	0.8209
A	198.6168	7.3095	4.9927	0.3418	0.5095
A	140.3891	5.1971	0.4538	0.7416	0.8516
A	127.1505	0.6778	0.4679	0.5466	0.7068
A	109.2325	1.5649	0.3613	0.4229	0.5944

A	91.0343	0.7022	0.6729	0.7476	0.8556
A	50.1665	1.3362	1.1750	0.6893	0.8161
A	33.8572	0.4192	0.3130	0.6953	0.8203
A	19.7079	0.0445	0.1802	0.7496	0.8569

Processing auphexdienoat6xprod6psd1pbedcms.log
PG=C01

WARNING: Imaginary frequencies

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	1

HF Energy
-861.6514869

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
93.02068	100.124	110.329	107.196	100.143	43.383	31.980

20

O	2.895936	-0.923574	-0.141313
C	1.694982	-0.176743	-0.122205
C	1.744740	1.156376	-0.220462
C	3.048569	1.890913	-0.281555
C	4.110392	1.092785	0.467357
C	4.102025	-0.356586	0.078382
C	0.526235	-1.089619	-0.034326
Au	-1.361898	-0.226490	0.004783
P	-3.510551	0.674927	0.057627
O	5.088646	-1.056361	-0.012812
H	0.647191	-1.711753	0.865998
H	0.576156	-1.796440	-0.876949
H	0.805073	1.698572	-0.247950
H	-4.547630	-0.139415	0.552316
H	-3.718847	1.834109	0.829802
H	-4.081565	1.086808	-1.162058
H	3.358542	2.050277	-1.324981
H	2.953559	2.884614	0.167273
H	5.121160	1.477819	0.318722
H	3.896226	1.120974	1.545393

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3236.1067	10.8058	227.8253	0.2257	0.3682	12.4860
A	3165.0795	11.5816	239.3057	0.4342	0.6055	
A	3122.5375	21.5166	263.6850	0.4189	0.5904	
A	3068.1657	15.8947	283.1342	0.7373	0.8488	

A	3067.4774	11.7723	175.6740	0.2106	0.3479
A	3043.2402	40.7157	490.9281	0.1362	0.2397
A	3032.0301	51.7096	500.0238	0.0770	0.1430
A	2532.1584	10.0401	304.2274	0.7415	0.8516
A	2529.7539	9.6569	325.3917	0.7171	0.8353
A	2514.8932	52.6989	926.4117	0.0300	0.0583
A	1817.9292	727.7872	43.3727	0.4009	0.5724
A	1758.8448	97.1683	132.4807	0.1127	0.2026
A	1465.9011	7.7567	41.1647	0.5784	0.7329
A	1440.4907	22.5926	16.1597	0.7413	0.8514
A	1432.1848	7.4421	56.1458	0.6581	0.7938
A	1377.8475	95.0789	3.1641	0.6605	0.7956
A	1346.0748	10.0845	13.0810	0.3176	0.4821
A	1312.8996	88.3148	65.4733	0.5788	0.7332
A	1249.5462	75.4478	35.6796	0.1308	0.2313
A	1244.6895	121.3956	16.6162	0.7314	0.8448
A	1185.4027	207.0540	78.0486	0.3473	0.5156
A	1171.7754	158.0639	7.5177	0.7497	0.8569
A	1154.6871	17.3708	4.0900	0.6185	0.7643
A	1124.1470	14.8435	46.9231	0.7095	0.8301
A	1119.9950	19.8820	50.6243	0.6194	0.7650
A	1118.7587	95.8987	72.4032	0.1631	0.2805
A	1065.1042	278.2601	5.1052	0.1994	0.3325
A	1044.7203	9.3459	11.0573	0.3402	0.5077
A	995.6457	265.2972	57.8381	0.7459	0.8545
A	981.5541	41.3457	3.2061	0.3548	0.5238
A	950.5847	21.2030	9.1511	0.3894	0.5605
A	914.3818	7.5822	3.2031	0.4545	0.6249
A	824.1033	49.1733	8.8270	0.6776	0.8078
A	781.1967	28.0139	18.7124	0.0664	0.1244
A	706.7264	26.1733	12.6074	0.0868	0.1598
A	693.7570	2.1141	4.6008	0.3489	0.5174
A	644.0852	9.2955	11.3267	0.2489	0.3986
A	603.5834	4.5949	4.1013	0.1386	0.2434
A	545.1926	9.0478	6.7916	0.7236	0.8396
A	533.1121	6.4227	4.0312	0.7394	0.8502
A	478.7137	1.1444	0.4762	0.2618	0.4150
A	469.6262	5.7199	9.6262	0.4367	0.6080
A	463.7313	5.6152	5.2926	0.3253	0.4909
A	436.0876	7.5109	3.4209	0.3083	0.4713
A	294.8914	0.5424	11.3767	0.0877	0.1612
A	232.9675	3.1998	2.8140	0.7486	0.8562
A	198.5866	11.9072	5.1197	0.4116	0.5832
A	139.8332	6.7002	0.5615	0.7355	0.8476
A	133.2744	3.2669	0.8181	0.6769	0.8073
A	114.0950	2.6281	0.8826	0.6437	0.7832
A	97.3649	0.7387	1.2983	0.7499	0.8571

