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Supporting Information

Difunctionalization of Ketone via *gem*-bis(boronate) to Synthesize Quaternary Carbon with High Selectivity

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1. General Considerations.

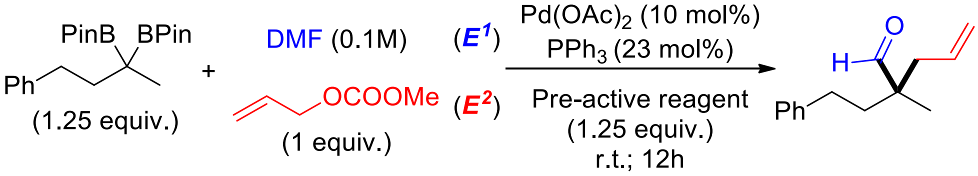
All commercially available compounds were used as received. ^{1}H and ^{13}C spectra were recorded on a Bruker Avance 400, 600 spectrometer, and $CDCl_3$ was purchased from Aldrich. The chemical shifts (δ) are given in parts per million relative to internal standard TMS (0 ppm for ^{1}H), $CDCl_3$ (77.0 ppm for ^{13}C). Flash column chromatography was performed on silica gel 60 (particle size 200-400 mesh ASTM, purchased from Yantai, China) and eluted with petroleum ether/ethyl acetate. Solvents were dried and purified according to the procedure from 'Purification of Laboratory Chemicals book'. Unless otherwise noted, all other reagents and starting materials were purchased from commercial sources and used without further purification.

2. Screening Results.

The Standard condition was listed below and the screening experiments were tested by changing the relevant parameters based on this procedure:

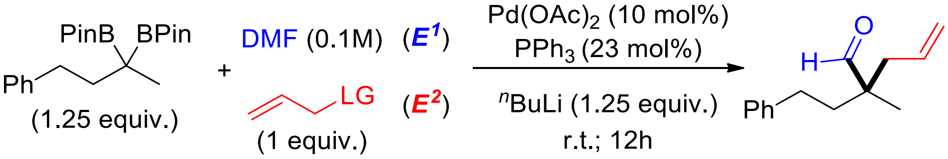
Under argon atmosphere, a 5 mL Shlenk tube was charged with the *gemi*-bis(boronates) compound **1a** (48.2 mg, 0.125 mmol, 1.25 equiv) and anhydrous THF (0.2 mL). The mixture was stirred for 10 min to dissolve, then cooled down to -78 °C. The ^{n}BuLi (0.125 mmol, 50uL, 2.5M in hexane) was added to the solution in one portion and the reaction mixture was stirred for 30 min. The mixture was then allowed to warm to 0 °C and stirred for another 30 min. Another 5 mL sealed tube was charged with $Pd(OAc)_2$ (2.2 mg, 0.01 mmol, 10 mol%), PPh_3 (6.0 mg, 0.023 mmol, 23 mol%) and anhydrous *N,N*-dimethylformamide (1 mL) under argon atmosphere. The mixture was stirred for 10 min and the above lithium organoborate solution was added to this tube with stirring for another 10 min. Allyl methyl carbonate **2a** (11.6 mg, 0.1 mmol) was added to the mixture. The tube was sealed with stirring at room temperature for 12 h. The reaction mixture was quenched by saturated aq. NH_4Cl (2 mL) and extracted by ethyl acetate (2 mL ×3). The organic layers were combined, dried over anhydrous Na_2SO_4, concentrated under vacuo. CH_2Br_2 (17.2 mg, 0.1 mmol) as internal standard and $CDCl_3$ were added. The solution was analyzed by ^{1}H NMR to give the yield of the product **3a**.

Table S1 screening results on pre-active reagent.



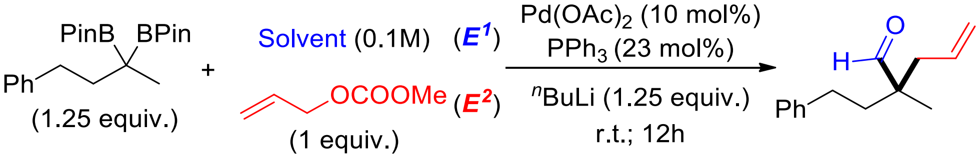
Entry	Pre-active reagent	Yield
1	^{n}BuLi	89%
2	NaO^{t}Bu	0
3	LiO^{t}Bu	0
4	MeLi	4%
5	No Pre-active reagent	0

Table S2 screening results on leaving group.



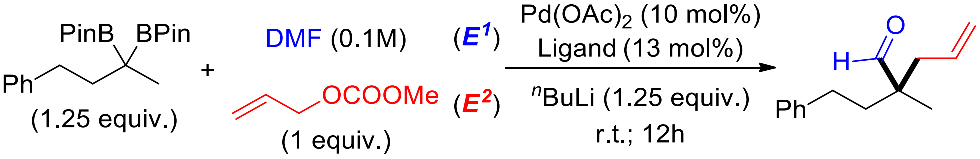
Entry	LG	Yield
1	OCOOMe	89%
2	Cl	76%
3	Br	70%
4	OBz	88%
5	OTs	80%
6	$OPO(OPh)_2$	62%

Table S3 screening results on aldehyde source and mixed solvent.



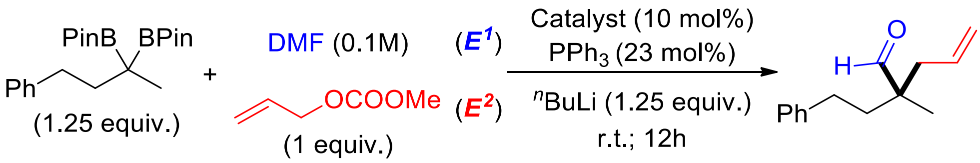
Entry	Solvent	Yield
1	THF/DMF (v/v 1/5)	89%
2	THF/DMF (v/v 10/1)	18%
3	THF/HCOOBu (v/v 1/5)	0
4	THF/HCOOBn (v/v 1/5)	0
5	THF/HCOOBn (v/v 1/1)	0

Table S4 screening results on ligand.



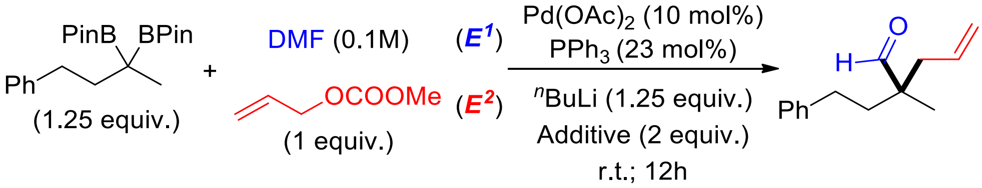
Entry	Ligand	Yield
1	PPh_3 (23 mol%)	89%
2	Bipyridine	44%
3	1,10-Phenanthroline	16%
4	dppbz	46%
5	dppm	16%
6	dppe	60%
7	dppf	54%
8	No ligand	30%

Table S5 screening results on catalyst.



Entry	Catalyst	Yield
1	$Pd(OAc)_2$	89%
2	$PdCl_2$	89%
3	$Pd(PPh_3)_2Cl_2$	77%
4	$Pd(PhCN)_2Cl_2$	76%
5	$NiBr_2$(dme)	0
6	$Cu(OAc)_2$	Trace
7	CuI	0
8	$Fe(OAc)_2$	0
9	$Pd(OAc)_2$ (5 mol%), PPh_3 (12 mol%)	80%
10	No catalyst	0
11	No catalyst, no ligand	0

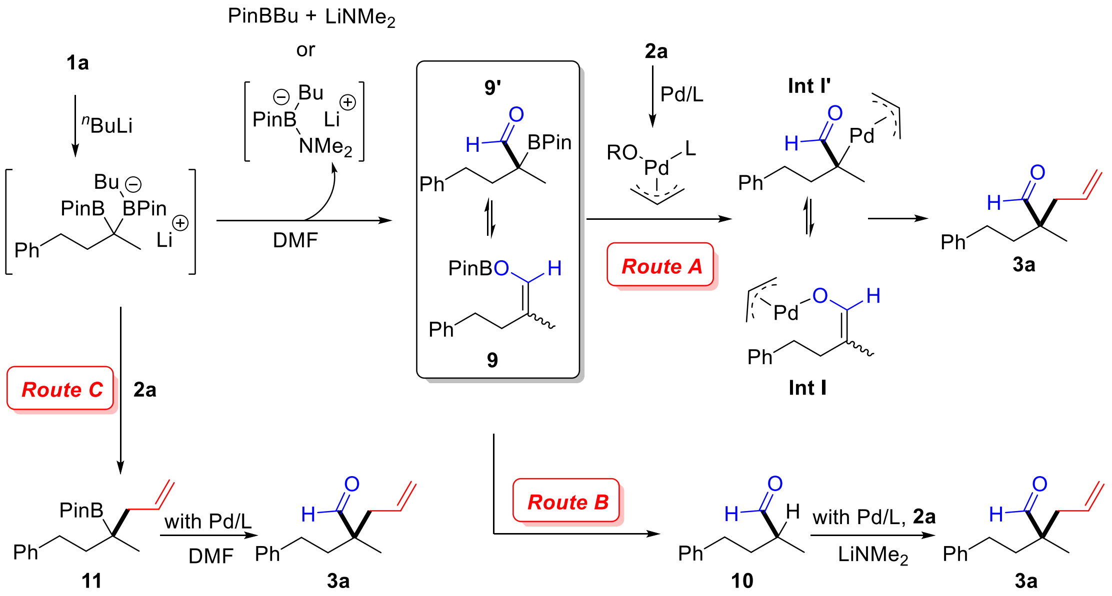
Table S6 screening results on additive.



Entry	Additive	Yield
1	No additive	89%
2	LiBr	25%
3	LiCl	15%
4	KI	79%
5	K_3PO_4	11%

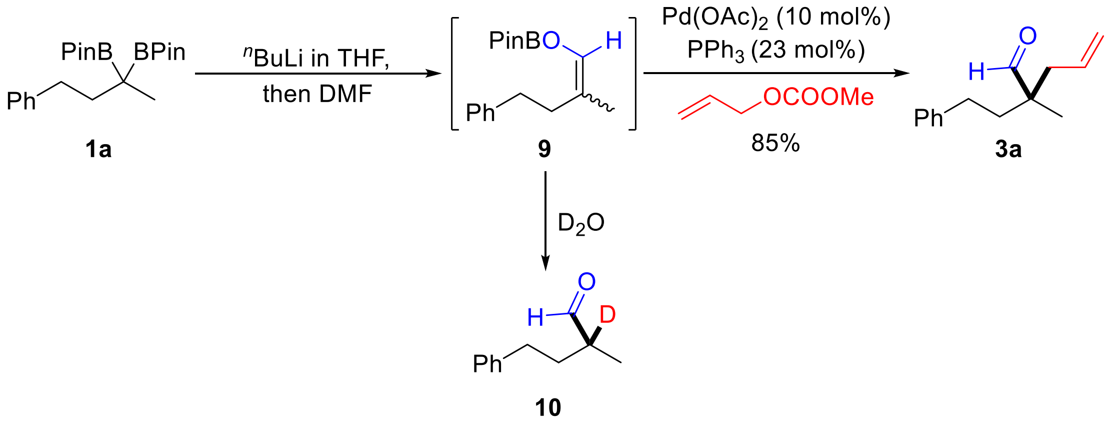
3. Mechanism study.

A proposed mechanism was listed in **Scheme S1**. The lithium organoborate was obtained *in situ* by mixing the compound **1a** with ^{n}BuLi. It reacted with DMF to give the two isomers **9** and **9'** through the *C*/*O* isomerization. In this process, another lithium organoborate salt was produced. It was also possible existing as the mixture of PinBBu and $LiNMe_2$. The two isomers **9** and **9'** reacted with π-allylic palladium species to give the intermediate **I** and **I'**. The reductive elimination of the species afforded the product **3a** (***Route A***). Another two possibilities were involved **10** (***Route B***) or **11** (***Route C***) as the intermediate in which the α-boron aldehyde or *C*/*O* isomerization was not vital process in this transformation.



Scheme S1 The proposed mechanism.

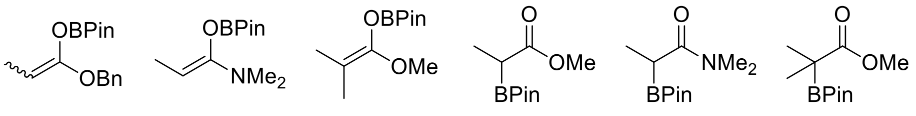
In order to gain some insights on this mechanism, some experiments as listed below were conducted.



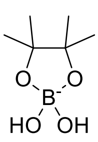
Under argon atmosphere, a 5 mL Shlenk tube was charged with the *gemi*-bis(boronates) compound **1a** (96.5 mg, 0.25 mmol) and anhydrous THF (0.4 mL). The mixture was stirred for 10 min to dissolve, then cooled down to -78 ºC. The ^{n}BuLi (0.25 mmol, 100uL, 2.5M in hexane) was added to the solution in one portion and the reaction mixture was stirred for 30 min. The mixture was then allowed to warm to 0 ºC and stirred for another 30 min. Then DMF (2 mL) was added and stirred for another 12 h. The mixture was transferred to NMR tube and immediately checked by ^{11}B NMR (34.1 ppm, 23.8 ppm, Figure S1, top).[S1] D$_2$O (0.2 mL) was added to the NMR tube, then the mixture was checked by ^{11}B NMR (5.2 ppm, Figure S1, bottom).[S2, S3] According to the literature, it was proposed as PinB(OD)$_2$Li. After flash column chromatography, compound **10** was isolated in 83% and the spectrum was listed below (Figure S2, top).

[S1] E. W. H. Ng, K.-H. Low, P. Chiu, *J. Am. Chem. Soc.* **2018**, *140*, 3537.
[S2] S. Nave, R. P. Sonawane, T. G. Elford, V. K. Aggarwal, *J. Am. Chem. Soc.* **2010**, *132*, 17096.
[S3] W. G. Henderson, M. J. How, G. R. Kennedy, E. F. Mooney, *Carbohydr. Res.* **1973**, *28*, 1.

Chemical shifts in pure C_6D_6 (ref. S1):

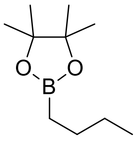


21.9 ppm 21.8 ppm 21.9 ppm 32.5 ppm 32.6 ppm 33.0 ppm

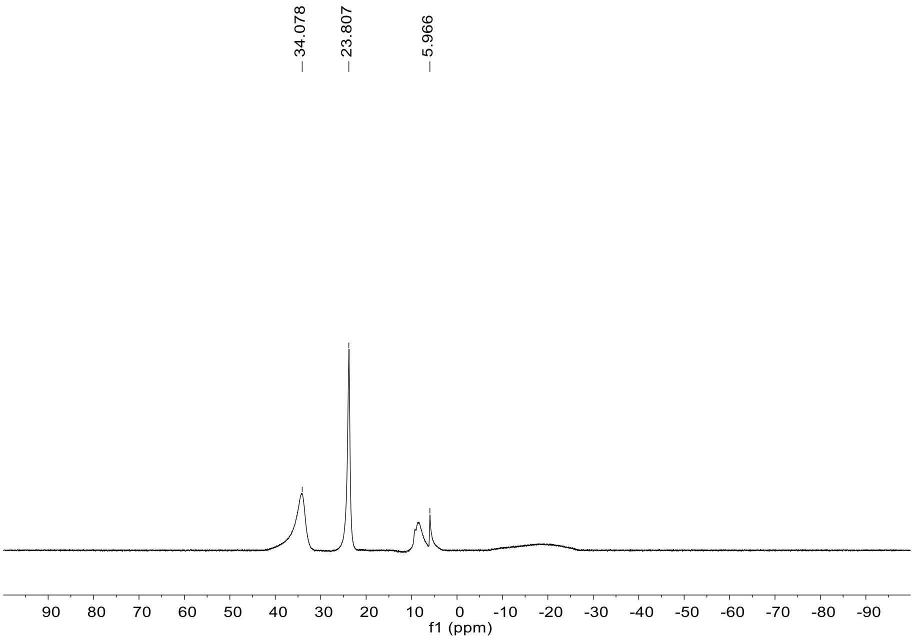


Chemical shifts in reaction solution
THF (ref. S2): 4.0 ppm

Chemical shifts in pure
H_2O (ref. S3): 5.2 ppm



(ref. S1) 37 ppm



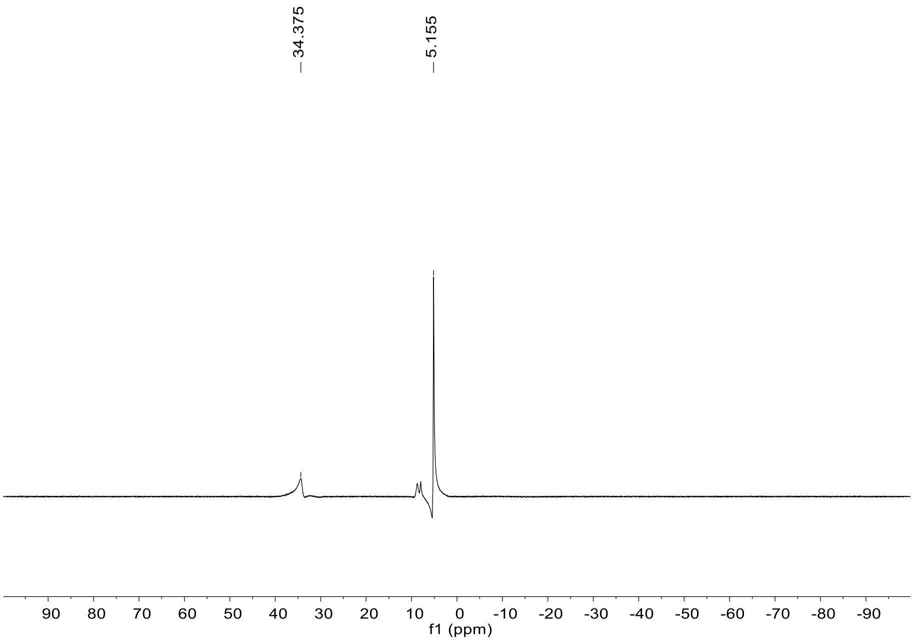


Figure S1: The ^{11}B NMR spectrum.

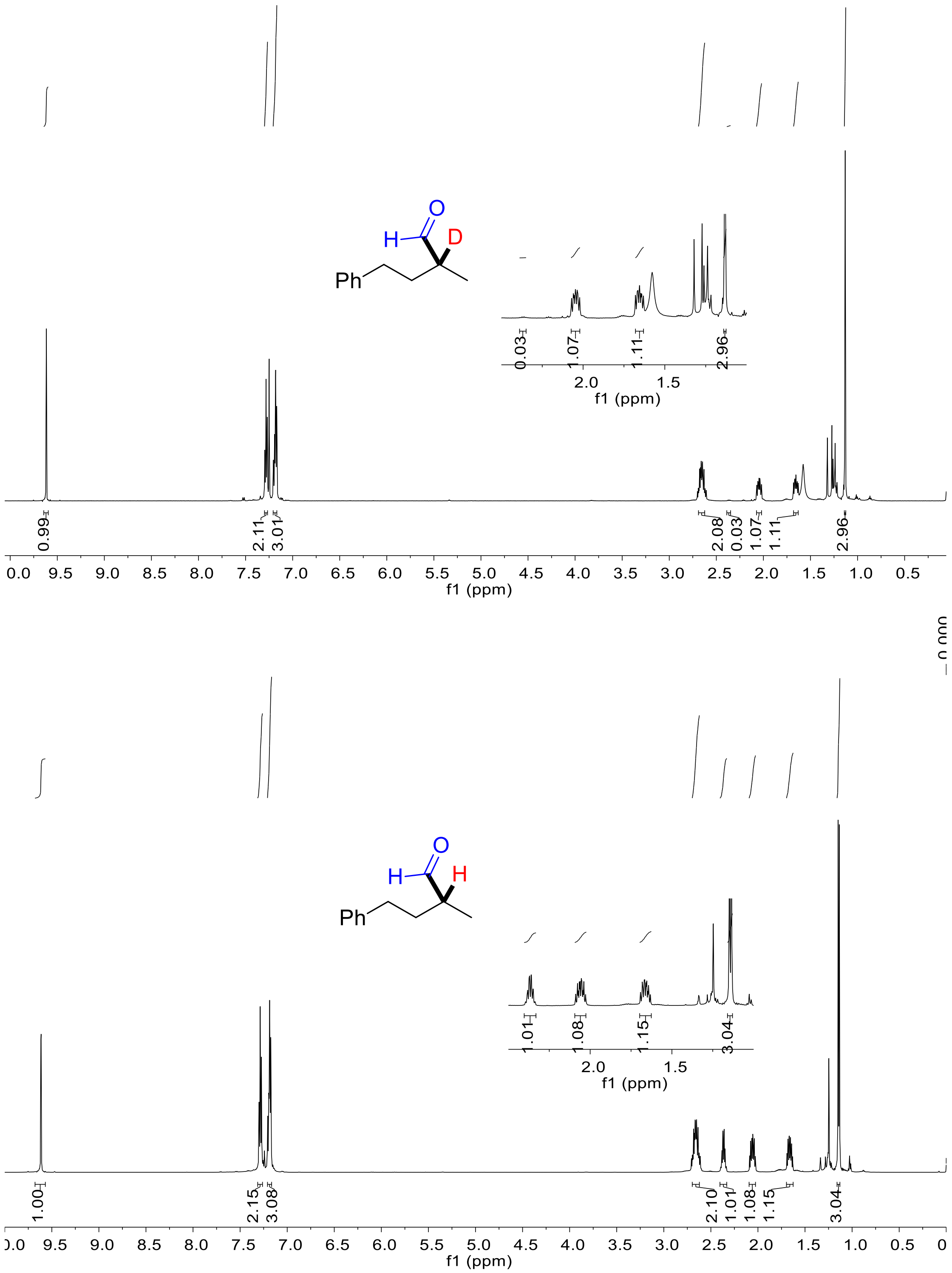


Figure S2: The ^{1}H NMR spectrum of compound **10**.

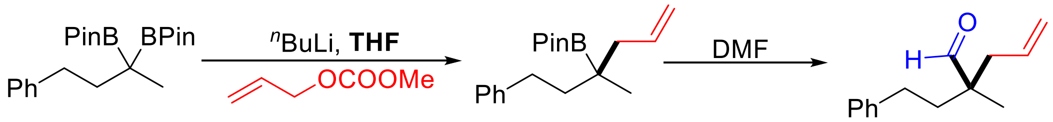
To exclude the possibility that compound **10** as an intermediate and the product was obtained from **10** with allyl methyl carbonate in the presence of the $LiNMe_2$ and palladium catalyst, some control experiments as listed below were conducted.