A	56.1621	3.1494	0.9884	0.7440	0.8532
A	37.2144	0.1885	0.1106	0.7499	0.8571
A	-1.3556	0.2025	0.0368	0.5954	0.7464

6-exo-dig prod2 for 4,5-Au-PH3 complex of hexa-4,5-dienoic acid carboxylate:

Processing auphexdienoat6xprod26psdm6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	GenECP	0

HF Energy
-861.9584258

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
92.44617	100.181	116.664	111.406	100.207	43.383	31.991

20

C	0.544060	-1.102255	0.011849
C	1.703836	-0.180909	0.104006
C	1.737753	1.152426	0.200053
C	3.035468	1.893252	0.276036
C	4.101402	1.101025	-0.468923
C	4.112916	-0.347797	-0.064316
O	5.104329	-1.021249	0.054608
Au	-1.353216	-0.234567	-0.008409
P	-3.552780	0.692031	-0.034831
O	2.896915	-0.920619	0.132692
H	-3.701673	2.094047	0.012455
H	-4.449524	0.350213	0.998841
H	-4.391496	0.428459	-1.138005
H	0.655410	-1.715658	-0.894410
H	0.593241	-1.809782	0.852421
H	0.792823	1.688308	0.221392
H	2.941868	2.893702	-0.162765
H	3.339375	2.048238	1.323876
H	3.879737	1.122429	-1.546725
H	5.113476	1.490848	-0.330915

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3201.3799	14.5450	9.7625
A	3130.9761	12.6016	
A	3080.4071	22.4280	
A	3074.4393	3.6401	
A	3033.6033	15.0428	

A	3029.5860	16.8829
A	3004.7471	38.7466
A	2501.2921	18.4057
A	2501.2036	17.9128
A	2487.5387	88.6267
A	1875.5458	515.3726
A	1755.9023	61.9098
A	1461.9621	4.4782
A	1432.8387	14.7950
A	1427.7434	8.7574
A	1363.0861	87.6249
A	1334.8646	3.9333
A	1302.6287	34.5488
A	1245.9959	100.1384
A	1236.1692	132.7568
A	1188.3464	204.9337
A	1159.4005	55.7997
A	1141.8025	9.8568
A	1133.3251	4.1819
A	1132.8493	3.7652
A	1117.1340	90.2121
A	1070.9425	117.1484
A	1036.9375	4.8894
A	1021.7727	213.2893
A	985.2924	19.9275
A	945.9206	4.6087
A	908.0400	6.6357
A	806.6614	16.5640
A	775.5128	11.9119
A	705.8386	7.9243
A	689.9479	0.2029
A	640.4301	4.0861
A	598.4212	3.8457
A	540.9724	6.2054
A	530.1605	1.4546
A	461.0245	3.1316
A	446.3906	2.7712
A	422.5768	1.1046
A	416.1808	2.6908
A	255.2641	0.6004
A	235.8977	1.0893
A	198.6342	7.3227
A	140.3835	5.2125
A	127.3979	0.6196
A	109.8434	1.6370
A	91.1632	0.5173
A	82.3466	0.2431

A	49.6935	1.6559
A	18.6216	0.0562

Processing auphexdienoat6xprod26psd1pbedcms.log
PG=C01

Method	BasisSet	Imaginary Freqs
RPBE1PBE	GenECP	0

HF Energy
-861.6515057

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
93.07073	100.718	117.752	110.639	100.744	43.383	31.980