Under argon atmosphere, a 5 mL Shlenk tube was charged with compound **10** (40.5 mg, 0.25 mmol, 1.25 equiv) and anhydrous THF (0.4 mL). The mixture was stirred for 10 min to dissolve, then cooled down to -78 ºC. The LDA (0.25 mmol, 2.0 M in THF) was added to the solution in one portion and the reaction mixture was stirred for 30 min. The mixture was then allowed to warm to 0 ºC and stirred for another 30 min. Then DMF (2 mL) was added and stirred for another 10 min. Another 5 mL sealed tube was charged with $Pd(OAc)_2$ (4.4 mg, 0.02 mmol, 10 mol%), PPh_3 (12.0 mg, 0.046 mmol, 23 mol%) and anhydrous *N,N*-dimethylformamide (2 mL) under argon atmosphere. The mixture was stirred for 10 min and the above mixture of compound **10** and LDA was added to this tube following another 10 min stirring. Allyl methyl carbonate **2a** (23.2 mg, 0.2 mmol) was added to the mixture. The tube was sealed and stirred at room temperature for 12 h. The reaction mixture was quenched by saturated aq. NH_4Cl (2 mL) and extracted by ethyl acetate (2 mL ×3). The organic layers were combined, dried over anhydrous Na_2SO_4, concentrated under vacuo. CH_2Br_2 (17.2 mg, 0.1 mmol) as internal standard and $CDCl_3$ were added. The solution was analyzed by ^1H NMR to give the yield of the product **3a**. Some variation on this process and the results were summarized on Table S7.

*Table S7 mechanism study on compound **10**.*

Condition	NMR Yield
With LDA, with $Pd(OAc)_2/PPh_3$	15 %
With LDA, without $Pd(OAc)_2/PPh_3$	0
Without LDA, with $Pd(OAc)_2/PPh_3$	0
Without LDA, without $Pd(OAc)_2/PPh_3$	0

Theoretically, in the first step, compound **9** was synthesized accompany with equal equivalent Me_2NLi in solution. From the above results, it indeed gave the product **3a** by reacting compound **10** with allyl methyl carbonate **2a** in the presence of LDA but with very low yield. In addition, considering the basic reaction solution, if compound **10** was produced by quenching with acidic proton, it should quenched the Me_2NLi firstly. So these results could exclude that **3a** was produced through the process with compound **10** as intermediate based on these experiments.



1a **11** **3a**

without $Pd(OAc)_2/PPh_3$: <5%
with $Pd(OAc)_2/PPh_3$: 34%

Not detected

Under argon atmosphere, a 5 mL Shlenk tube was charged with the *gemi*-bis(boronates) compound **1a** (96.5 mg, 0.25 mmol, 1.25 equiv). Anhydrous THF (1 mL) was added to this vial. The mixture was stirred for 10 min to dissolve, then cooled down to -78 ºC. The ⁿBuLi (0.25 mmol, 100uL, 2.5M in hexane) was added to the solution in one portion and the reaction mixture was stirred for 30 min. The mixture was then allowed to warm to 0 °C and stirred for another 30 min. Then $Pd(OAc)_2$ (4.4 mg, 0.02 mmol, 10 mol%), PPh_3 (12.0 mg, 0.046 mmol, 23 mol%) and allyl methyl carbonate **2a** (23.2 mg, 0.2 mmol) were added to the mixture. The tube was sealed with stirring at room temperature for 12 h. DMF (4 mL) was added and the mixture was stirred for another 12h. The reaction mixture was quenched by saturated aq. NH_4Cl (2 mL) and extracted by ethyl acetate (2 mL ×3). The organic layers were combined, dried over anhydrous Na_2SO_4, concentrated under vacuo. CH_2Br_2 (17.2 mg, 0.1 mmol) as internal standard and $CDCl_3$ were added. The solution was analyzed by ^1H NMR to show no product **3a** was detected.

If the reaction was conducted in the absence of $Pd(OAc)_2/PPh_3$, only trace product **11** was detected in the first step. No further experiment was conducted to study the synthesis of product **3a** in the second step.

4. General Procedure for Experiments.

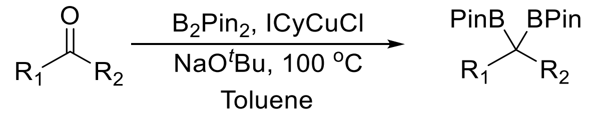
4.1 General procedure for difunctionalizaiton

Under argon atmosphere, a 5 mL Shlenk tube was charged with the *gemi*-bis(boronates) compound **1** (0.25 mmol, 1.25 equiv). Anhydrous THF (0.4 mL) was added to this vial. The mixture was stirred for 10 min to dissolve, then cooled down to -78 °C. The ^{n}BuLi (0.25 mmol, 100uL, 2.5M in hexane) was added to the solution in one portion and the reaction mixture was stirred for 30 min. The mixture was then allowed to warm to 0 °C and stirred for another 30 min. Another 5 mL sealed tube was charged with $Pd(OAc)_2$ (4.4 mg, 0.02 mmol, 10 mol%), PPh_3 (12.0 mg, 0.046 mmol, 23 mol%) and anhydrous *N,N*-dimethylformamide (2 mL) under argon atmosphere. The mixture was stirred for 10 min and the above lithium organoborate solution was added to this tube following another 10 min stirring. Allyl methyl carbonate **2** (0.2 mmol) was added to the mixture. The tube was sealed and stirred at room temperature for 12 h. The reaction mixture was quenched by saturated aq. NH_4Cl (2 mL) and extracted with ethyl acetate (2 mL ×3). The organic layers were combined, dried over anhydrous Na_2SO_4, concentrated under vacuo. The residue was purified carefully by column chromatography on silica gel with a gradient eluent of petroleum ether/ethyl acetate affording the product (**3** or **4**).

4.2 Procedures for diborylation of ketones.

Procedure A[S4]:

$$\text{ICyCl} + \text{CuCl} + \text{NaO}^t\text{Bu} \xrightarrow{\text{THF}} \text{ICyCuCl}$$



Under argon atmosphere, a 25 mL sealed tube equipped with a Teflon-coated magnetic stir bar was charged with CuCl (0.05 mmol), ICyCl (0.05 mmol), NaO^{t}Bu (0.06 mmol). THF (0.5 mL) was added and the tube was stirred at room temperature

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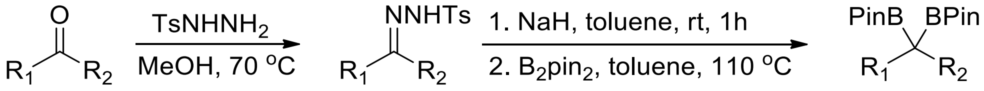
[S4] L. Wang, T. Zhang, W. Sun, Z. He, C. Xia, Y. Lan, C. Liu, *J. Am. Chem. Soc.* **2017**, *139*, 5257.

for 1 h. Then THF was evaporated. The tube was filled with argon again. B_2Pin_2 (2.2 mmol), NaO^{t}Bu (2.6 mmol), ketone (1 mmol) and toluene (10 mL) were added. The tube was sealed and stirred for 12 h at 100 °C. After cooling to room temperature, the reaction was diluted with ethyl acetate (5 mL) and filtered through Celite. The filtrate was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel with a gradient eluent of petroleum ether/ethyl acetate affording the product.

Procedure B [S5]:

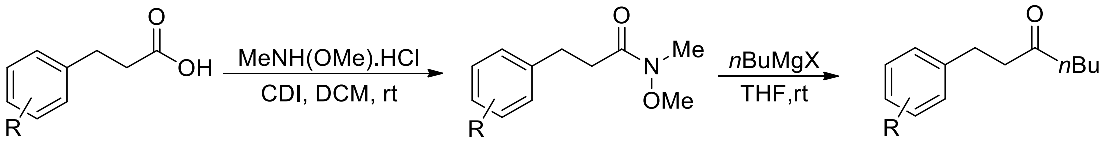


Tosylhydrazine (1.82 g, 10 mmol) was dissolved in methanol (10 ml). Ketone (10 mmol) was added. The mixture was heated to 70 °C and stirred overnight. The precipitate was collected, washed with petroleum ether (5 mL ×3) and dried in vacuum to give the *N*-tosylhydrazone which was used directly in the next step.

60% NaH (240 mg, 6 mmol) was added carefully to *N*-tosylhydrazone (5 mmol) in dry toluene (10 mL) under argon atmosphere, and the mixture was stirred for 1 h. Then B_2pin_2 (1.52g, 6 mmol) was added. The reaction mixture was stirred at 100 °C for 12 h and then quenched with water (20 mL) and ethyl acetate (10 mL). The aqueous layer was then extracted with ethyl acetate (20 mL ×3). The organic layers ware combined and dried over anhydrous Na_2SO_4, concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel with a gradient eluent of petroleum ether/ethyl acetate affording the product.

4.3 Procedures for synthesis of ketones.

Procedure C[S6]:



To a stirred solution of carboxylic acid (11 mmol) in dry CH_2Cl_2 (40 mL) at room temperature, CDI (11 mmol) was added carefully. The mixture was stirred for 30 min then *N,O*-Dimethylhydroxylamine hydrochloride (10 mmol) was added. The reaction mixture was stirred at room temperature until completion (monitored by TLC analysis). The mixture was washed with saturated aq. $NaHCO_3$, brine, dried over anhydrous Na_2SO_4, concentrated under reduced pressure to give the weinreb amide without further purification.

The weinreb amide (5 mmol) was dissolved in THF (10 mL) under argon atmosphere. After the reaction mixture wad cooled to 0 °C, the Grignard reagent was added dropwise to the reaction mixture. After stirring for 10-14 h. the reaction mixture was diluted with ethyl acetate and quenched by saturated aq. NH_4Cl. The mixture was

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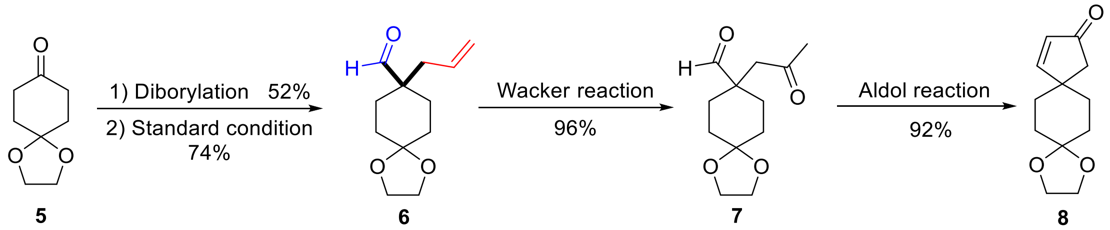
[S5] H. Li, X. Shangguan, Z. Zhang, S. Huang, Y. Zhang, J. Wang, *Org. Lett.* **2014**, *16*, 448.

[S6] K. Kubota, S. Osaki, M. Jin, H. Ito, *Angew. Chem. Int. Ed.* **2017**, *56*, 6646.

then exacted with ethyl acetate and dried over anhydrous Na_2SO_4, concentrated under reduced pressure. The residue was purified by flash column chromatography with a gradient eluent of hexane and ethyl acetate to give the corresponding ketone.

4.4 Procedures for synthesis of compound 8.



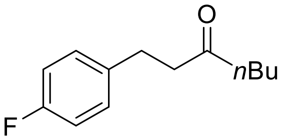
The *gemi*-bis(boronates) compound was prepared according to General Procedure A from the starting compound **5** to give 52% isolated yield on 1 mmol scale.

Under Arogon atmosphere, a 25 mL Shlenk tube was charged with the *gemi*-bis(boronates) compound (0.5 mmol, 1.25 equiv) Anhydrous THF (0.8 mL) was added to this vial. The mixture was stirred for 10 min to dissolve, then cooled down to -78 °C. The ^{n}BuLi (0.5 mmol, 200uL, 2.5M in hexane) was added to the solution in one portion and the reaction mixture was stirred for 30 min. The mixture was then allowed to warm to 0 °C and stirred for another 30 min. Another 25 mL sealed tube was charged with $Pd(OAc)_2$ (8.8 mg, 0.04 mmol, 10 mol%), PPh_3 (24.0 mg, 0.092 mmol, 23 mol%) and anhydrous *N,N*-dimethylformamide (4 mL) under argon atmosphere. The mixture was stirred for 10 min and the above lithium organoborate solution was added to this tube following another 10 min stirring. Allyl methyl carbonate **2** (0.4 mmol) was added to the mixture. The tube was sealed and stirred at room temperature for 24 h. The reaction mixture was quenched by saturated aq. NH_4Cl (4 mL) and extracted with ethyl acetate (4 mL ×3). The organic layers were combined, dried over anhydrous Na_2SO_4, concentrated under vacuo. The residue was purified carefully by column chromatography on silica gel (eluent solution: petroleum ether/ethyl acetate, 20/1 v/v) affording the product **6** as a colorless oil in 74% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.40 (s, 1H), 5.58 (ddt, *J* = 17.5, 10.2, 7.5 Hz, 1H), 4.99 (dd, *J* = 17.5, 10.2 Hz, 2H), 3.86 (s, 4H), 2.14 (d, *J* = 7.5 Hz, 2H), 1.96-1.88 (m, 2H), 1.64-1.58 (m, 2H), 1.54-1.44 (m, 4H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.8, 132.4, 118.7, 108.2, 64.3, 48.8, 40.0, 31.2, 28.0; HRMS: m/z (ESI) calculated $[M+Na]^+$:233.1154, measured: 233.1128.

A 25 mL Shlenk tube was charged with CuCl (3.9 mg, 0.04 mmol, 20 mol%), $PdCl_2$ (1.4 mg, 0.008 mmol, 4 mol%). After degassed and filled with oxygen three times, the mixed solution of *N,N*-dimethylformamide (2.5 mL) and water (1 mL) was added. After stirring for 30 min, **6** (42 mg, 0.2 mmol) was added to the reaction mixture under oxgen atmosphere and the mixture was stirred for 12 h. Upon completion, the solution was filtered through Celite and washed with ethyl acetate (2 mL ×3). The filtrate was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent solution: petroleum ether/ethyl acetate, 20/1 v/v) affording the product **7** as a colorless oil in 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 3.94 (s, 4H), 2.78 (s, 2H), 2.13 (s, 3H), 2.09-2.01 (m, 2H), 1.72-1.55 (m, 6H).

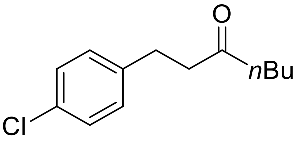
To a stirred solution of the keto aldehyde **7** (0.2 mmol) in THF (2 mL) at room temperature, 1N KOH aqueous solution (0.24 mL, 0.24 mmol, 1.2 equiv) was added carefully. The reaction mixture was stirred at room temperature overnight. Unpon completion, the mixture was then diluted with ethyl acetate (2 mL), washed with brine, dried over anhydrous Na_2SO_4 and concentrated under vacuo. The residue was purified by column chromatography on silica gel (eluent solution: petroleum ether/ethyl acetate, 20/1 v/v) affording the final product **8** as a pale-yellow solid in 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 5.6 Hz, 1H), 6.08 (d, *J* = 5.6 Hz, 1H), 3.97 (s, 4H), 2.28 (s, 2H), 1.86-1.76 (m, 4H), 1.70-1.60 (m, 2H), 1.59-1.50 (m, 2H).^{1}H NMR was in agreement with the literature [S7].

5 The characterization of the new products



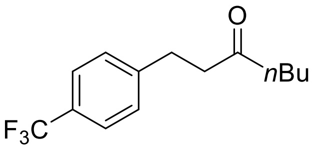
The title compound was synthesized according to General Procedure C from 3-(4-fluorophenyl)propanoic acid. The overall yield (2 steps) was 87%.

1H NMR (600 MHz, CDCl3) δ 7.16-7.10 (m, 2H), 6.98-6.91 (m, 2H), 2.86 (t, J = 7.6 Hz, 2H), 2.70 (t, J = 7.6 Hz, 2H), 2.37 (t, J = 7.5 Hz, 2H), 1.56-1.49 (m, 2H), 1.31-1.23 (m, 2H), 0.88 (t, J = 7.4 Hz, 3H); 13C NMR (151 MHz, CDCl3) δ 210.0 , 161.2 (d, J = 243.8 Hz), 136.7 (d, J = 3.3 Hz), 129.6 (d, J = 7.8 Hz), 115.1 (d, J = 21.1 Hz), 44.1, 42.7, 28.8, 25.8, 22.2, 13.7; HRMS: m/z (ESI) calculated $[M+Na]^+$:231.1161, measured: 231.1132.



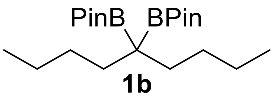
The title compound was synthesized according to General Procedure C from 3-(4-chlorophenyl) propanoic acid. The overall yield (2 steps) was 96%.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.23 (d, *J* = 8.4 Hz, 2H), 7.11 (d, *J* = 8.4 Hz, 2H), 2.85 (t, *J* = 7.5 Hz, 2H), 2.70 (t, *J* = 7.5 Hz, 2H), 2.37 (t, *J* = 7.5 Hz, 2H), 1.56-1.50 (m, 2H), 1.31-1.24 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 209.8, 139.6, 131.7, 129.6, 128.4, 43.9, 42.7, 28.9, 25.8, 22.2, 13.8; HRMS: m/z (ESI) calculated $[M+H]^+$:225.1046, measured: 225.1036.



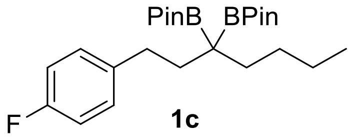
[S7] A. Srikrishna, P. P. Kumar, *Tetrahedron* **2000**, *56*, 8189.

The title compound was synthesized according to General Procedure C from 3-(4-(trifluoromethyl)phenyl) propanoic acid. The overall yield (2 steps) was 78%.
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 2.95 (t, *J* = 7.5 Hz, 1H), 2.75 (t, *J* = 7.5 Hz, 1H), 2.39 (t, *J* = 7.5 Hz, 1H), 1.57-1.51 (m, 1H), 1.32-1.24 (m, 1H), 0.89 (t, *J* = 7.3 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 209.7, 145.3, 128.7, 128.4 (q, *J* = 32.2 Hz),125.3 (q, *J* = 3.8 Hz), 124.4 (q, *J* = 271.9 Hz), 43.6, 42.7, 29.4, 25.8, 22.3, 13.8; HRMS: m/z (ESI) calculated $[2M+Na]^+$:539.2361, measured: 539.2358.



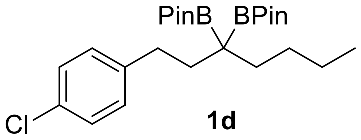
1b

The title compound **1b** was synthesized according to General Procedure B from nonan-5-one. The yield was 55%.
^{1}H NMR (600 MHz, $CDCl_3$) δ 1.64-1.57 (m, 4H), 1.29 (q, *J* = 7.4 Hz, 4H), 1.22 (s, 24H), 1.20-1.14 (m, 4H), 0.88 (t, *J* = 7.4 Hz, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 82.8, 29.4, 28.4, 24.7, 23.5, 14.3; HRMS: m/z (ESI) calculated $[M+Na]^+$: 403.3167, measured: 403.3165.



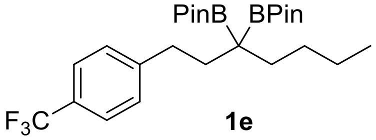
1c

The title compound **1c** was synthesized according to General Procedure B from 3-(4-fluorophenyl) propan-3-one. The yield was 37%.
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.17-7.11 (m, 2H), 6.95-6.90 (m, 2H), 2.50-2.42 (m, 2H), 1.89-1.84 (m, 2H), 1.73-1.66 (m, 2H), 1.33 (q, *J* = 7.3 Hz, 2H), 1.26-1.20 (m, 26H), 0.91 (t, *J* = 7.3 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.0 (d, *J* = 242.7 Hz), 139.4 (d, *J* = 3.3 Hz), 129.7 (d, *J* = 7.7 Hz), 114.7 (d, *J* = 20.8 Hz), 83.0, 33.0, 31.9, 29.5, 28.5, 24.8, 24.7, 23.4, 14.3; HRMS: m/z (ESI) calculated $[M+Na]^+$: 469.3073, measured: 469.3075.



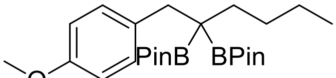
1d

The title compound **1d** was synthesized according to General Procedure B from 3-(4-chlorophenyl) propan-3-one. The yield was 30%.
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.20 (d, *J* = 8.3 Hz, 2H), 7.12 (d, *J* = 8.3 Hz, 2H), 2.52-2.41 (m, 2H), 1.90-1.82 (m, 2H), 1.75-1.66 (m, 2H), 1.33 (q, *J* = 7.3 Hz, 2H), 1.26-1.19 (m, 26H), 0.91 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.2, 131.0, 129.8, 128.1, 83.0, 33.1, 31.7, 29.5, 28.5, 24.8, 24.7, 23.4, 14.3; HRMS: m/z (ESI) calculated $[M+Na]^+$:485.2777, measured: 485.2787.



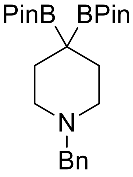
1e

The title compound **1e** was synthesized according to General Procedure B from 3-(4-(trifluoromethyl)phenyl) propan-3-one. The yield was 67%.
^{1}H NMR (600 MHz, CDCl$_3$) δ 7.49 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 2.61-2.48 (m, 2H), 1.94-1.85 (m, 2H), 1.75-1.67 (m, 2H), 1.34 (q, *J* = 7.3 Hz, 2H), 1.28-1.21 (m, 26H), 0.91 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 148.0, 128.8, 127.7 (q, *J* = 32.1 Hz), 125.0 (q, *J* = 3.7 Hz), 124.5 (q, *J* = 271.5 Hz), 83.0, 33.7, 31.6, 29.5, 28.6, 24.8, 24.7, 23.4, 14.3; HRMS: m/z (ESI) calculated [M+Na]$^+$:519.3041, measured: 519.3042.



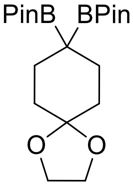
1f

The title compound **1f** was synthesized according to General Procedure A from 1-(4-methoxyphenyl)hexan-2-one. The yield was 50%.
^{1}H NMR (600 MHz, CDCl$_3$) δ 7.15 (d, *J* = 8.6 Hz, 2H), 6.75 (d, *J* = 8.6 Hz, 2H), 3.76 (s, 3H), 2.91 (s, 2H), 1.55-1.48 (m, 2H), 1.36-1.26 (m, 2H), 1.24 (s,12H), 1.21 (s, 12H), 0.88 (t, *J* = 7.2 Hz, 2H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 157.5, 134.0, 130.6, 113.0, 83.1, 55.2, 33.5, 29.5, 28.3, 25.0, 24.7, 23.4, 14.3; HRMS: m/z (ESI) calculated [M+Na]$^+$:467.3116, measured: 467.3114.



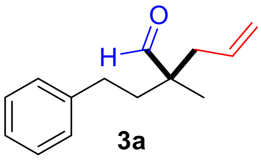
1g

The title compound **1g** was synthesized according to General Procedure B from 1-benzylpiperidin-4-one. The yield was 35%.
^{1}H NMR (600 MHz, CDCl$_3$) δ 7.31-7.25 (m, 4H), 7.24-7.18 (m, 1H), 3.44 (s, 2H), 2.50-2.25 (m, 4H), 1.85-1.75 (m, 4H), 1.20 (s, 24H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 138.2, 129.3, 127.9, 126.6, 82.9, 63.9, 54.1, 28.7, 24.8, 24.6; HRMS: m/z (ESI) calculated [M+H]$^+$:428.3143, measured: 428.3147.



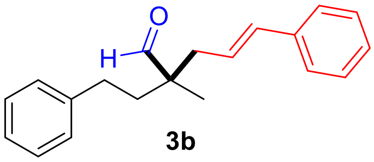
1h

The title compound **1h** was synthesized according to General Procedure A from 1,4-dioxaspiro[4.5]decan-8-one. The yield was 52%.
^{1}H NMR (600 MHz, $CDCl_3$) δ 3.92 (s, 4H), 1.82 (t, *J* = 6.0 Hz, 4H), 1.61 (t, *J* = 6.0 Hz, 4H), 1.21 (s, 24H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 109.2, 83.0, 64.0, 34.9, 26.8, 24.6; HRMS: m/z (ESI) calculated [2M+Na]$^{+}$: 811.5294, measured: 811.5289.



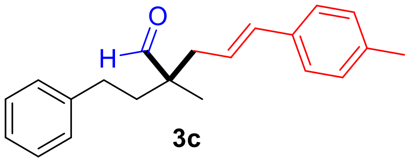
3a

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.51 (s, 1H), 7.28 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.19 (t, *J* = 7.8 Hz, 1H), 7.16 (d, *J* = 7.2 Hz, 2H), 5.77-5.68 (m, 1H), 5.16-5.09 (m, 2H), 2.56-2.47 (m, 2H), 2.36-2.27 (m, 2H), 1.87-1.81 (m, 1H), 1.80-1.74 (m, 1H), 1.12 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.8, 141.9, 132.8, 128.5, 128.3, 126.0, 118.8, 49.0, 39.6, 37.3, 30.5, 18.6; HRMS: m/z (ESI) calculated [M+Na]$^{+}$: 225.1255, measured: 225.1249.



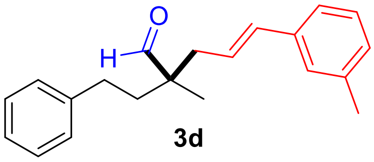
3b

^{1}H NMR (600 MHz, $CDCl_3$)δ 9.55 (s, 1H), 7.33 (d, *J* = 7.2 Hz, 2H), 7.29 (dd, *J* = 7.2, 5.4 Hz, 2H), 7.27 (dd, *J* = 7.8, 4.8 Hz, 2H), 7.24-7.17 (m, 2H), 7.16 (d, *J* = 7.8 Hz, 2H), 6.45 (d, *J* = 15.5 Hz, 1H), 6.11 (dt, *J* = 15.5, 7.6 Hz, 1H), 2.60-2.49 (m, 2H), 2.49-2.39 (m, 2H), 1.92-1.84 (m, 1H), 1.84-1.76 (m, 1H), 1.17 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.7, 141.7, 137.0, 133.6, 128.5, 128.4, 128.2 , 127.3, 126.1, 126.0, 124.4, 49.6, 38.8, 37.4, 30.5, 18.7; HRMS: m/z (ESI) calculated [M+Na]$^{+}$: 301.1568, measured: 301.1567.



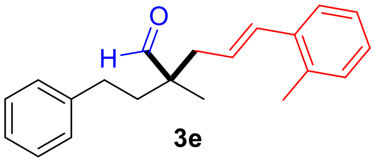
3c

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.56 (s, 1H), 7.28 (dd, *J* =7.8, 7.2 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.19 (t, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 7.8 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 6.42 (d, *J* = 15.7 Hz, 1H), 6.06 (dt, *J* = 15.7, 7.6 Hz, 1H), 2.60-2.50 (m, 2H), 2.49-2.39 (m, 2H), 2.33 (s, 3H), 1.92-1.87 (m, 1H), 1.84-1.78 (m, 1H), 1.17 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.9, 141.8, 137.2, 134.3, 133.5, 129.2, 128.5, 128.3, 126.0, 123.3, 49.6, 38.9, 37.4, 30.5, 21.2, 18.7; HRMS: m/z (ESI) calculated [M+Na]$^{+}$: 315.1725, measured: 315.1741.



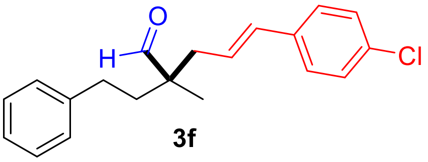
3d

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.56 (s, 1H), 7.28 (dd, J = 7.8, 7.2 Hz, 2H), 7.22-7.17 (m, 2H), 7.17-7.14 (m, 3H), 7.13 (d, J = 7.8 Hz, 1H), 7.04 (d, J = 7.4 Hz, 1H), 6.42 (d, J = 15.5 Hz, 1H), 6.09 (dt, J = 15.5, 7.6 Hz, 1H), 2.61-2.50 (m, 2H), 2.50-2.39 (m, 2H), 2.33 (s, 3H), 1.93-1.86 (m, 1H), 1.84-1.77 (m, 1H), 1.17 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.8, 141.7, 138.1, 136.9, 133.7, 128.5, 128.4, 128.2, 128.1, 126.8, 126.0, 124.1, 123.3, 49.6, 38.9, 37.4, 30.5, 21.4, 18.7; HRMS: m/z (ESI) calculated $[M+Na]^+$: 315.1725, measured: 315.1747.



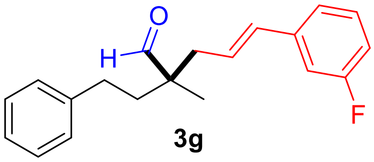
3e

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.56 (s, 1H), 7.37 (dd, J = 4.8, 3.6 Hz, 1H), 7.27 (dd, J = 7.8, 7.2 Hz, 2H), 7.21-7.10 (m, 4H), 6.65 (d, J = 15.5 Hz, 1H), 5.97 (dt, J = 15.5, 7.6 Hz, 1H), 2.61-2.51 (m, 2H), 2.51-2.42 (m, 2H), 2.31 (s, 3H), 1.94-1.86 (m, 1H), 1.86-1.78 (m, 1H), 1.18 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.71 , 141.7, 136.3, 135.0, 131.7, 130.2, 128.5, 128.2, 127.3, 126.04, 126.02, 125.9, 125.7, 49.5, 39.0, 37.3, 30.5, 19.8, 18.7; HRMS: m/z (ESI) calculated $[M+Na]^+$: 315.1725, measured: 315.1711.



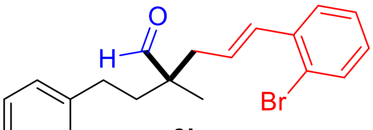
3f

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.55 (s, 1H), 7.31-7.24 (m, 6H), 7.19 (t, J = 7.4 Hz, 1H), 7.16 (d, J = 6.9 Hz, 2H), 6.39 (d, J = 15.5 Hz, 1H), 6.08 (dt, J = 15.5, 7.6 Hz, 1H), 2.60-2.49 (m, 2H), 2.49-2.38 (m, 2H), 1.93-1.85 (m, 1H), 1.84-1.76 (m, 1H), 1.17 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.6, 141.6, 135.5, 132.9, 132.4, 128.6, 128.5, 128.2, 127.3, 126.1, 125.2, 49.5, 38.7, 37.4, 30.5, 18.7; HRMS: m/z (ESI) calculated $[M+Na]^+$: 335.1179, measured: 335.1177.



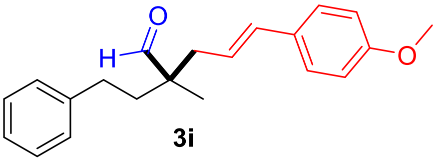
3g

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.55 (s, 1H), 7.28 (dd, J = 7.8, 7.8 Hz, 2H), 7.28-7.22 (m, 1H), 7.19 (t, J = 7.2 Hz, 1H), 7.16 (d, J = 7.2 Hz, 2H), 7.09 (d, J = 7.8 Hz, 1H), 7.03 (ddd, J = 10.2, 2.4, 1.8 Hz, 1H), 6.91 (tdd, J = 8.4, 2.4, 0.6 Hz, 1H), 6.42 (d, J = 15.5 Hz, 1H), 6.12 (dt, J = 15.5, 7.6 Hz, 1H), 2.60-2.50 (m, 2H), 2.50-2.41 (m, 2H), 1.93-1.85 (m, 1H), 1.84-1.77 (m, 1H), 1.18 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.5, 163.0 (d, J = 245.2 Hz), 141.6, 139.3 (d, J = 7.7 Hz), 132.6 (d, J = 2.4 Hz), 132.0 (d, J = 8.4 Hz), 128.5, 128.2, 126.1, 126.0 (d, J = 15.7 Hz), 122.0 (d, J = 2.7 Hz), 114.1 (d, J = 21.4 Hz), 112.6 (d, J = 21.7 Hz), 49.5, 38.7, 37.4, 30.5, 18.8; HRMS: m/z (ESI) calculated $[M+Na]^+$: 319.1474, measured: 319.1468.



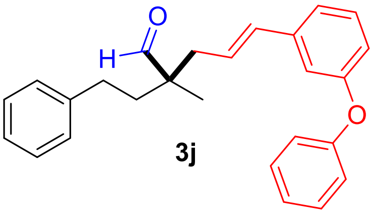
3h

^{1}H NMR (600 MHz, CDCl$_3$) δ 9.50 (s, 1H), 7.46 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.38 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.21 (dd, *J* = 8.1, 6.9 Hz, 2H), 7.20-7.16 (m, 1H), 7.13-7.09 (m, 4H), 7.02 (ddd, *J* = 7.8, 7.8, 1.7 Hz, 1H), 6.73 (d, *J* = 15.4 Hz, 1H), 5.97 (dt, *J* = 15.4, 7.6 Hz, 1H), 2.53-2.47 (m, 2H), 2.48-2.38 (m, 2H), 1.86-1.80 (m, 1H), 1.79-1.72 (m, 1H), 1.12 (s, 3H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 205.7, 141.7, 137.0, 132.8, 132.6, 128.7, 128.5, 128.3, 127.8, 127.5, 127.1, 126.1, 123.2, 49.5, 38.6, 37.4, 30.5, 18.9; HRMS: m/z (ESI) calculated [M+Na]$^+$: 379.0673, measured: 379.0667.



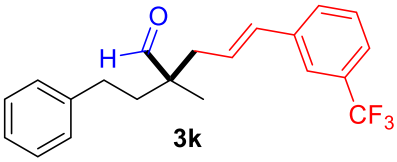
3i

^{1}H NMR (600 MHz, CDCl$_3$) δ 9.56 (s, 1H), 7.30-7.24 (m, 4H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.16 (d, *J* = 7.7 Hz, 3H), 6.84 (d, *J* = 8.3 Hz, 2H), 6.39 (d, *J* = 15.4 Hz, 1H), 5.96 (dt, *J* = 15.4, 7.5 Hz, 1H), 3.80 (s, 2H), 2.61-2.49 (m, 3H), 2.48-2.39 (m, 2H), 1.93-1.85 (m, 1H), 1.84-1.77 (m, 1H), 1.17 (s, 3H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 205.9, 159.0, 141.8, 133.0, 129.9, 128.5, 128.2, 127.3, 126.0, 122.0, 113.9, 55.3， 49.6, 38.9, 37.4, 30.5, 18.7; HRMS: m/z (ESI) calculated [M+Na]$^+$: 331.1674, measured: 331.1666.



3j

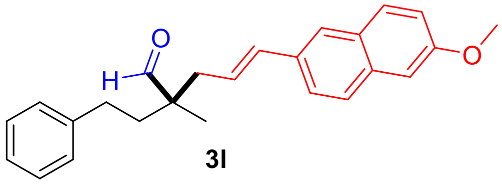
^{1}H NMR (600 MHz, CDCl$_3$) δ 9.54 (s, 1H), 7.33 (dd, *J* = 8.5, 7.5 Hz, 2H), 7.30-7.21 (m, 3H), 7.18 (t, *J* = 7.8 Hz, 1H), 7.15 (d, *J* = 7.2 Hz, 2H), 7.12-7.06 (m, 2H), 7.02-7.98 (m, 3H), 6.85 (ddd, *J* = 8.2, 2.5, 1.0 Hz, 1H), 6.40 (d, *J* = 15.5 Hz, 1H), 6.09 (dt, *J* = 15.5, 7.6 Hz, 1H), 2.60-2.49 (m, 2H), 2.48-2.36 (m, 2H), 1.91-1.85 (m, 1H), 1.83-1.75 (m, 1H), 1.16 (s, 3H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 205.6, 157.4, 157.1, 141.6, 138.9, 133.1, 129.8, 129.7, 128.5, 128.2, 126.0, 125.3, 123.2, 121.1, 118.7, 117.8, 116.6, 49.5, 38.7, 37.4, 30.5, 18.7; HRMS: m/z (ESI) calculated [M+Na]$^+$: 393.1830, measured: 393.1818.



3k

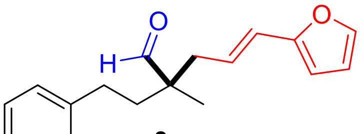
^{1}H NMR (600 MHz, CDCl$_3$) δ 9.56 (s, 1H), 7.56 (s, 1H), 7.49 (d, *J* = 7.7 Hz, 1H), 7.47 (d, *J* = 7.7 Hz, 1H), 7.41 (dd, *J* = 7.7, 7.7 Hz, 1H), 7.28 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.20

(t, *J* = 7.2 Hz, 1H), 7.17 (d, *J* = 7.8 Hz, 2H), 6.47 (d, *J* = 15.5 Hz, 1H), 6.19 (dt, *J* = 15.5, 7.6 Hz, 1H), 2.63-2.53 (m, 2H), 2.53-2.42 (m, 2H), 1.94-1.87 (m, 1H), 1.85-1.79 (m, 1H), 1.19 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.5, 141.6, 137.7, 132.3, 130.9 (q, *J* = 32.1 Hz), 129.2 (d, *J* = 0.8 Hz), 129.0, 128.5, 128.2, 126.6, 126.1, 124.1 (q, *J* = 272.3 Hz), 123. 9 (q, *J* = 3.7 Hz), 122.8 (q, *J* = 3.8 Hz), 49.6, 38.7, 37.5, 30.5, 18.8; HRMS: m/z (ESI) calculated [M+Na]$^+$: 369.1442, measured: 369.1455.



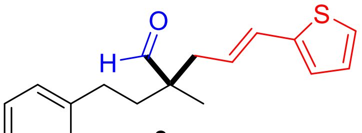
3l

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.59 (s, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.67 (d, *J* = 8.6 Hz, 1H), 7.61 (s, 1H), 7.52 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.28 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H), 7.17 (d, *J* = 7.8 Hz, 2H), 7.12 (dd, *J* = 8.8, 2.5 Hz, 1H), 7.10 (d, *J* = 2.5 Hz, 1H), 6.58 (d, *J* = 15.4 Hz, 1H), 6.18 (dt, *J* = 15.4, 7.6 Hz, 1H), 3.91 (s, 3H), 2.63-2.54 (m, 2H), 2.54-2.45 (m, 2H), 1.96-1.89 (m, 1H), 1.87-1.80 (m, 1H), 1.20 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.9, 157.6, 141.8, 134.0, 133.8, 132.4, 129.4, 128.9, 128.5, 128.3, 127.0, 126.0, 125.7, 124.0, 123.6, 119.0, 105.8, 55.3, 49.7, 39.0, 37.4, 30.5, 18.7; HRMS: m/z (ESI) calculated [M+K]$^+$: 397.1570, measured: 397.1557.



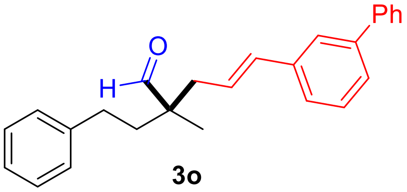
3m

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.55 (s, 1H), 7.36 (d, *J* = 12.4 Hz, 2H), 7.31-7.24 (m, 3H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 2H), 6.49 (s, 1H), 6.30 (d, *J* = 15.4 Hz, 1H), 5.81 (dt, *J* = 15.4, 7.6 Hz, 1H), 2.60-2.48 (m, 2H), 2.45-2.35 (m, 2H), 1.93-1.84 (m, 1H), 1.83-1.76 (m, 1H), 1.16 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.8, 143.4, 141.7, 139.9, 128.5, 128.2, 126.1, 123.91, 123.86, 123.3, 107.5, 49.5, 38.8, 37.4, 30.5, 18.7; HRMS: m/z (ESI) calculated [M+Na]$^+$: 291.1361, measured: 291.1357.



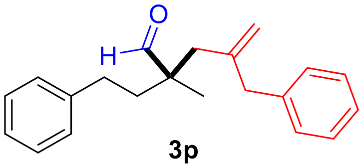
3n

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.55 (s, 1H), 7.28 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.19 (t, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 7.8 Hz, 2H), 7.11 (d, *J* = 5.0 Hz, 1H), 6.94 (dd, *J* = 5.0, 3.5 Hz, 1H), 6.89 (d, *J* = 3.5 Hz, 1H), 6.57 (d, *J* = 15.4 Hz, 1H), 5.95 (dt, *J* = 15.4, 7.6 Hz, 1H), 2.61-2.49 (m, 2H), 2.47-2.34 (m, 2H), 1.92-1.85 (m, 1H), 1.84-1.77 (m, 1H), 1.17 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.7, 142.1, 141.7, 128.5, 128.2, 127.3, 126.8, 126.1, 125.0, 124.2, 123.8, 49.6, 38.6, 37.4, 30.5, 18.8; HRMS: m/z (ESI) calculated $[M+Na]^+$: 307.1133, measured: 307.1126.



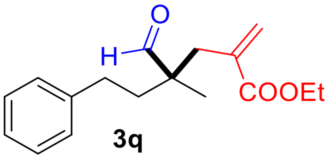
3o

^1H NMR (600 MHz, $CDCl_3$) δ 9.57 (s, 1H), 7.58 (d, *J* = 7.3 Hz, 2H), 7.53 (s, 1H), 7.47-7.41 (m, 3H), 7.40-7.34 (m, 2H), 7.33 (dd, *J* = 7.8, 6.0 Hz, 1H), 7.27 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.21-7.14 (m, 3H), 6.51 (d, *J* = 15.7 Hz, 1H), 6.18 (dt, *J* = 15.4, 7.6 Hz, 1H), 2.61-2.52 (m, 2H), 2.52-2.42 (m, 2H), 1.94-1.87 (m, 1H), 1.86-1.78 (m, 1H), 1.18 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.7, 141.7, 141.6, 141.0, 137.5, 133.6, 129.0, 128.7, 128.5, 128.2, 127.3, 127.1, 126.3, 126.0, 125.1, 125.0, 124.8, 49.6, 38.9, 37.4, 30.5, 18.7; HRMS: m/z (ESI) calculated $[M+Na]^+$: 377.1881, measured: 377.1876.



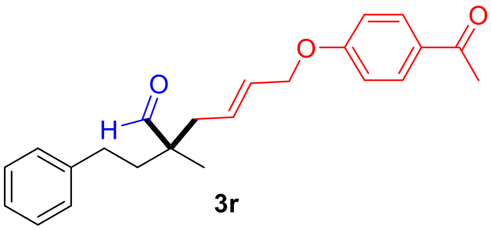
3p

^1H NMR (600 MHz, $CDCl_3$) δ 9.52 (s, 1H), 7.32-7.24 (m, 4H), 7.21 (t, *J* =7.2 Hz, 1H), 7.18 (t, *J* = 7.2 Hz, 1H), 7.16-7.12 (m, 4H), 4.90 (s, 1H), 4.87 (s, 1H), 3.32-3.18 (m, 2H), 2.54 (td, *J* = 13.2, 4.9 Hz, 1H), 2.43 (td, *J* = 13.2, 4.9 Hz, 1H), 2.36 (d, *J* = 14.4 Hz, 1H), 2.18 (d, *J* = 14.4 Hz, 1H), 1.87 (td, *J* = 13.2, 4.9 Hz, 1H), 1.72 (td, *J* = 13.2, 4.9 Hz, 1H), 1.15 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 206.1, 144.2, 141.7, 138.9, 129.0, 128.4, 128.4, 128.2, 126.3, 126.0, 116.6, 49.6, 43.9, 41.4, 38.0, 30.4, 18.2; HRMS: m/z (ESI) calculated $[M+Na]^+$: 315.1725, measured: 315.1719.



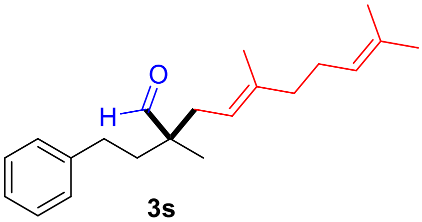
3q

^1H NMR (600 MHz, $CDCl_3$) δ 9.52 (s, 1H), 7.28 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.19 (t, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 7.8 Hz, 2H), 6.27 (s, 1H), 5.58 (s, 1H), 4.18 (q, *J* = 7.2 Hz, 2H), 2.72 (d, *J* = 13.8 Hz, 1H), 2.61-2.55 (m, 1H), 2.53 (d, *J* = 13.8 Hz, 1H), 2.51-2.44 (m, 1H), 1.95-1.86 (m, 1H), 1.74-1.66 (m, 1H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.09 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 205.0, 167.1, 141.6, 136.3, 128.9, 128.4, 128.2, 126.0, 61.0, 49.4, 37.9, 37.7, 30.4, 17.7, 14.0; HRMS: m/z (ESI) calculated $[2M+Na]^+$: 517.3036, measured: 517.3009.



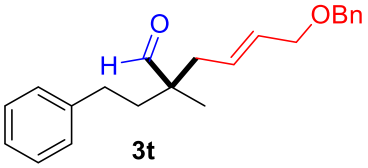
3r

^{1}H NMR (600 MHz, CDCl$_3$) δ 9.51 (s, 1H), 7.92 (d, *J* = 8.4 Hz, 2H), 7.28 (dd, *J* = 7.6, 7.2 Hz, 2H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.14 (d, *J* = 7.2 Hz, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 5.82-5.73 (m, 2H), 4.56 (d, *J* = 4.2 Hz, 2H), 2.55 (s, 3H), 2.53-2.48 (m, 2H), 2.37-2.31 (m, 2H), 1.86-1.79 (m, 1H), 1.79-1.71 (m, 1H), 1.13 (s, 3H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 205.4, 196.8, 162.3, 141.6, 130.5, 130.3, 129.5, 128.5, 128.3, 128.2, 126.1, 114.3, 68.2, 49.1, 37.9, 37.4, 30.4, 26.3, 18.7; HRMS: m/z (ESI) calculated [M+Na]$^+$: 373.1774, measured: 373.1812.



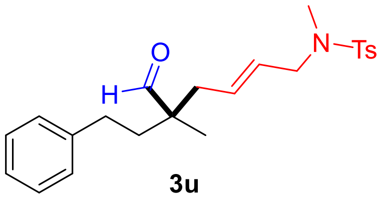
3s

^{1}H NMR (600 MHz, CDCl$_3$) δ 9.51 (s, 1H), 7.28 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 7.8 Hz, 2H), 5.08 (t, *J* = 7.6 Hz, 1H), 5.05 (t, *J* = 6.9 Hz, 1H), 2.57-2.50 (m, 1H), 2.50-2.43 (m, 1H), 2.25 (d, *J* = 7.6 Hz, 2H), 2.10-2.04 (m, 2H), 2.04-1.99 (m, 2H), 1.89-1.82 (m, 1H), 1.80-1.73 (m, 1H), 1.66 (s, 3H), 1.62 (s, 3H), 1.59 (s, 3H), 1.10 (s, 3H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 206.4, 142.0, 138.4, 131.56, 128.4, 128.2, 126.0, 124.0, 118.3, 49.9, 39.9, 37.2, 33.9, 30.6, 26.5, 25.7, 18.3, 17.7, 16.2; HRMS: m/z (ESI) calculated [M+Na]$^+$: 321.2194, measured: 321.2154.