20

C	-0.526312	-1.089218	-0.028825
C	-1.694913	-0.176395	-0.119309
C	-1.744554	1.156839	-0.215968
C	-3.048267	1.891454	-0.278664
C	-4.111820	1.091937	0.466349
C	-4.102438	-0.356741	0.074815
O	-5.088791	-1.056347	-0.020467
Au	1.362055	-0.226676	0.005801
P	3.510610	0.675063	0.052222
O	-2.895723	-0.923327	-0.142420
H	3.633398	2.077533	0.093481
H	4.366604	0.385716	-1.028042
H	4.345353	0.323699	1.130728
H	-0.646835	-1.708086	0.873832
H	-0.576751	-1.798979	-0.868928
H	-0.804867	1.699141	-0.240718
H	-2.954269	2.884293	0.172291
H	-3.355850	2.052852	-1.322480
H	-3.900127	1.118219	1.544921
H	-5.122248	1.477207	0.316035

WARNING: Geometry optimization converged in opt job, but not in freq job

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3236.0847	10.8005	228.0794	0.2257	0.3682	12.4852
A	3165.0293	11.5820	239.3735	0.4337	0.6051	
A	3122.5390	21.5024	263.5141	0.4194	0.5909	
A	3068.2273	15.0376	284.4552	0.7451	0.8539	
A	3067.2460	12.7633	170.8632	0.1969	0.3290	
A	3043.3324	40.6155	491.6258	0.1359	0.2393	

A	3032.0579	51.6557	497.5003	0.0767	0.1424
A	2530.6694	9.4289	304.5449	0.7464	0.8548
A	2529.5158	9.1402	320.1575	0.7494	0.8568
A	2514.2045	52.8718	931.9311	0.0280	0.0544
A	1817.9333	727.8820	43.3922	0.4006	0.5720
A	1758.8714	97.2836	131.7649	0.1126	0.2025
A	1466.0310	7.7659	41.1474	0.5787	0.7332
A	1440.4738	22.4976	16.0638	0.7421	0.8520
A	1432.9392	7.4078	56.0616	0.6585	0.7941
A	1377.8276	95.0466	3.1394	0.6651	0.7988
A	1346.1135	10.1731	13.1138	0.3162	0.4805
A	1312.9323	88.0371	65.4512	0.5781	0.7326
A	1249.5615	76.0745	35.8702	0.1273	0.2259
A	1244.7183	120.7172	16.7839	0.7282	0.8428
A	1185.4909	205.5494	77.6563	0.3403	0.5078
A	1171.7686	160.0846	7.9343	0.7500	0.8571
A	1155.1292	16.8105	2.9595	0.6172	0.7633
A	1123.2524	10.2712	46.5118	0.7288	0.8431
A	1121.7975	26.0517	57.3814	0.5826	0.7363
A	1118.5293	94.0147	67.2072	0.1473	0.2569
A	1065.1277	278.3596	5.1017	0.2025	0.3367
A	1044.7102	9.2906	11.0656	0.3426	0.5103
A	994.6719	266.0070	57.3495	0.7477	0.8556
A	981.5478	40.7522	3.1688	0.3525	0.5212
A	950.5932	21.2167	9.0801	0.3909	0.5621
A	914.4221	7.5233	3.2352	0.4483	0.6190
A	824.4222	48.8971	8.6306	0.6720	0.8038
A	781.3119	27.8673	18.6545	0.0656	0.1231
A	706.9384	26.0146	12.6638	0.0859	0.1582
A	694.3236	1.9169	4.3619	0.3222	0.4874
A	644.1358	9.2512	11.6518	0.2437	0.3919
A	603.7833	4.4696	4.1089	0.1359	0.2393
A	545.4886	8.7601	6.7671	0.7272	0.8420
A	533.4194	6.7946	4.0651	0.7369	0.8485
A	475.4326	1.3052	1.2014	0.7463	0.8547
A	470.3356	6.1588	8.9585	0.3994	0.5708
A	463.7001	4.8499	5.5131	0.3256	0.4912
A	435.8965	7.7767	3.1497	0.3003	0.4620
A	294.7844	0.5388	11.3835	0.0862	0.1588
A	233.4817	3.2309	2.7708	0.7482	0.8560
A	198.6312	11.9407	5.1429	0.4132	0.5848
A	140.5652	6.6471	0.5901	0.7370	0.8486
A	133.2324	3.2894	0.8090	0.6736	0.8050
A	114.2730	2.6754	0.9276	0.6439	0.7834
A	95.8289	0.7539	1.2923	0.7500	0.8571
A	66.2317	0.2724	0.1848	0.7377	0.8491
A	56.7896	3.1370	0.9608	0.7450	0.8539

A	7.5673	0.1562	0.0552	0.6738	0.8051