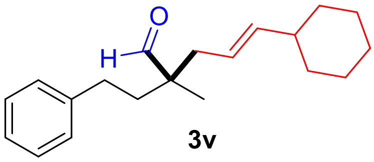
3t

^{1}H NMR (600 MHz, CDCl$_3$) δ 9.50 (s, 1H), 7.34-7.31 (m, 4H), 7.28-7.24 (m, 3H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.15 (d, *J* = 7.2 Hz, 2H), 5.69 (dt, *J* = 15.0, 5.8 Hz, 1H), 5.62 (dt, *J* = 15.0, 7.1 Hz, 1H), 4.48 (s, 2H), 3.98 (d, *J* = 5.8 Hz, 2H), 2.56-2.46 (m, 2H), 2.36-2.27 (m, 2H), 1.87-1.81 (m, 1H), 1.79-1.72 (m, 1H), 1.20 (s, 3H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 205.6, 141.7, 138.2, 130.6, 128.4, 128.3, 128.2, 128.0, 127.7, 127.6, 126.0, 71.9, 70.3, 49.1, 38.1, 37.2, 30.4, 18.6; HRMS: m/z (ESI) calculated [M+Na]$^+$: 345.1830, measured: 345.1793.



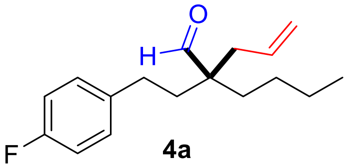
3u

^{1}H NMR (600 MHz, CDCl$_3$) δ 9.45 (s, 1H), 7.65 (d, *J* = 7.9 Hz, 2H), 7.30 (d, *J* = 7.9 Hz, 2H), 7.27 (dd, *J* = 7.2, 7.2 Hz, 2H), 7.18 (t, *J* = 7.2 Hz, 1H), 7.13 (d, *J* = 7.2 Hz, 2H), 5.59-5.33 (m, 2H), 3.56 (d, *J* = 5.8 Hz, 2H), 2.61 (s, 3H), 2.53-2.43 (m, 2H), 2.42 (s, 3H), 2.33-2.21 (m, 2H), 1.83-1.76 (m, 1H), 1.75-1.68 (m, 1H), 1.08 (s, 3H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 205.3, 143.3, 141.4, 134.1, 129.7, 129.6, 128.4, 128.3, 128.1, 127.3, 126.0, 52.1, 49.0, 37.8, 37.2, 34.1, 30.2, 21.4, 18.5; HRMS: m/z (ESI) calculated [M+H]$^+$: 400.1946, measured: 400.1956.



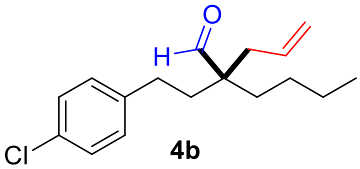
3v

^{1}H NMR (600 MHz, CDCl$_3$) δ 9.50 (s, 1H), 7.29 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H), 7.17 (d, *J* = 7.8 Hz, 2H), 5.47 (dd, *J* = 15.3, 6.8 Hz, 1H), 5.28 (dtd, *J* = 15.3, 7.5, 1.2 Hz, 1H), 2.58-2.44 (m, 2H), 2.28-2.19 (m, 2H), 1.98-1.89 (m, 1H), 1.84-1.78 (m, 1H), 1.77-1.71 (m, 1H), 1.71-1.65 (m, 4H), 1.66-1.62 (m, 1H), 1.30-1.22 (m, 2H), 1.19-1.13 (m, 1H), 1.10 (s, 3H), 1.09-1.02 (m, 2H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 206.2, 142.0, 140.9, 128.4, 128.2, 125.9, 121.2, 49.2, 40.8, 38.5, 37.1, 33.0, 30.4, 26.1, 25.9, 18.4. HRMS: m/z (ESI) calculated [M+Na]$^+$: 307.2038, measured: 307.2057.



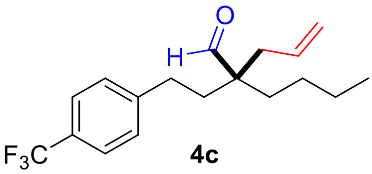
4a

^{1}H NMR (600 MHz, CDCl$_3$) δ 9.49 (s, 1H), 7.13-7.07 (m, 2H), 6.96 (t, *J* = 8.6 Hz, 2H), 5.70 (m, 1H), 5.15 (dd, *J* = 15.0, 7.4 Hz, 1H), 2.51-2.40 (m, 2H), 2.39-2.29 (m, 2H), 1.76 (t, *J* = 8.7 Hz, 2H), 1.58-1.52 (m, 2H), 1.35-1.28 (m, 2H), 1.23-1.17 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 206.2, 161.3 m(d, *J* = 243.8 Hz), 137.5 (d, *J* = 3.1 Hz), 132.8, 129.5 (d, *J* = 7.8 Hz), 118.5, 115.2 (d, *J* = 21.1 Hz), 52.0, 35.9, 34.4, 32.2, 29.1, 25.7, 23.2, 13.9; HRMS: m/z (ESI) calculated [M+Na]$^+$: 285.1631, measured: 285.1631.



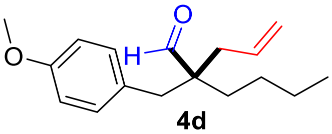
4b

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.49 (s, 1H), 7.24 (d, *J* = 8.1 Hz, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 5.70 (m, 1H), 5.13 (dd, *J* = 15.6, 8.4 Hz, 1H), 2.51-2.39 (m, 2H), 2.39-2.30 (m, 2H), 1.75 (t, *J* = 9.0 Hz, 2H), 1.58-1.53 (m, 2H), 1.35-1.28 (m, 2H), 1.23-1.16 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 206.1, 140.4, 132.7, 131.7, 129.5, 128.5, 118.6, 52.0, 36.0, 34.1, 32.2, 29.3, 25.7, 23.2, 13.9; HRMS: m/z (ESI) calculated [M+Na]$^+$: 301.1335, measured: 301.1344.



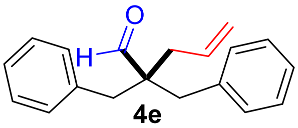
4c

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.43 (s, 1H), 7.45 (d, *J* = 7.8 Hz, 2H), 7.19 (d, *J* = 7.8 Hz, 2H), 5.67-5.59 (m, 1H), 5.10-5.05 (m, 2H), 2.52-2.40 (m, 2H), 2.33-2.24 (m, 2H), 1.74-1.67 (m, 2H), 1.55-1.45 (m, 2H), 1.24 (q, *J* = 7.3 Hz, 2H), 1.16-1.09 (m, 2H), 0.83 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 206.0, 146.1, 132.6, 128.5, 128.4 (q, *J* = 32.4 Hz), 125.3 (q, *J* = 3.6 Hz), 124.2 (q, *J* = 271.9 Hz), 118.6, 52.0, 36.0, 33.9, 32.2, 29.8, 25.7, 23.2, 13.9; HRMS: m/z (ESI) calculated [M+Na]$^+$: 335.1599, measured: 335.1597.



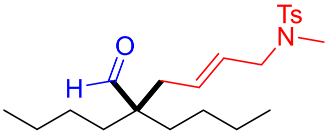
4d

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.50 (s, 1H), 6.93 (d, *J* = 8.6 Hz, 2H), 6.73 (d, *J* = 8.6 Hz, 2H), 5.73-5.65 (m, 1H), 5.20-4.97 (m, 2H), 3.71 (s, 3H), 2.72 (q, *J* = 14.2 Hz, 2H), 2.23 (dd, *J* = 14.7, 7.3 Hz, 1H), 2.12 (dd, *J* = 14.7, 7.3 Hz, 1H), 1.49-1.42 (m, 1H), 1.42-1.35 (m, 1H), 1.22-1.10 (m, 4H), 0.83 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 206.8, 158.2, 133.1, 131.1, 128.6, 118.6, 113.6, 55.2, 53.3, 38.5, 35.8, 31.9, 25.7, 23.2, 14.0; HRMS: m/z (ESI) calculated [M+Na]$^+$: 283.1674, measured: 283.1675.



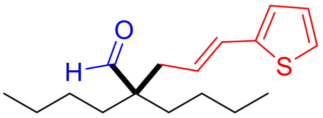
4e

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.68 (s, 1H), 7.29-7.25 (m, 4H), 7.24-7.20 (m, 2H), 7.13-7.09 (m, 4H), 5.94-5.84 (m, 1H), 5.21 (d, *J* = 10.1 Hz, 1H), 5.14 (d, *J* = 17.1 Hz, 1H), 2.99 (d, *J* = 14.1 Hz, 2H), 2.83 (d, *J* = 14.1 Hz, 2H), 2.27 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 206.5, 136.3, 133.2, 130.4, 128.3, 126.7, 119.3, 53.5, 40.2, 35.4; HRMS: m/z (ESI) calculated [M+Na]$^+$: 287.1412, measured: 287.1410.



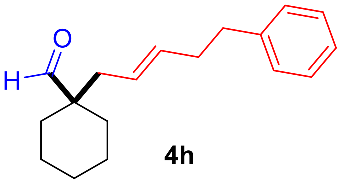
4f

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.32 (s, 1H), 7.59 (d, *J* = 8.2 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 5.39-5.27 (m, 2H), 3.48 (d, *J* = 4.5 Hz, 2H), 2.54 (s, 3H), 2.36 (s, 3H), 2.19-2.09 (m, 2H), 1.42-1.32 (m, 4H), 1.19 (q, *J* = 7.3 Hz, 4H), 1.11-0.97 (m, 4H), 0.81 (t, *J* = 7.3 Hz, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 206.5, 143.3, 134.1, 130.3, 129.6, 127.7, 127.4, 52.2, 52.1, 34.1, 34.0, 32.0, 25.5, 23.2, 21.5 13.9; HRMS: m/z (ESI) calculated $[M+Na]^+$: 416.2235, measured: 416.2202.



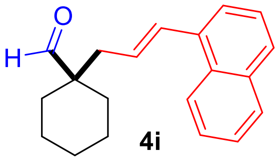
4g

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.42 (s, 1H), 7.04 (d, *J* = 5.1 Hz, 1H), 6.90-6.85 (m, 1H), 6.81 (d, *J* = 3.5 Hz, 1H), 6.47 (d, *J* = 15.4 Hz, 1H), 5.81 (dt, *J* = 15.4, 7.6 Hz, 1H), 2.30 (d, *J* = 7.6 Hz, 2H), 1.48-1.41 (m, 4H), 1.26-1.20 (m, 4H), 1.13-1.03 (m, 4H), 0.83 (t, *J* = 7.2 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 206.8, 142.4, 127.2, 126.2, 124.9, 124.7, 123.6, 52.5, 34.9, 32.3, 25.7, 23.3, 13.9; HRMS: m/z (ESI) calculated $[M+H]^+$: 279.1783, measured: 279.1776.



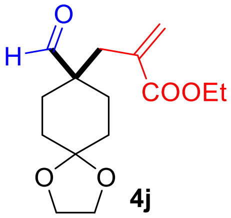
4h

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.31 (s, 1H), 7.20 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.13-1.07 (m, 3H), 5.38 (dt, *J* = 15.0, 6.7 Hz, 1H), 5.20 (dt, *J* = 15.0, 7.2 Hz, 2H), 2.58 (t, *J* = 7.5 Hz, 2H), 2.28-2.19 (m, 2H), 2.02 (d, *J* = 7.2 Hz, 2H), 1.76-1.71 (m, 2H), 1.51-1.46 (m, 2H), 1.46-1.40 (m, 1H), 1.25-1.17 (m, 4H), 1.16-1.11 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 207.3, 141.8, 133.4, 128.4, 128.2, 125.7, 124.6, 49.8, 39.5, 35.8, 34.4, 30.7, 25.6, 22.5; HRMS: m/z (ESI) calculated $[M+Na]^+$: 279.1725, measured: 279.1723.



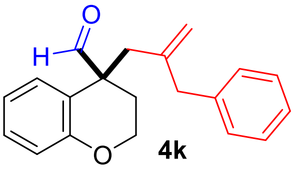
4i

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.56 (s, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 7.2 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.52-7.45 (m, 3H), 7.41 (dd, *J* = 7.8, 7.2 Hz, 1H), 7.12 (d, *J* = 15.4 Hz, 1H), 6.07 (dt, *J* = 15.4, 7.6 Hz, 1H), 2.45 (dd, *J* = 7.6, 1.4 Hz, 2H), 2.02-1.93 (m, 2H), 1.67-1.60 (m, 2H), 1.58-1.52 (m, 1H), 1.46-1.35 (m, 4H), 1.35-1.28 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 206.9, 135.0, 133.5, 131.0, 130.7, 128.4, 127.7, 127.7, 125.9, 125.7, 125.6, 123.8, 123.8, 50.2, 40.1, 30.9, 25.6, 22.5; HRMS: m/z (ESI) calculated $[M+Na]^+$: 301.1568, measured: 301.1556.



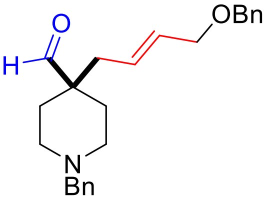
4j

^{1}H NMR (600 MHz, CDCl$_3$) δ 9.47 (s, 1H), 6.26 (d, *J* = 1.4 Hz, 1H), 5.55 (s, 1H), 4.17 (q, *J* = 7.1 Hz, 2H), 3.92 (s, 4H), 2.52 (s, 2H), 2.03-1.97 (m, 2H), 1.70-1.64 (m, 2H), 1.59-1.47 (m, 4H), 1.28 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 204.8, 166.8, 135.8, 129.0, 108.2, 64.25 , 64.22 , 61.0, 48.8, 38.3, 31.3, 28.4, 14.0; HRMS: m/z (ESI) calculated [M+H]$^+$: 283.1546, measured: 283.1547.



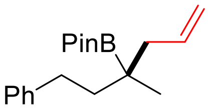
4k

^{1}H NMR (400 MHz, CDCl$_3$) δ 9.49 (s, 1H), 7.24-7.19 (m, 2H), 7.16-7.07 (m, 3H), 6.99 (d, *J* = 7.2 Hz, 2H), 6.87 (dd, *J* = 7.2, 7.2 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 1H), 4.83 (s, 1H), 4.80 (s, 1H), 4.17-4.09 (m, 1H), 4.04-3.96 (m, 1H), 3.08-2.97 (m, 2H), 2.66 (d, *J* = 14.4 Hz, 1H), 2.44 (d, *J* = 14.4 Hz, 1H), 2.27 (ddd, *J* = 14.4, 6.0, 2.8 Hz, 1H), 2.00-1.90 (m, 1H); ^{13}C NMR (101 MHz, CDCl$_3$ δ 200.6, 155.5, 143.9, 138.7, 129.0, 128.8, 128.5, 128.4, 126.3, 121.1, 120.5, 117.9, 117.6, 63.3, 49.1, 43.6, 41.5, 26.7; HRMS: m/z (ESI) calculated [M+Na]$^+$: 315.1361, measured: 315.1346.



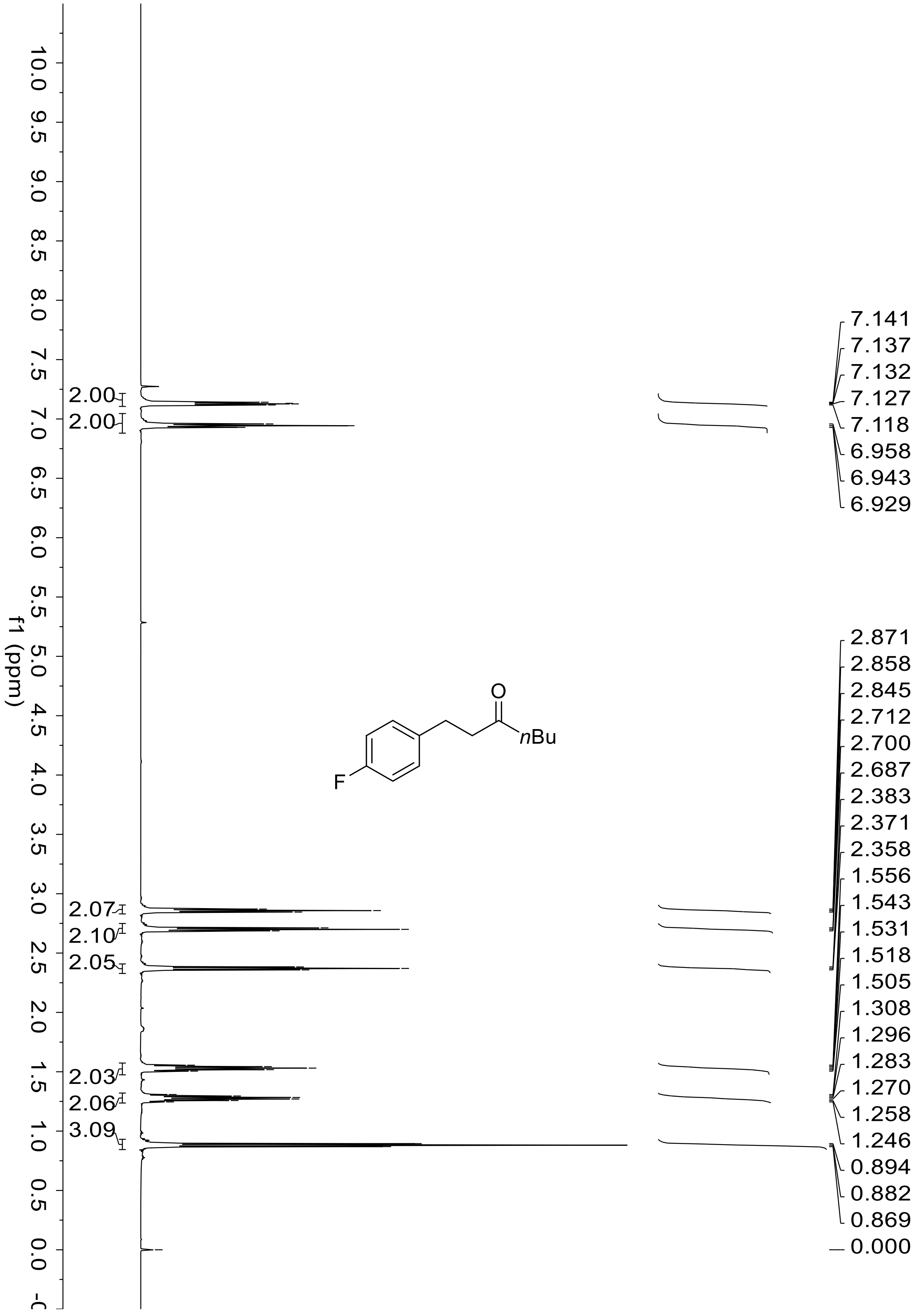
4l

^{1}H NMR (600 MHz, CDCl$_3$) δ 9.46 (s, 1H), 7.36-7.32 (m, 4H), 7.32-7.30 (m, 2H), 7.30-7.27 (m, 4H), 5.62 (dt, *J* = 15.0, 5.8 Hz, 1H), 5.55 (dt, *J* = 15.0, 7.2 Hz, 1H), 4.47 (s, 2H), 3.95 (d, *J* = 5.8 Hz, 2H), 3.45 (s, 2H), 2.71-2.61 (m, 2H), 2.23 (d, *J* = 7.2 Hz, 2H), 2.13-2.04 (m, 2H), 2.02-1.95 (m, 2H), 1.63-1.53 (m, 2H); ^{13}C NMR (151 MHz, CDCl$_3$) δ 206.1, 138.1, 130.7, 129.1, 128.3, 128.3, 128.2, 127.7, 127.6, 127.4, 127.0, 71.9, 70.2, 63.2, 50.3, 48.2, 30.5, 24.8; HRMS: m/z (ESI) calculated [M+Na]$^+$: 386.2096, measured: 386.2105.



11

^{1}H NMR (600 MHz, CDCl$_3$) δ 7.19 (t, *J* = 7.6 Hz, 2H), 7.09 (m, 3), 5.76 (ddt, *J* = 17.3, 10.1, 7.4 Hz, 1H), 4.97 (d, *J* = 17.3 Hz, 1H), 4.93 (d, *J* = 10.1 Hz, 1H), 2.55-2.43 (m, 2H), 2.16 (dd, *J* = 13.6, 7.6 Hz, 1H), 1.97 (dd, *J* = 13.6, 7.6 Hz, 1H), 1.64 (td, *J* = 12.9, 5.0 Hz, 1H), 1.43 (td, *J* = 12.9, 5.0 Hz, 1H), 1.18 (s, 12), 0.93 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.5, 136.4, 128.3, 128.2, 125.5, 116.4, 83.1, 43.3, 41.4, 32.4, 24.9, 24.8, 21.3; HRMS: m/z (ESI) calculated $[M+Na]^+$: 323.2158, measured: 323.2130.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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)
2.00
2.00
2.07
2.10
2.05
2.03
2.06
3.09
O
nBu
F
7.141
7.137
7.132
7.127
7.118
6.958
6.943
6.929
2.871
2.858
2.845
2.712
2.700
2.687
2.383
2.371
2.358
1.556
1.543
1.531
1.518
1.505
1.308
1.296
1.283
1.270
1.258
1.246
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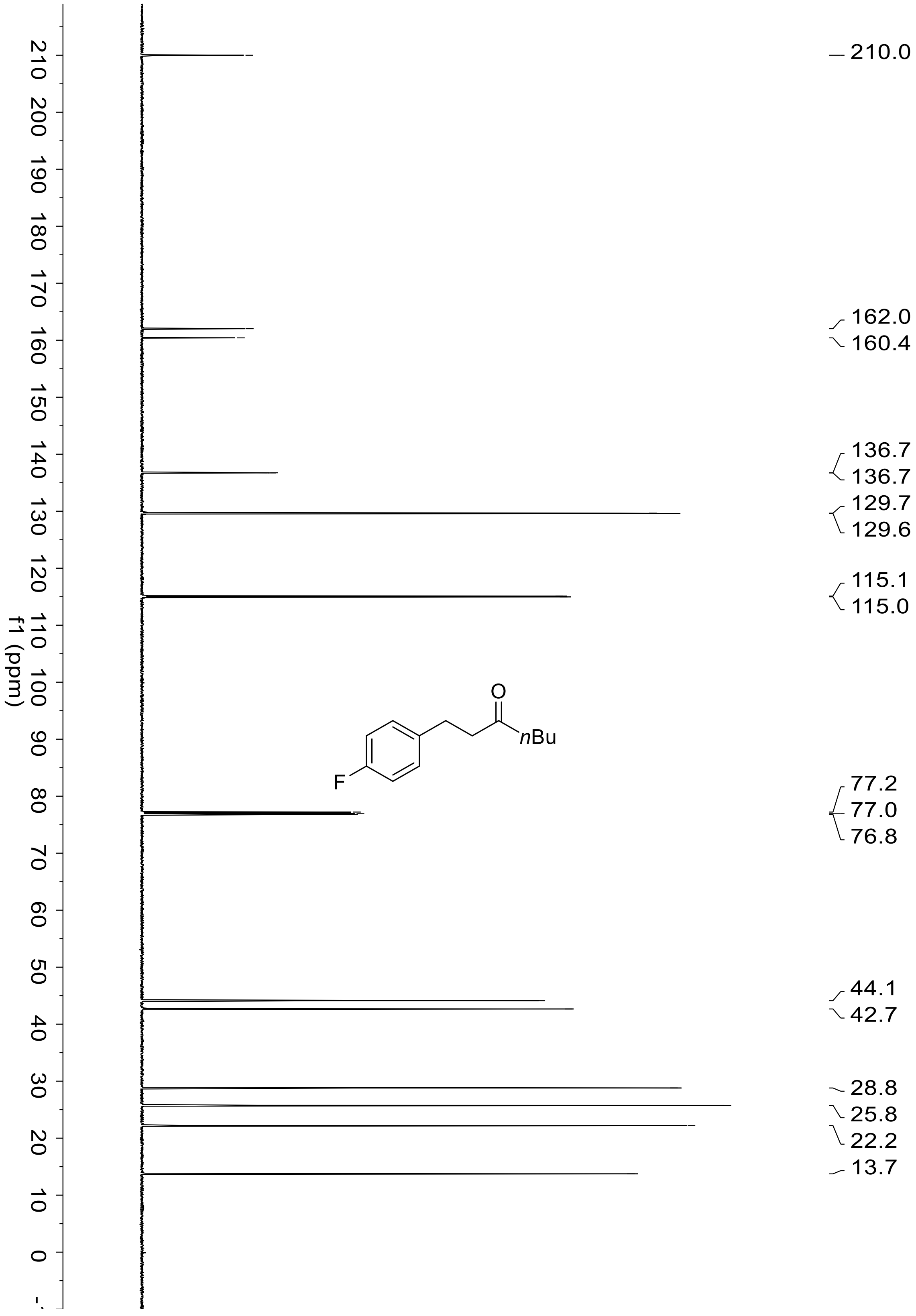
0.882
0.869
0.000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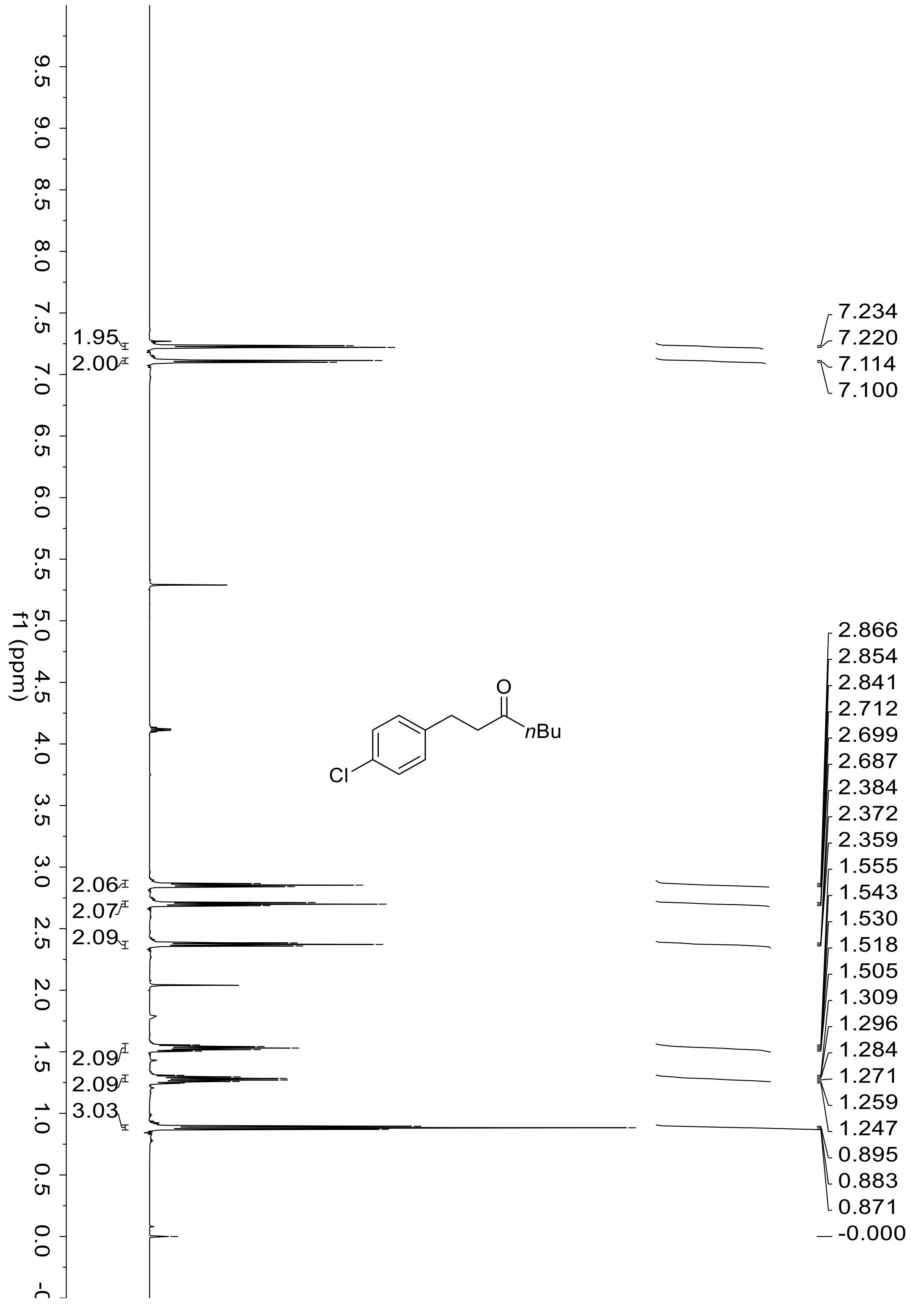
162.0
160.4
136.7
136.7
129.7
129.6
115.1
115.0
77.2
77.0
76.8
44.1
42.7
28.8
25.8
22.2
13.7
O
nBu
F
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
1.95
2.00
2.06
2.07
2.09
2.09
2.09
3.03
7.234
7.220
7.114
7.100
2.866
2.854
2.841
2.712
2.699
2.687
2.384
2.372
2.359
1.555
1.543
1.530
1.518
1.505
1.309
1.296
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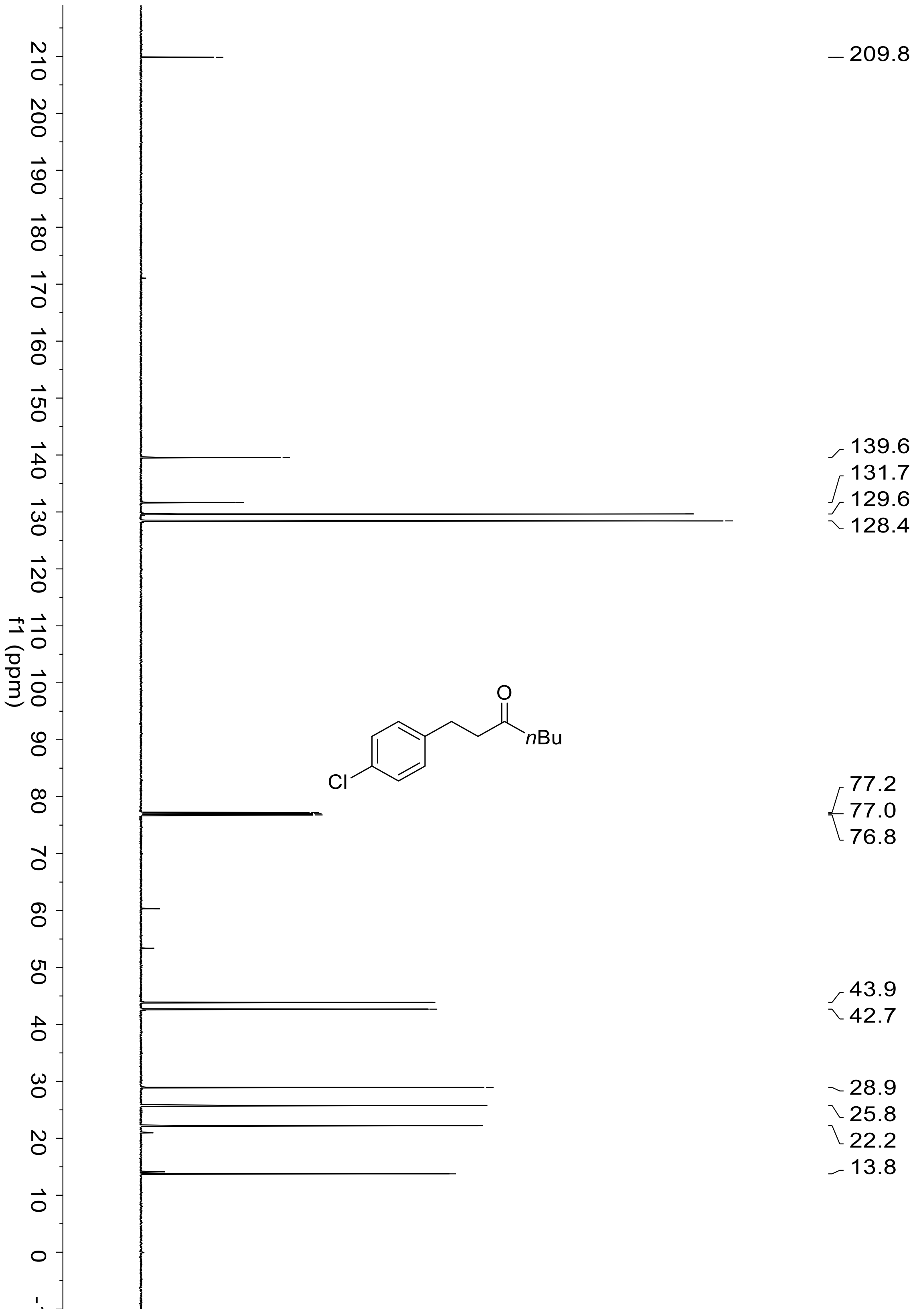
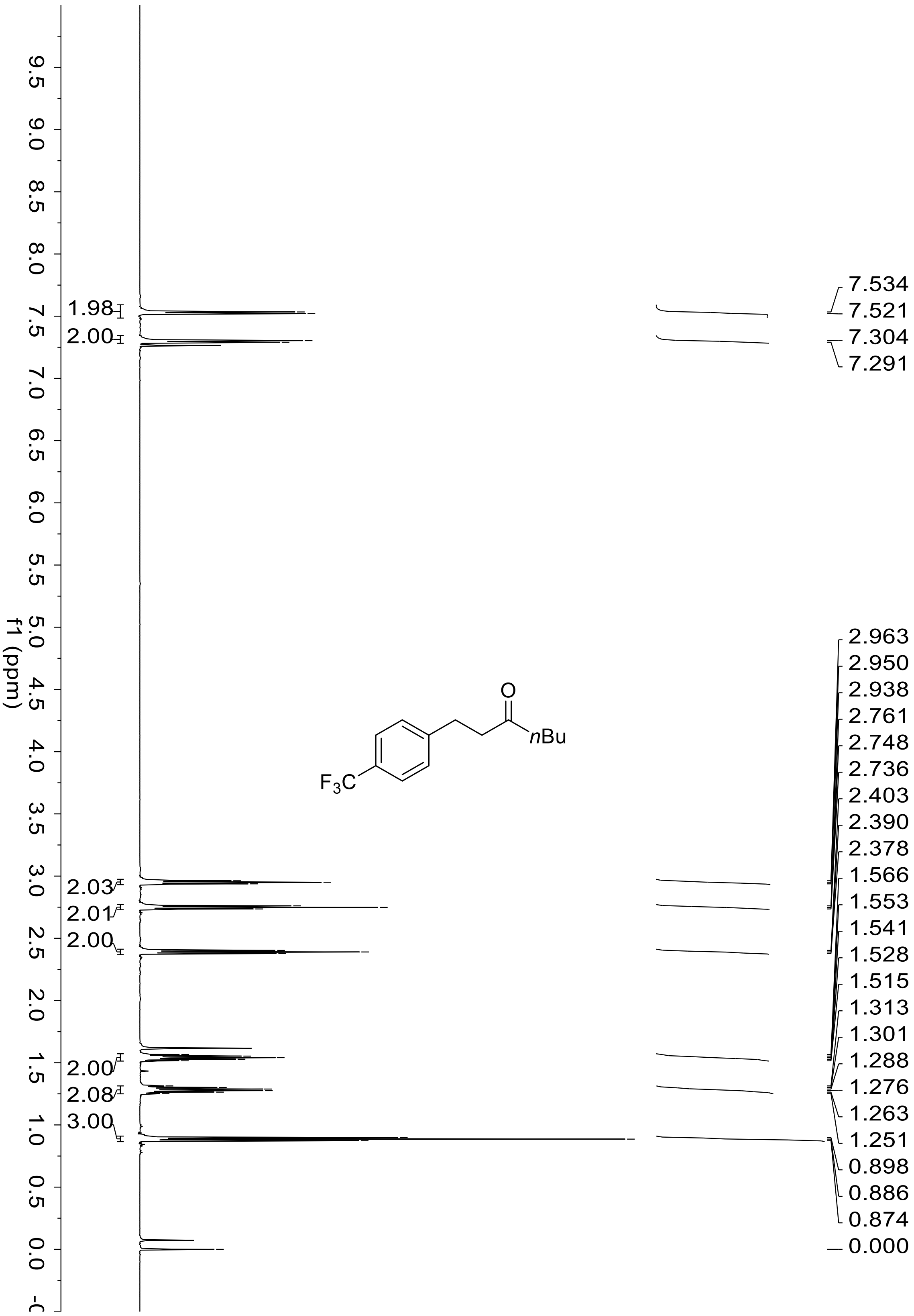
1.271
1.259
1.247
0.895
0.883
0.871
-0.000
O
nBu
Cl


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
209.8
139.6
131.7
129.6
128.4
77.2
77.0
76.8
43.9
42.7
28.9
25.8
22.2
13.8
O
nBu
Cl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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)
1.98
2.00
2.03
2.01
2.00
2.00
2.08
3.00
O
nBu
F3C
7.534
7.521
7.304
7.291
2.963
2.950
2.938
2.761
2.748
2.736
2.403
2.390
2.378
1.566
1.553
1.541
1.528
1.515
1.313
1.301
1.288
1.276
1.263
1.251
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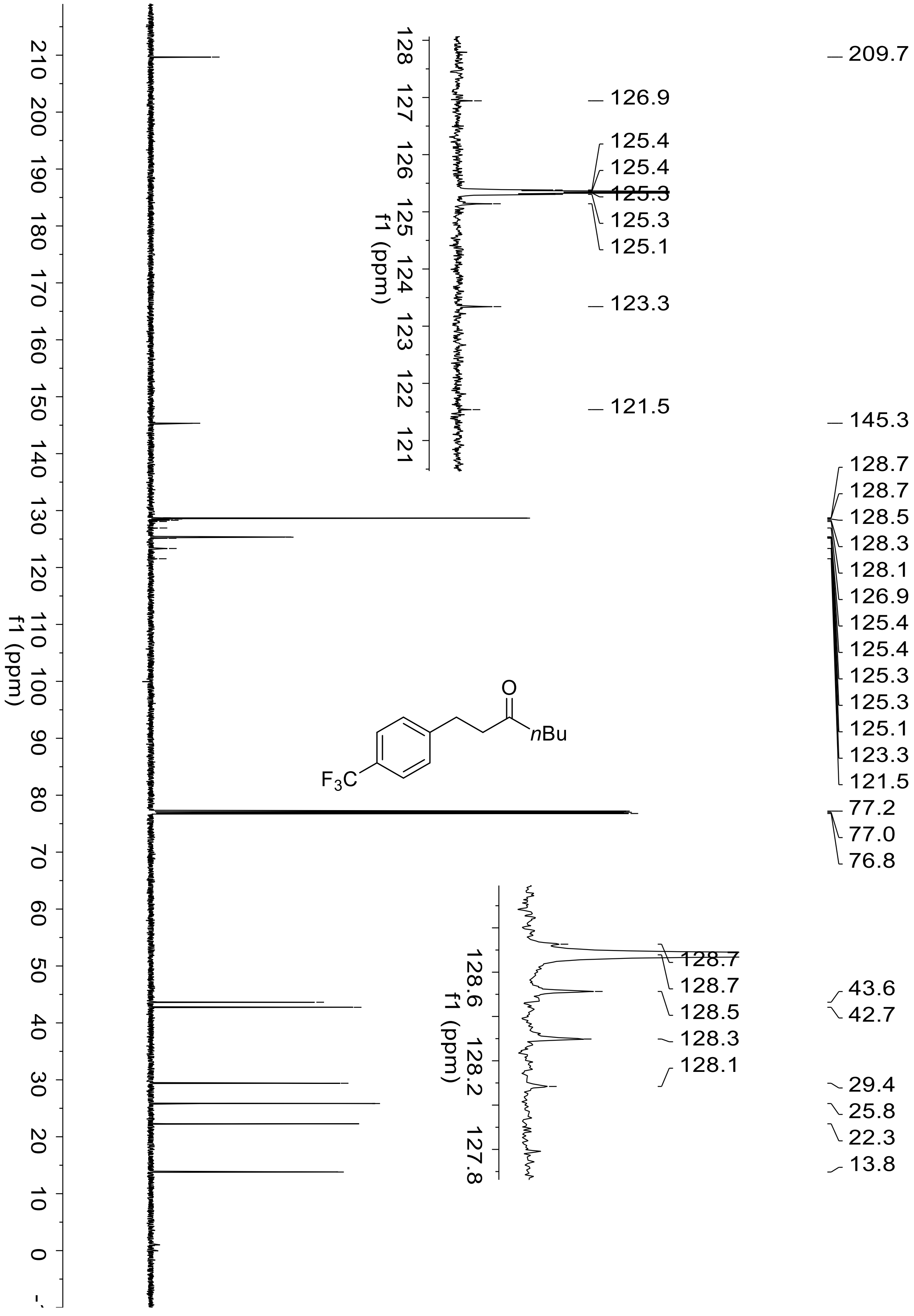
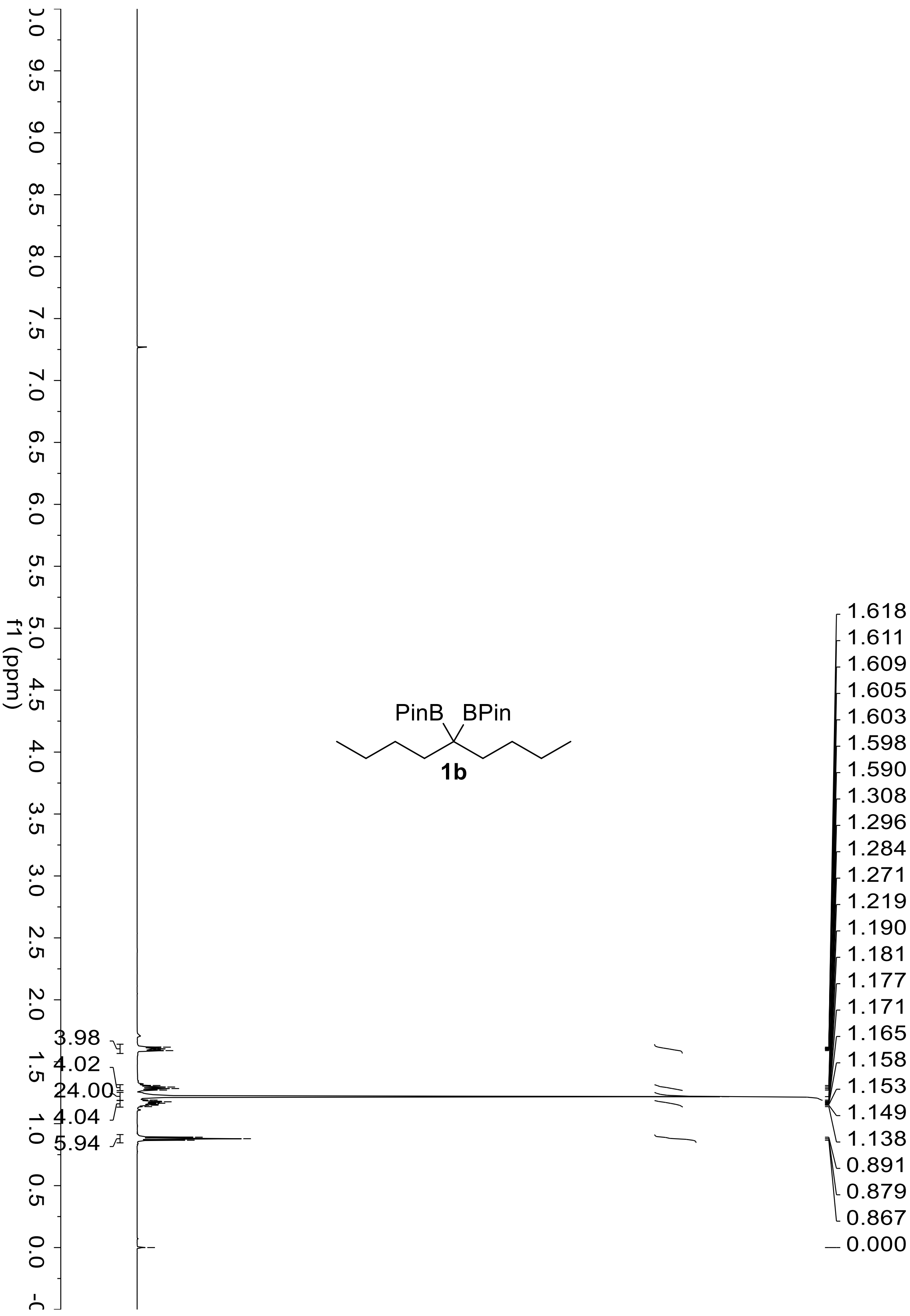
0.886
0.874
0.000


209.7
145.3
128.7
128.7
128.5
128.3
128.1
126.9
125.4
125.4
125.3
125.3
125.1
123.3
121.5
77.2
77.0
76.8
43.6
42.7
29.4
25.8
22.3
13.8
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
126.9
125.4
125.4
125.3
125.3
125.1
123.3
121.5
128 127 126 125 124 123 122 121
f1 (ppm)
128.7
128.7
128.5
128.3
128.1
128.6 128.2 127.8
f1 (ppm)
O
nBu
F3C


PinB
BPin
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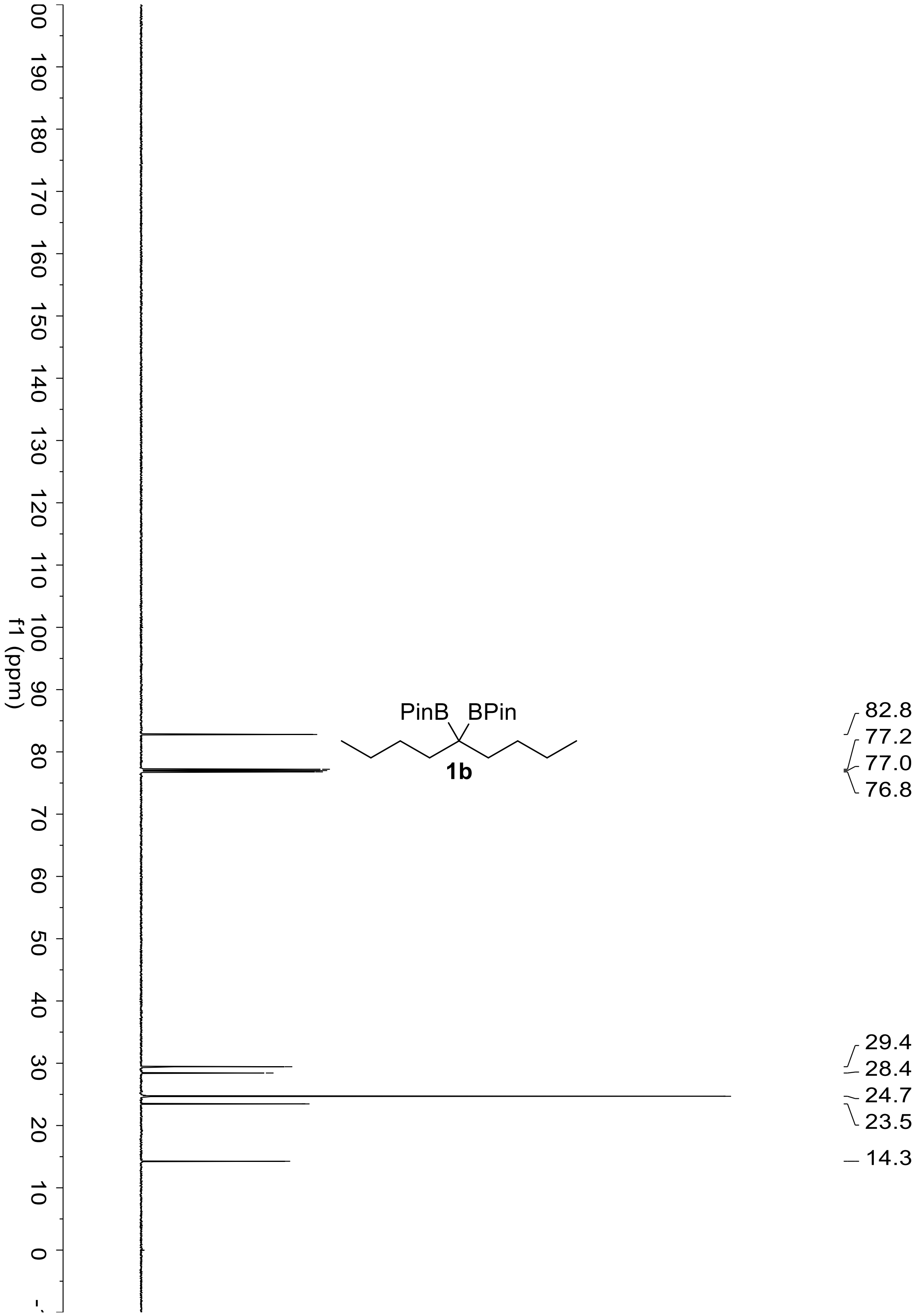
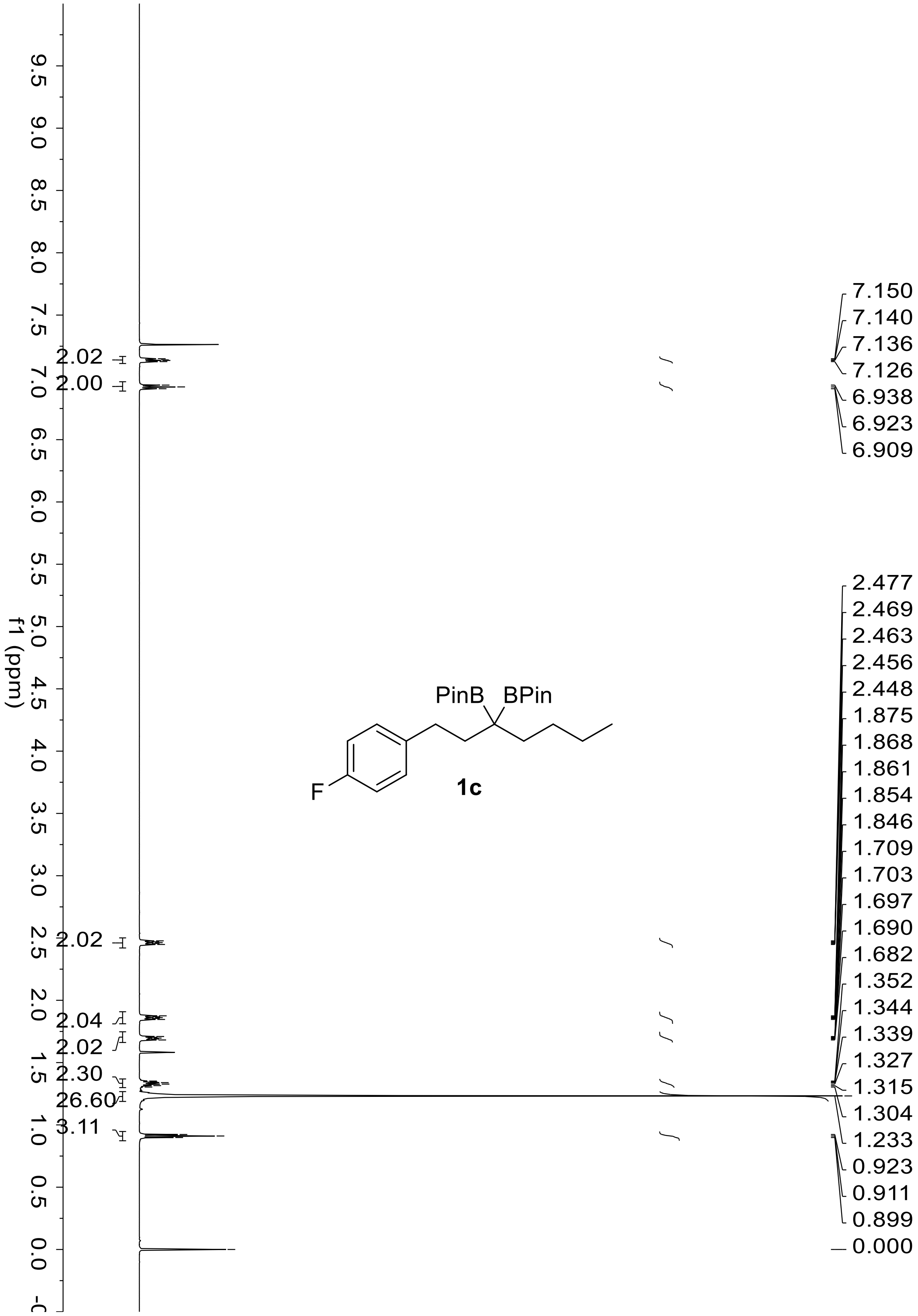
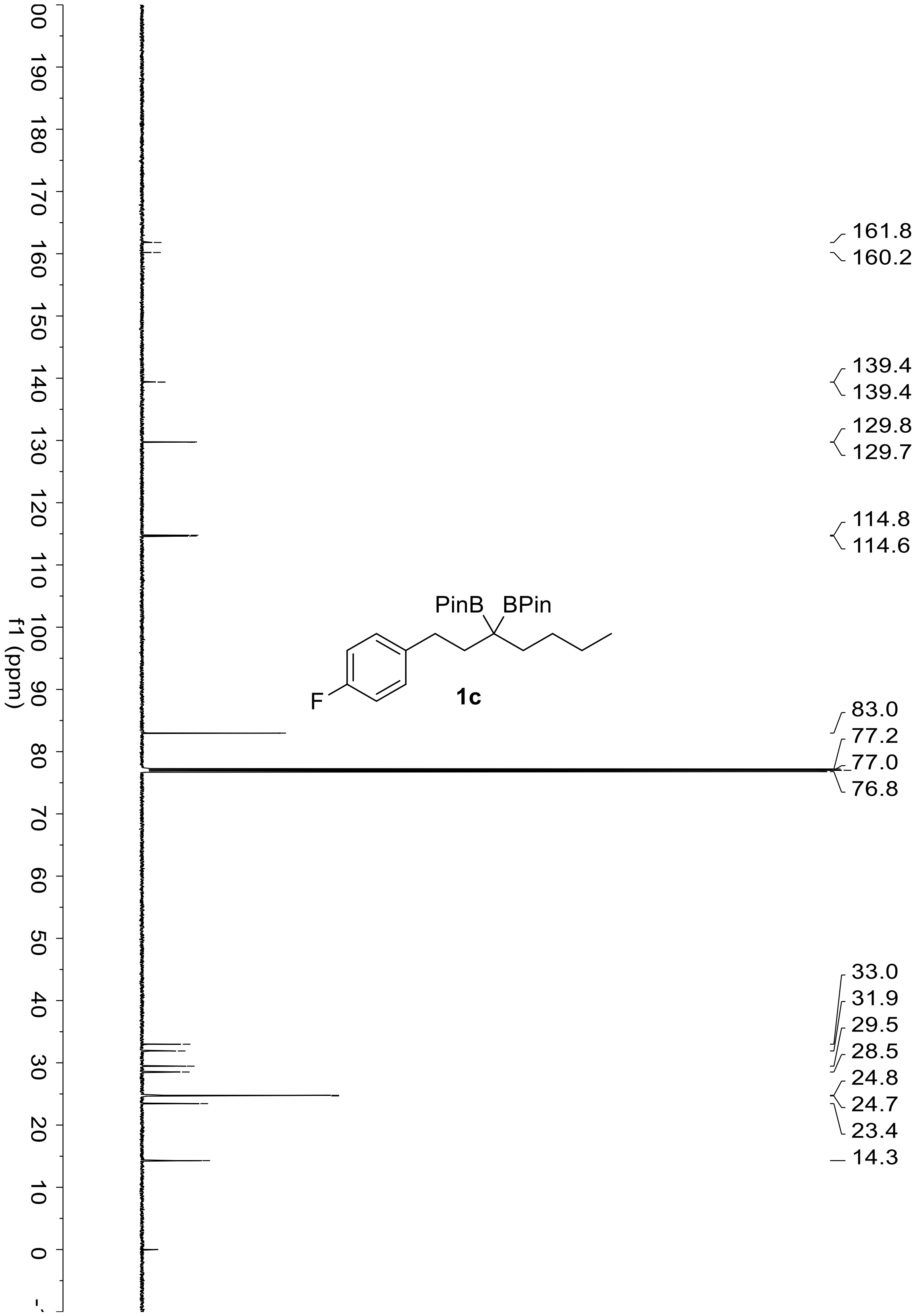
1.609
1.605
1.603
1.598
1.590
1.308
1.296
1.284
1.271
1.219
1.190
1.181
1.177
1.171
1.165
1.158
1.153
1.149
1.138
0.891
0.879
0.867
0.000
3.98
4.02
24.00
4.04
5.94
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



PinB
BPin
1b
82.8
77.2
77.0
76.8
29.4
28.4
24.7
23.5
14.3
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-
f1 (ppm)


7.150
7.140
7.136
7.126
6.938
6.923
6.909
2.477
2.469
2.463
2.456
2.448
1.875
1.868
1.861
1.854
1.846
1.709
1.703
1.697
1.690
1.682
1.352
1.344
1.339
1.327
1.315
1.304
1.233
0.923
0.911
0.899
0.000
PinB
BPin
F
1c
2.02
2.00
2.02
2.04
2.02
2.30
26.60
3.11
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)


PinB BPin
F
1c
161.8
160.2
139.4
139.4
129.8
129.7
114.8
114.6
83.0
77.2
77.0
76.8
33.0
31.9
29.5
28.5
24.8
24.7
23.4
14.3
f1 (ppm)
00
190
180
170
160
150
140
130
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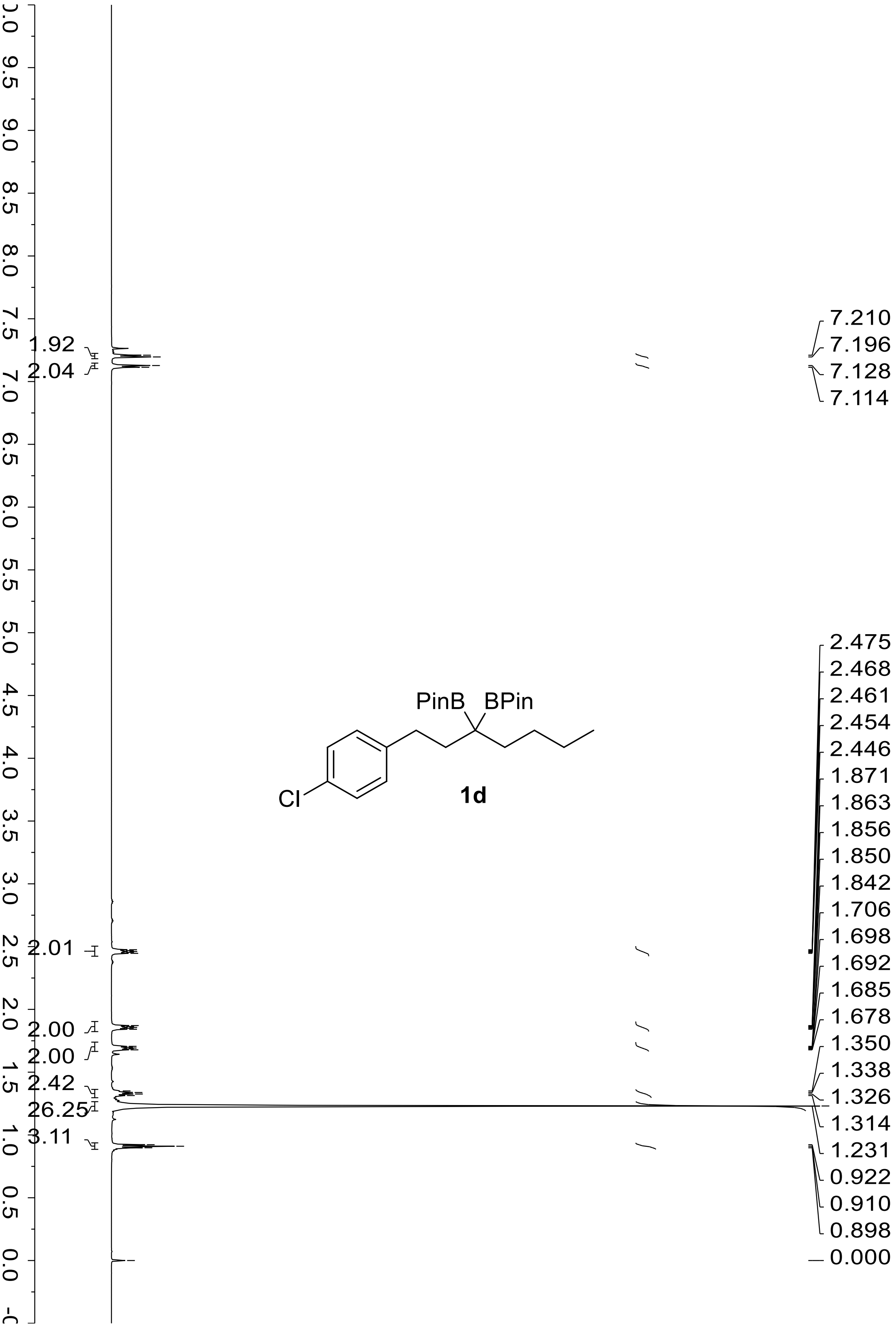
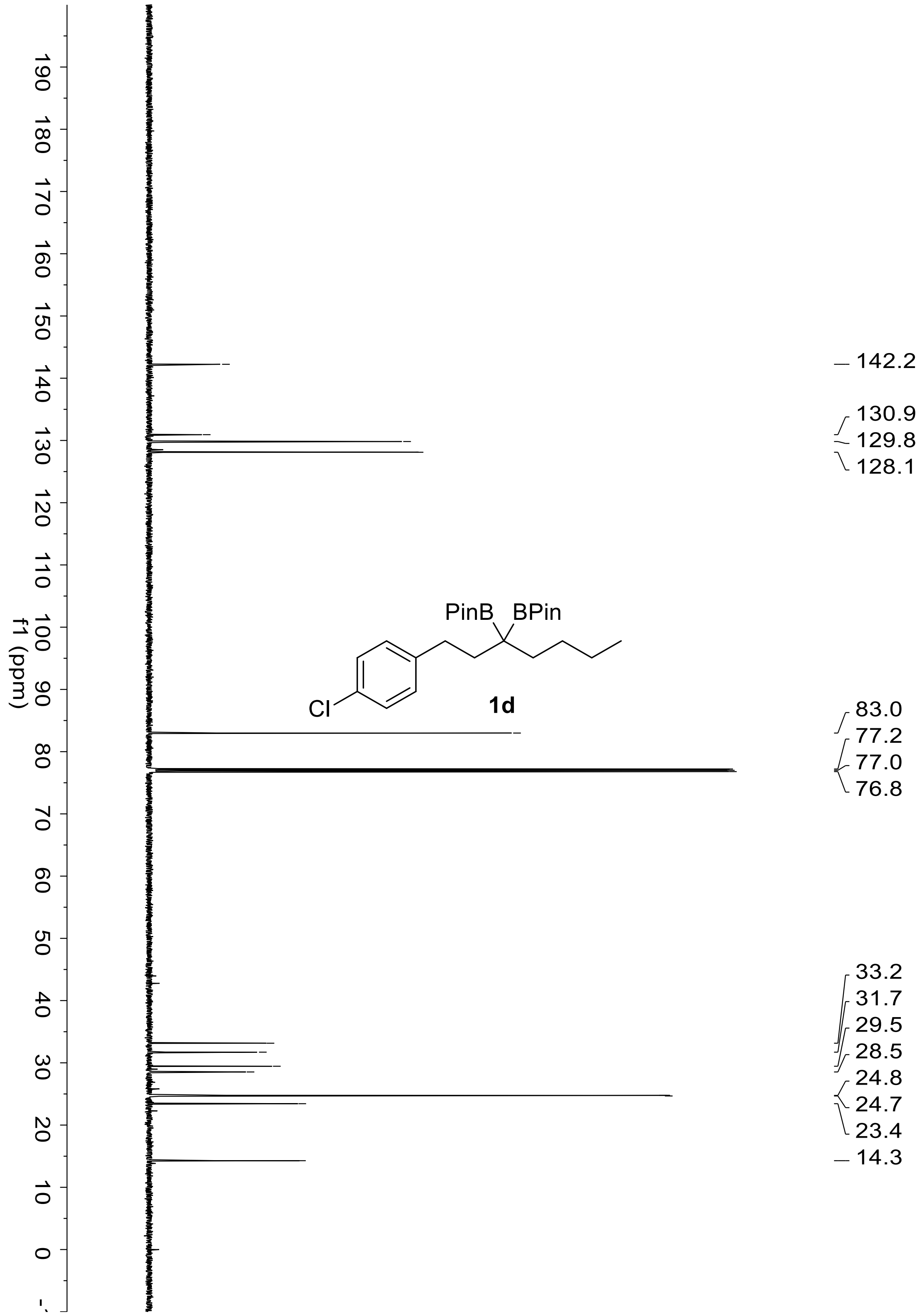
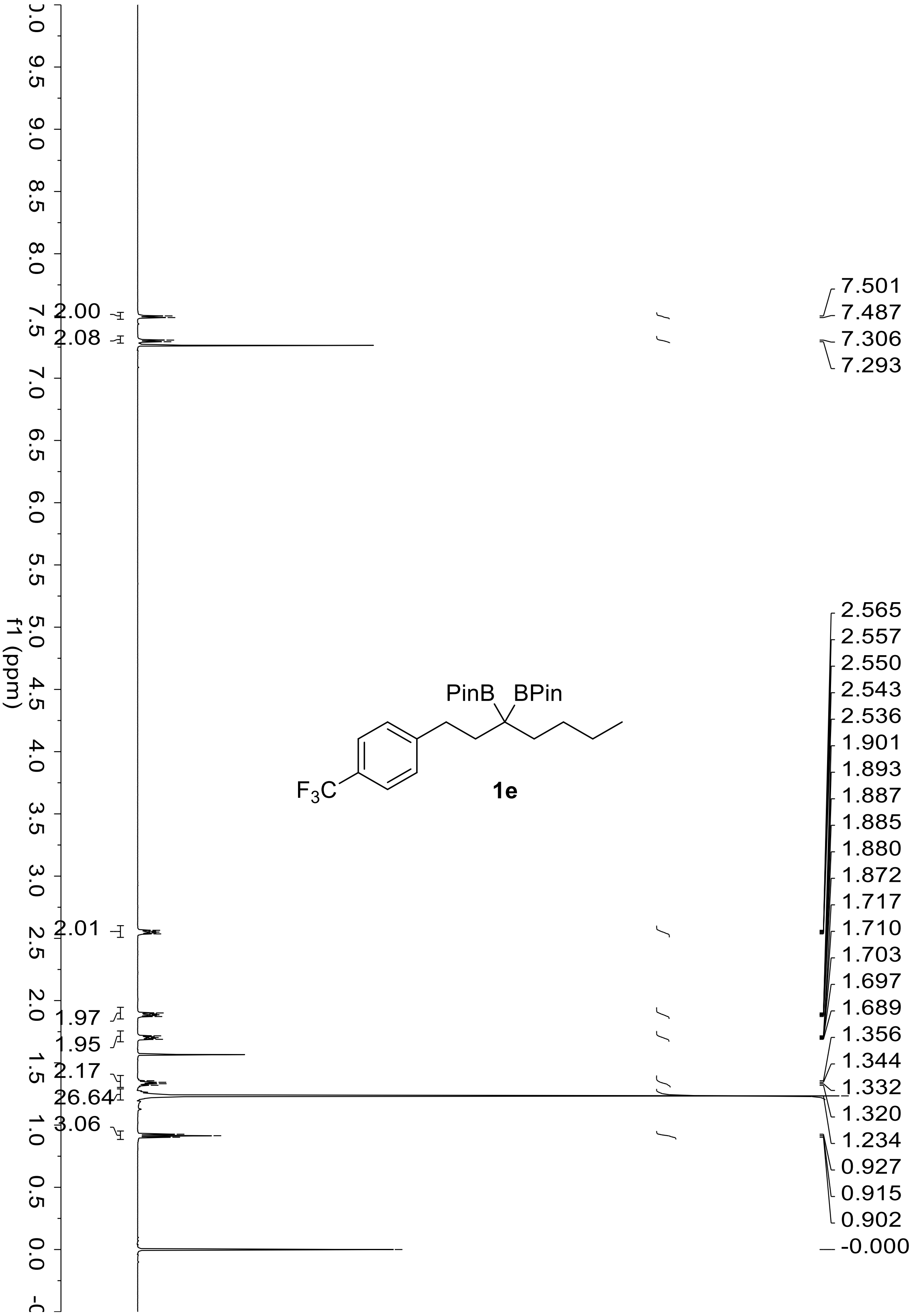
50
40
30
20
10
0



PinB
BPin
Cl
7.210
7.196
7.128
7.114
2.475
2.468
2.461
2.454
2.446
1.871
1.863
1.856
1.850
1.842
1.706
1.698
1.692
1.685
1.678
1.350
1.338
1.326
1.314
1.231
0.922
0.910
0.898
0.000
1.92
2.04
2.01
2.00
2.00
2.42
26.25
3.11
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

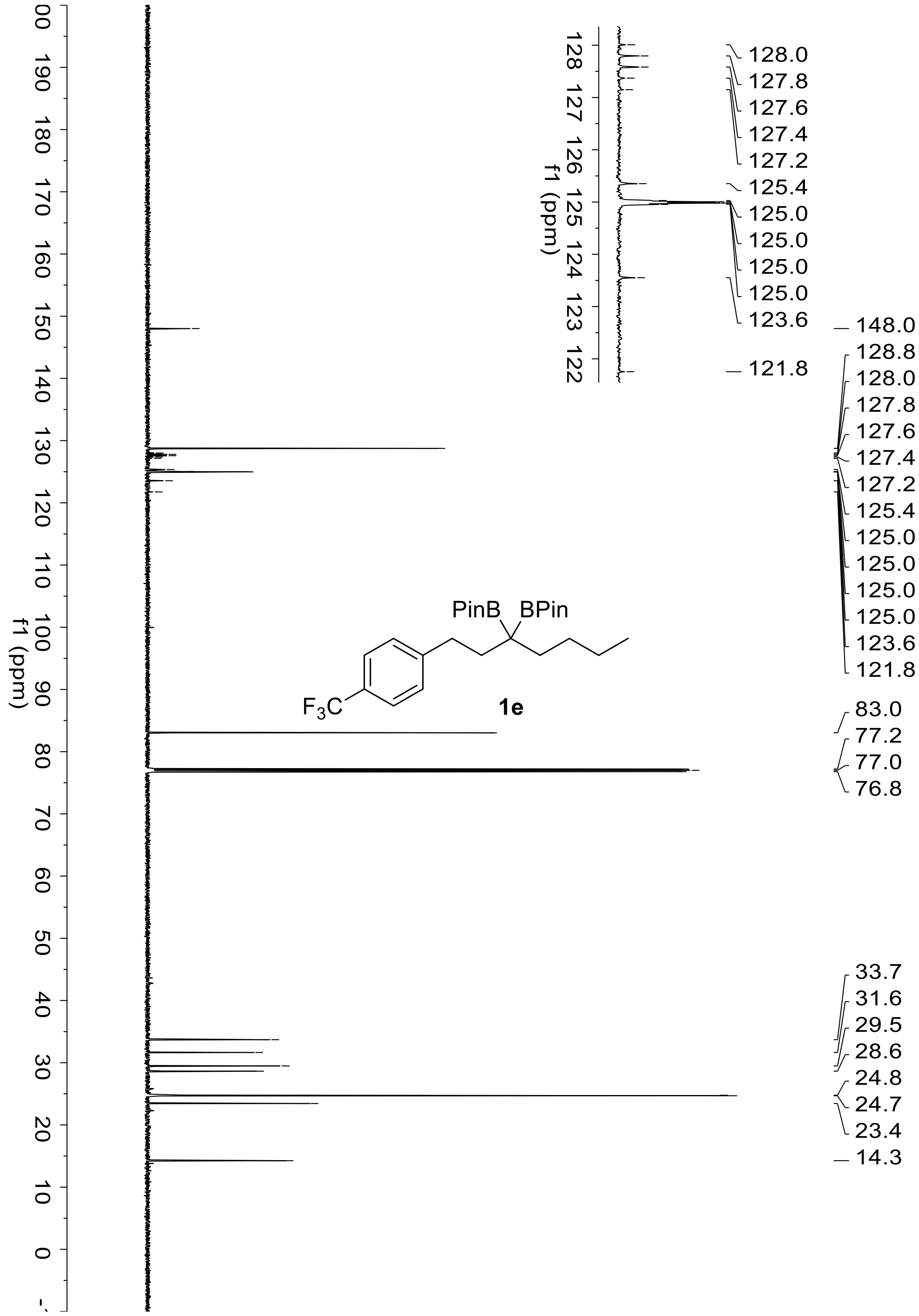
1d

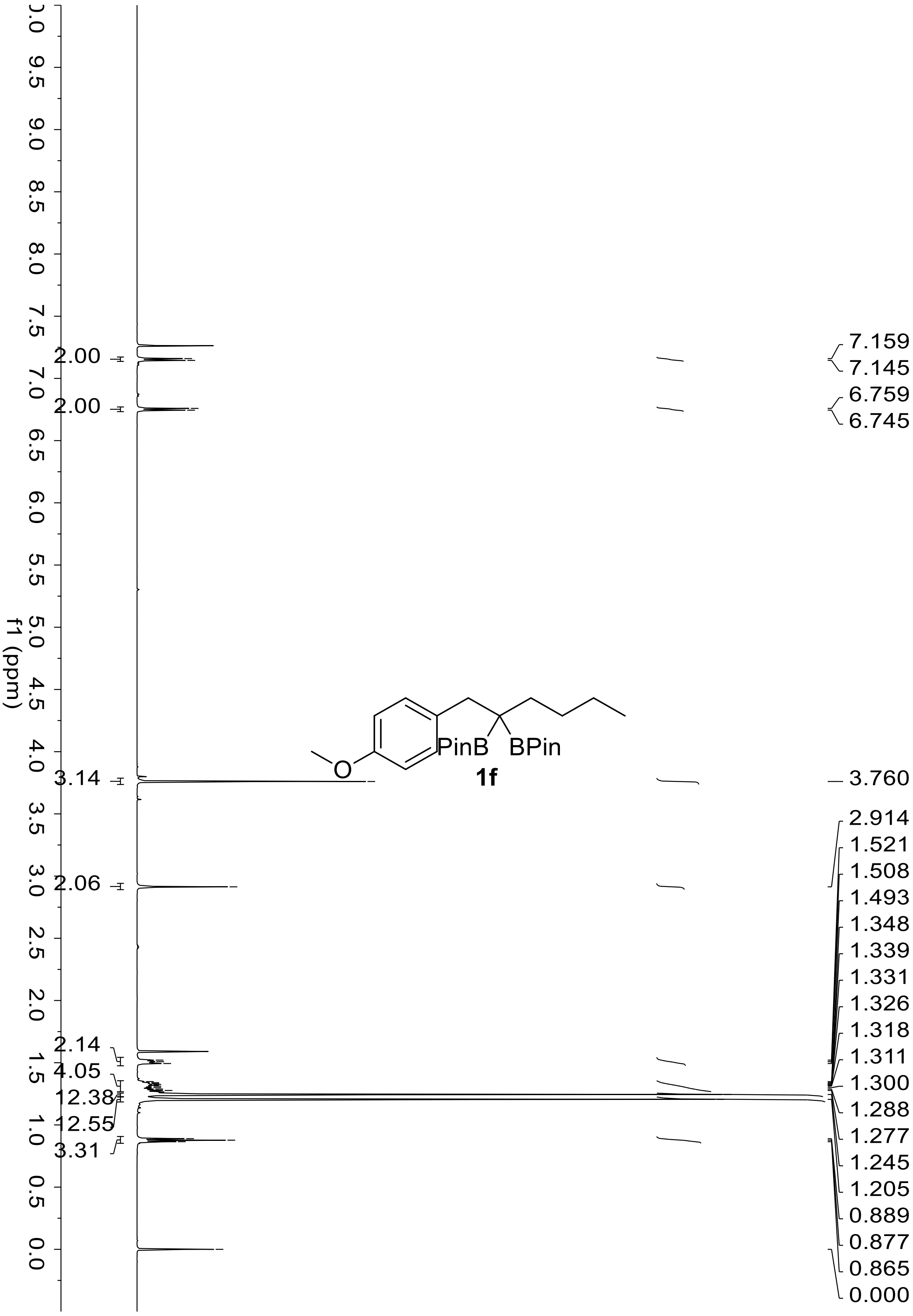

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
142.2
130.9
129.8
128.1
83.0
77.2
77.0
76.8
33.2
31.7
29.5
28.5
24.8
24.7
23.4
14.3
PinB
BPin
Cl
1d



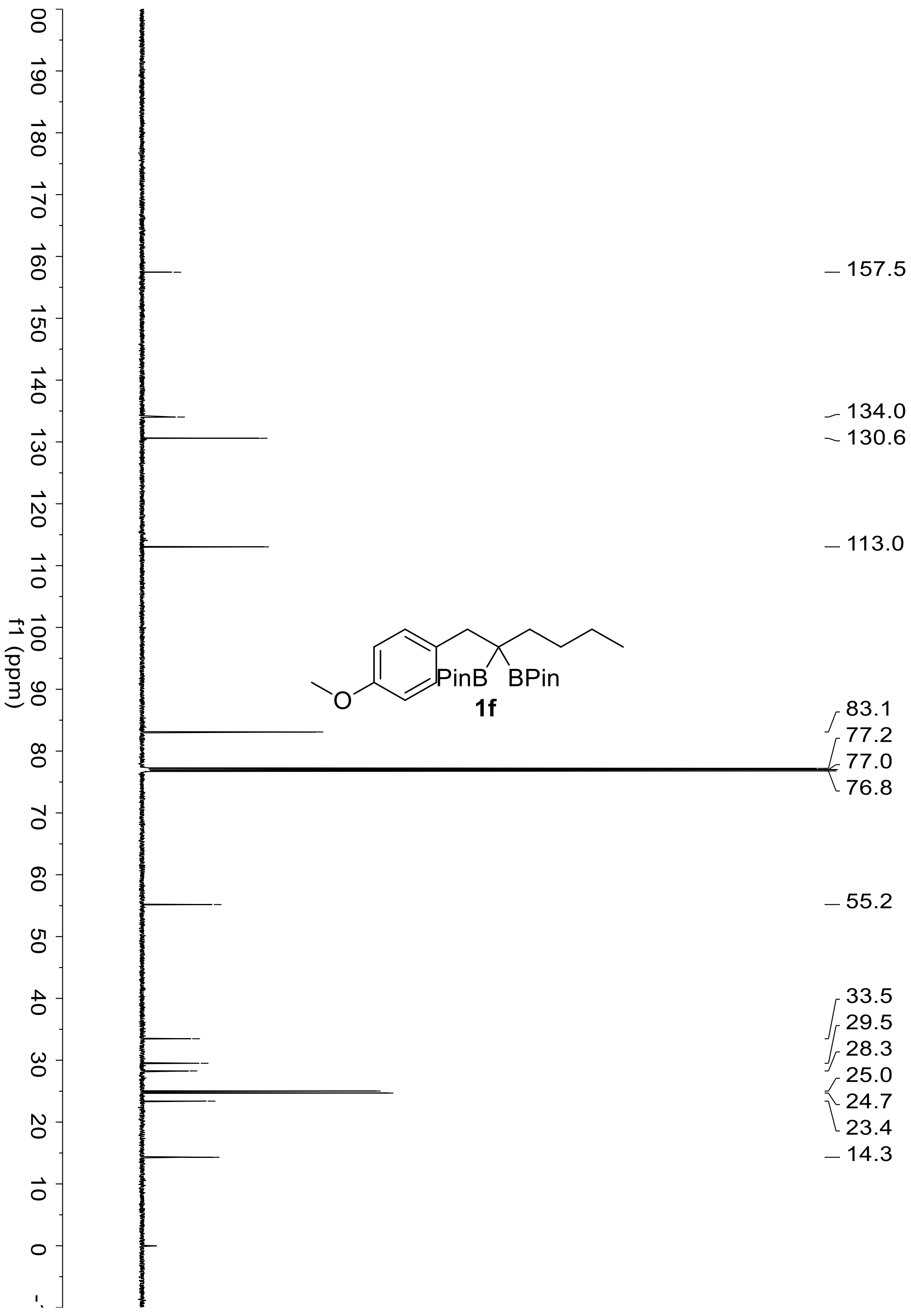
1e

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
2.00
2.08
2.01
1.97
1.95
2.17
26.64
3.06
7.501
7.487
7.306
7.293
2.565
2.557
2.550
2.543
2.536
1.901
1.893
1.887
1.885
1.880
1.872
1.717
1.710
1.703
1.697
1.689
1.356
1.344
1.332
1.320
1.234
0.927
0.915
0.902
-0.000
PinB
BPin
F_3C

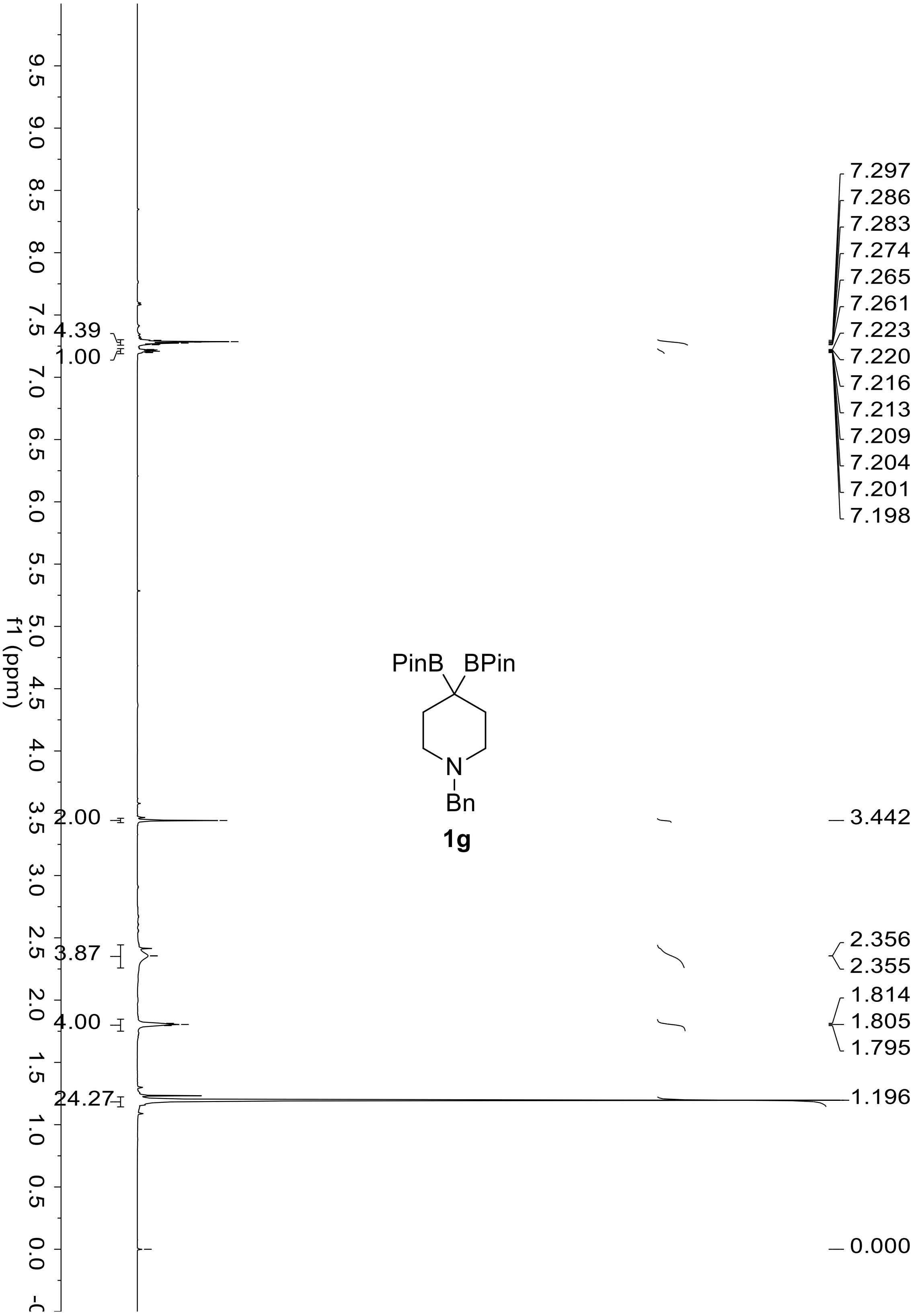

PinB BPin
F3C
1e
f1 (ppm)
128 127 126 125 124 123 122
128.0
127.8
127.6
127.4
127.2
125.4
125.0
125.0
125.0
125.0
123.6
121.8
148.0
128.8
128.0
127.8
127.6
127.4
127.2
125.4
125.0
125.0
125.0
125.0
123.6
121.8
83.0
77.2
77.0
76.8
33.7
31.6
29.5
28.6
24.8
24.7
23.4
14.3
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0



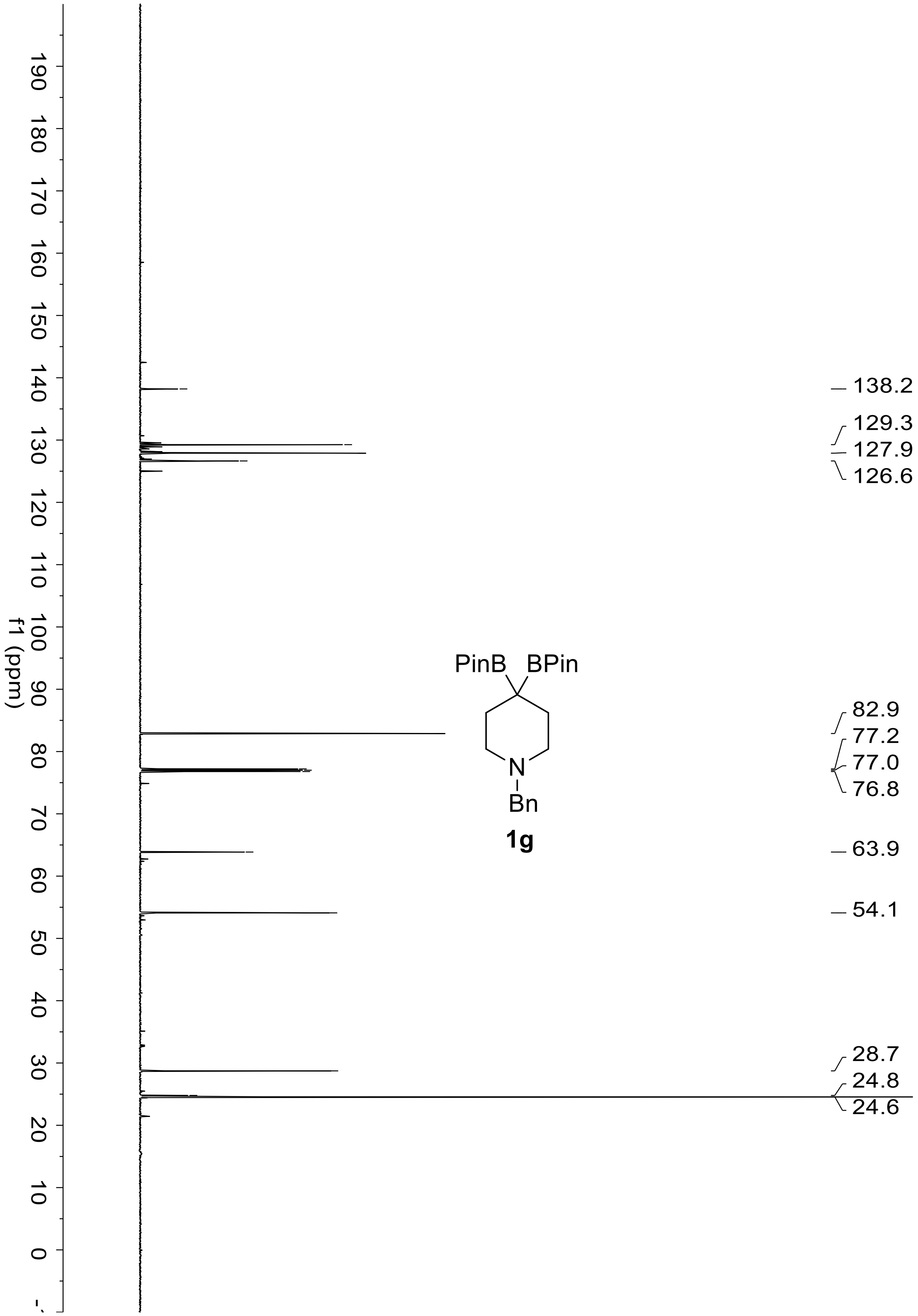
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
2.00
2.00
3.14
2.06
2.14
4.05
12.38
12.55
3.31
7.159
7.145
6.759
6.745
3.760
2.914
1.521
1.508
1.493
1.348
1.339
1.331
1.326
1.318
1.311
1.300
1.288
1.277
1.245
1.205
0.889
0.877
0.865
0.000
O
PinB
BPin
1f

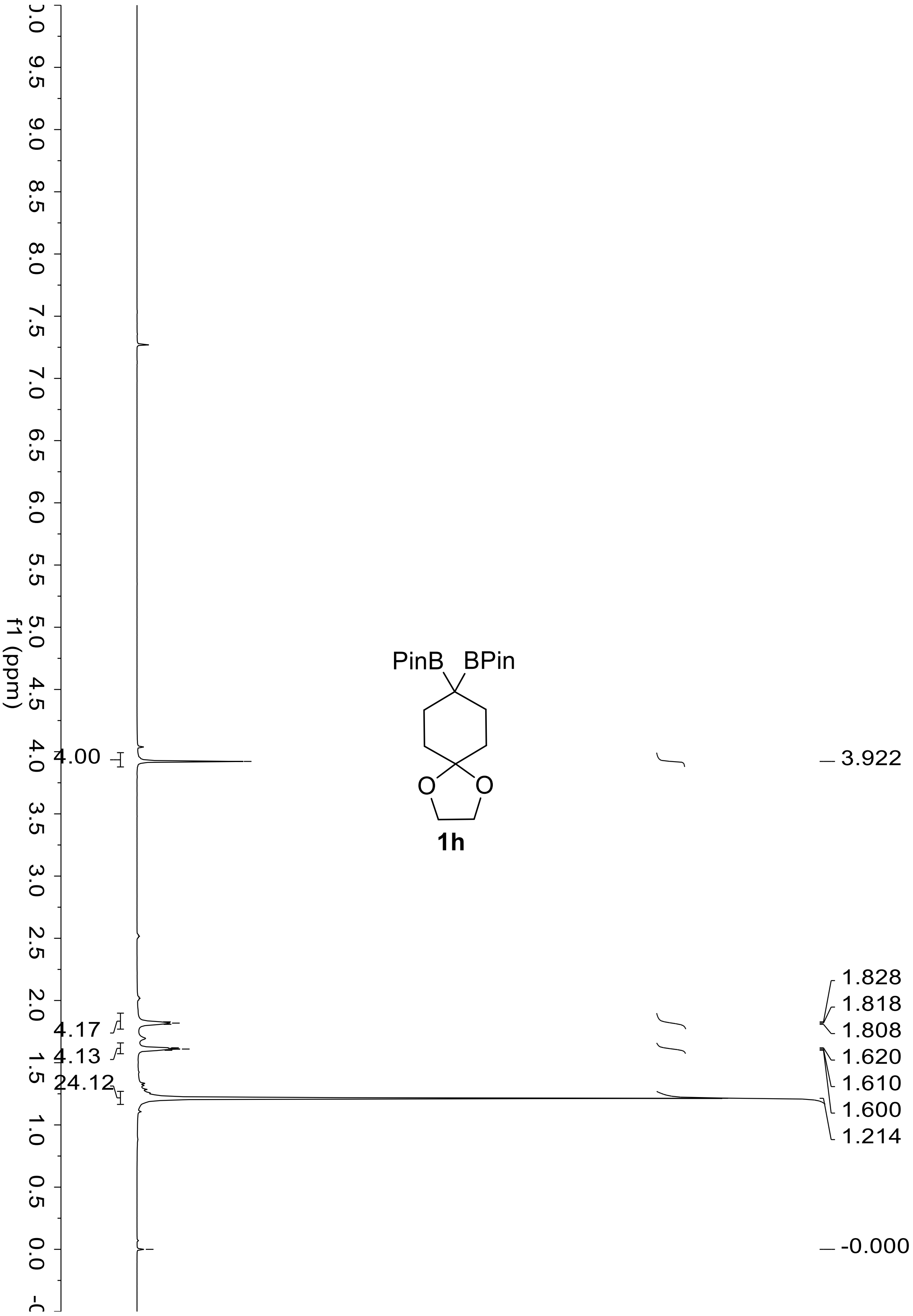


00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
157.5
134.0
130.6
113.0
83.1
77.2
77.0
76.8
55.2
33.5
29.5
28.3
25.0
24.7
23.4
14.3
O
PinB
BPin
1f


PinB
BPin
N
Bn
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)
4.39
1.00
2.00
3.87
4.00
24.27
7.297
7.286
7.283
7.274
7.265
7.261
7.223
7.220
7.216
7.213
7.209
7.204
7.201
7.198
3.442
2.356
2.355
1.814
1.805
1.795
1.196
0.000

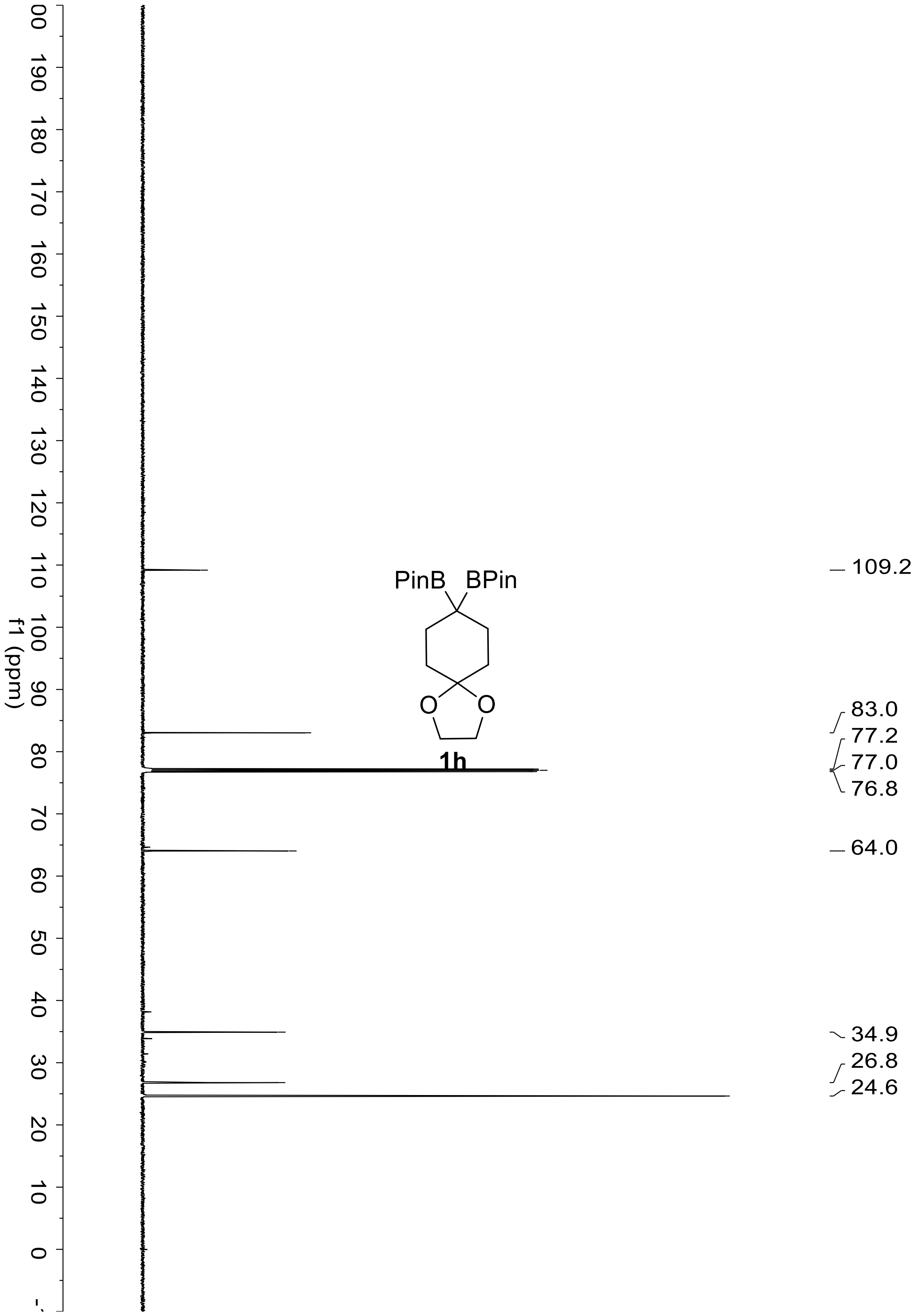
1g


PinB BPin
N
Bn
1g
138.2
129.3
127.9
126.6
82.9
77.2
77.0
76.8
63.9
54.1
28.7
24.8
24.6
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

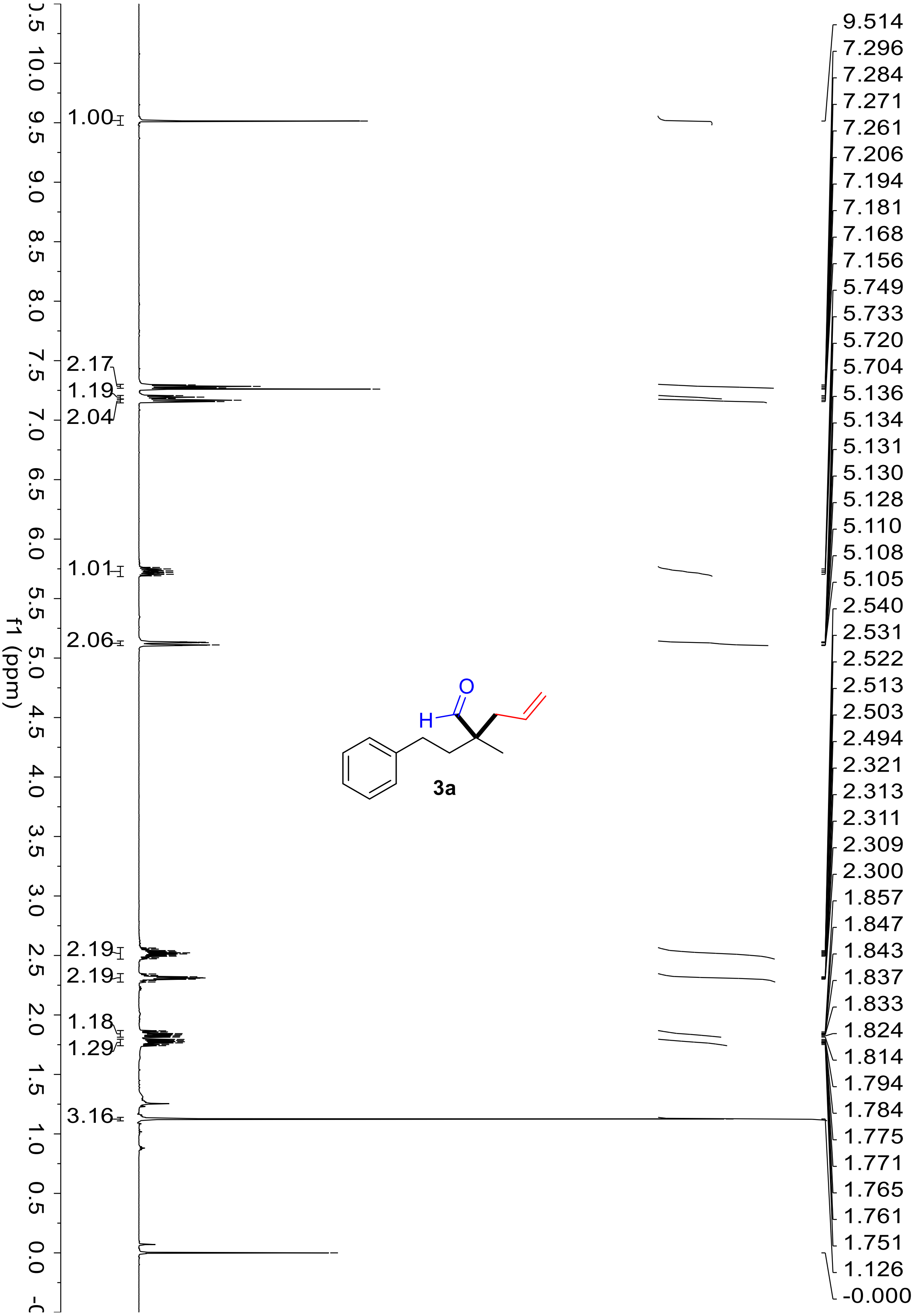


PinB BPin
O O
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
4.00
4.17
4.13
24.12
3.922
1.828
1.818
1.808
1.620
1.610
1.600
1.214
-0.000

1h

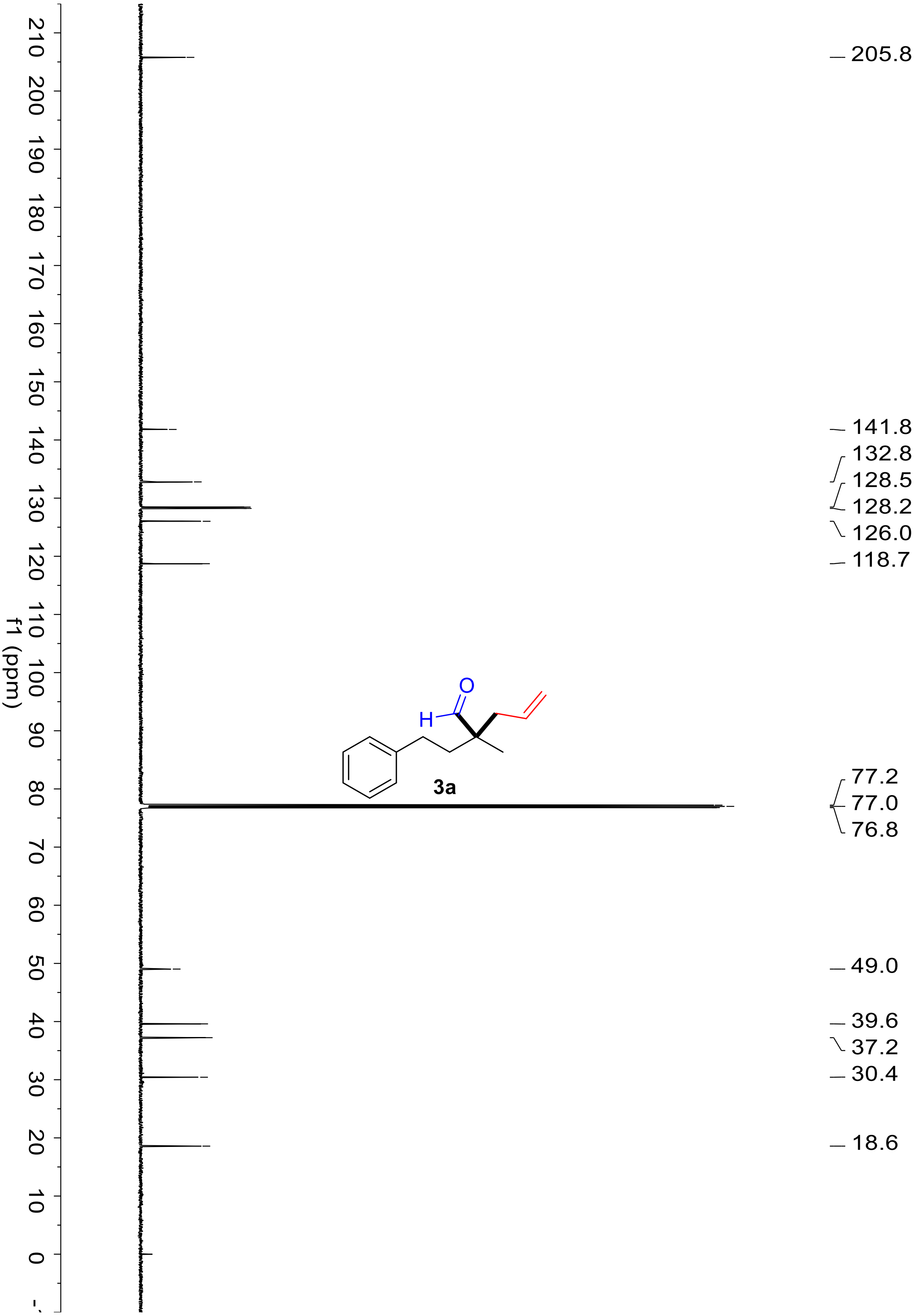

PinB
BPin
O
O
109.2
83.0
77.2
77.0
76.8
64.0
34.9
26.8
24.6
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

1h

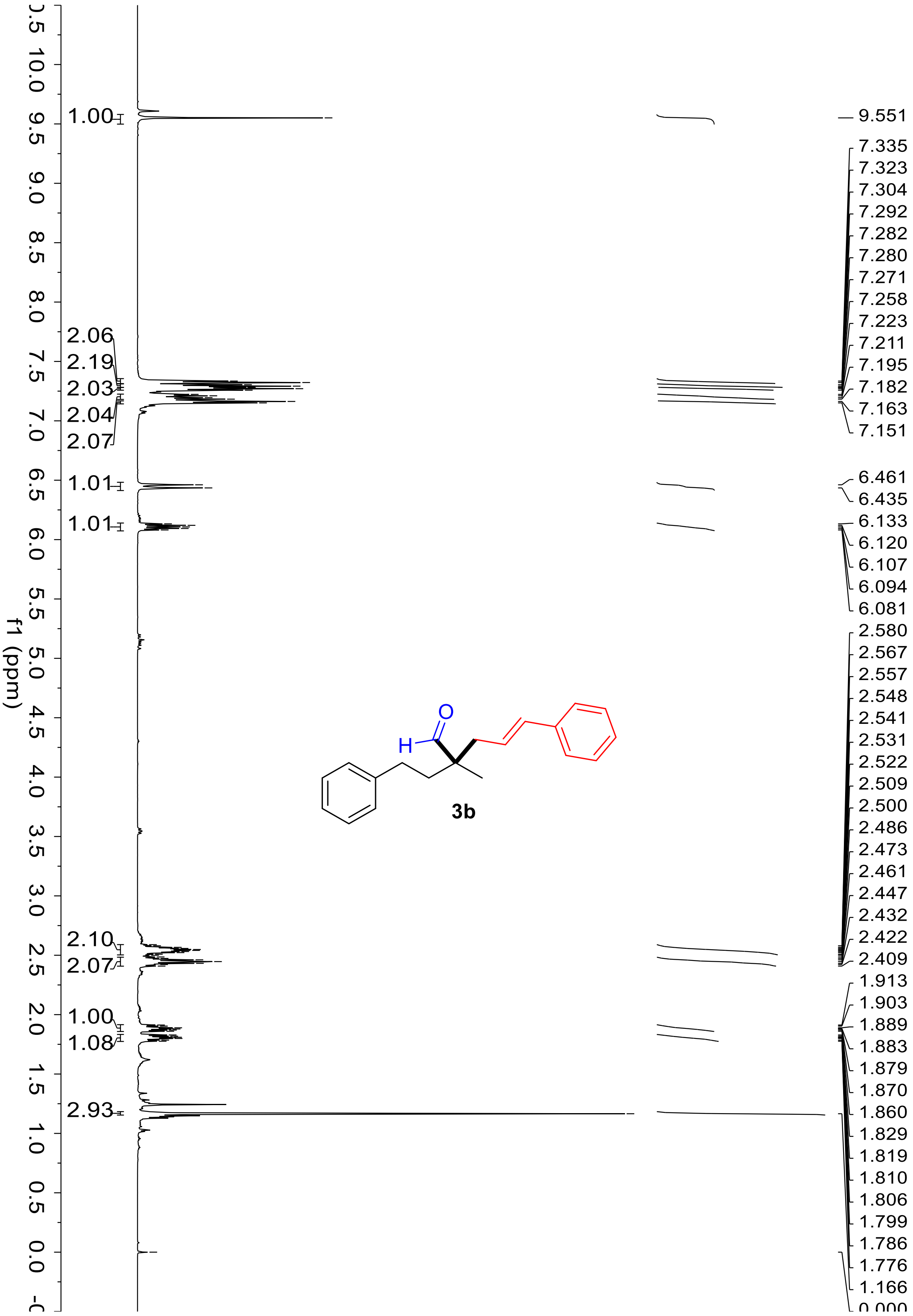


3a

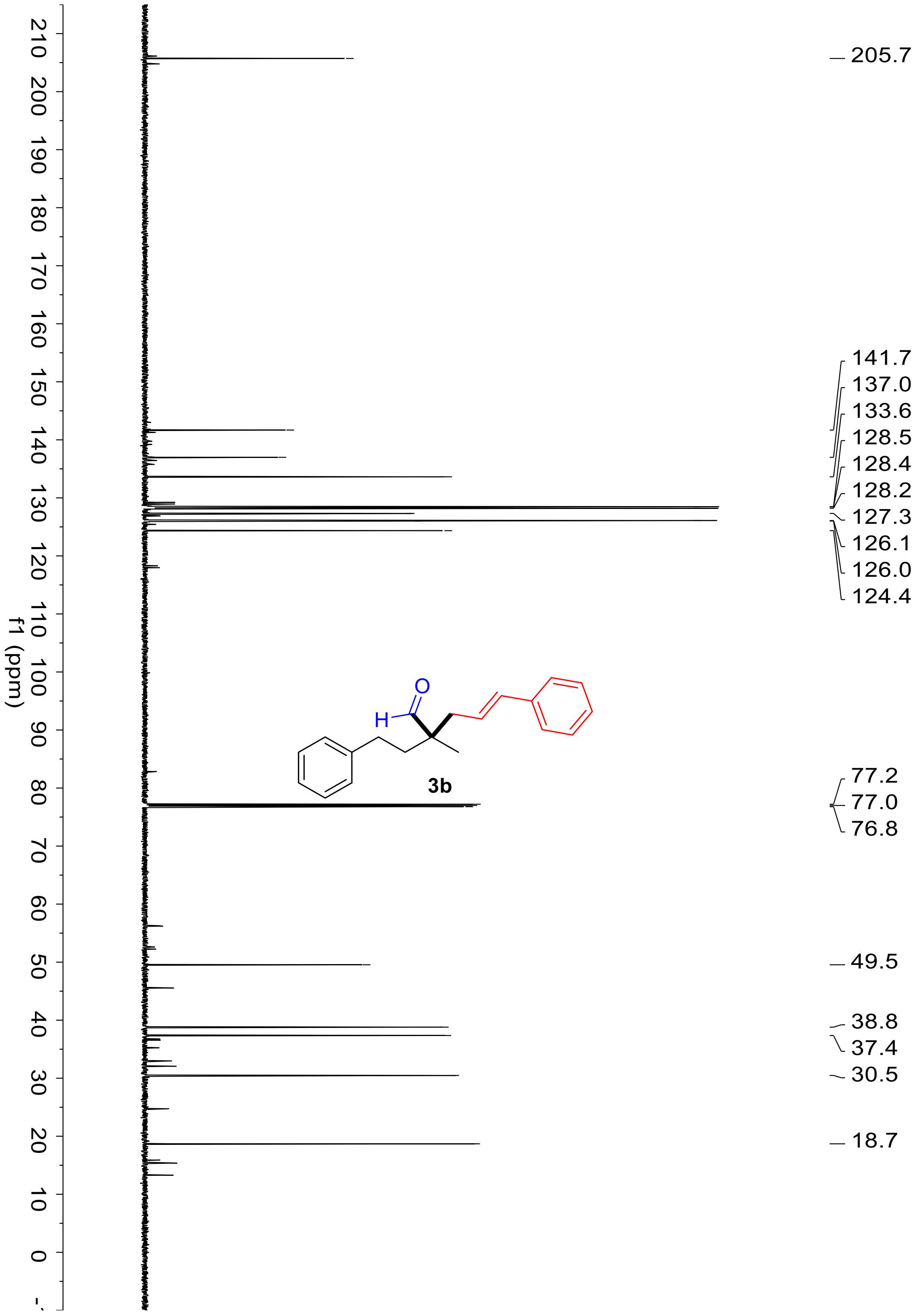
9.514
7.296
7.284
7.271
7.261
7.206
7.194
7.181
7.168
7.156
5.749
5.733
5.720
5.704
5.136
5.134
5.131
5.130
5.128
5.110
5.108
5.105
2.540
2.531
2.522
2.513
2.503
2.494
2.321
2.313
2.311
2.309
2.300
1.857
1.847
1.843
1.837
1.833
1.824
1.814
1.794
1.784
1.775
1.771
1.765
1.761
1.751
1.126
-0.000
1.00
2.17
1.19
2.04
1.01
2.06
2.19
2.19
1.18
1.29
3.16
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)
O
H

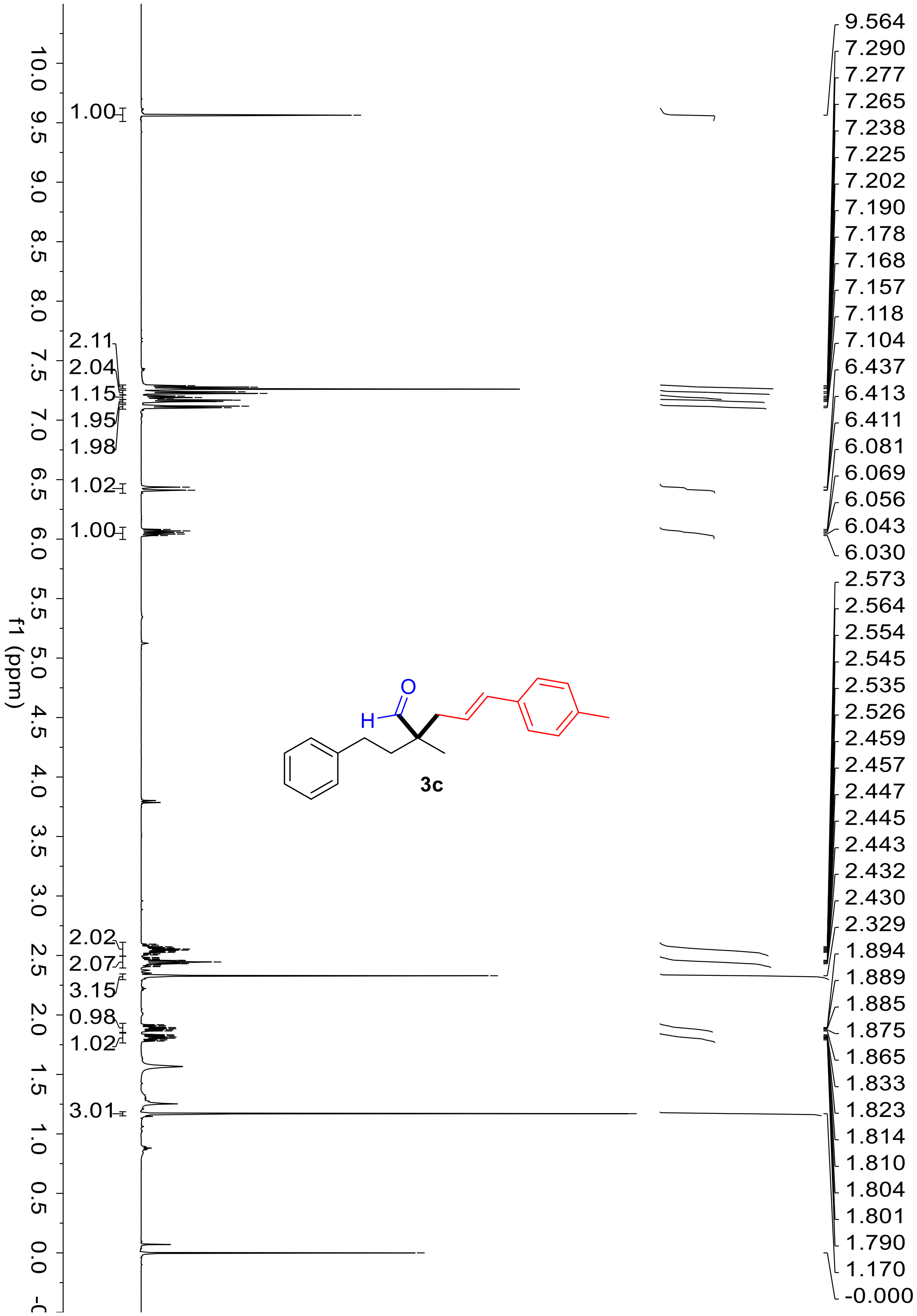

3a

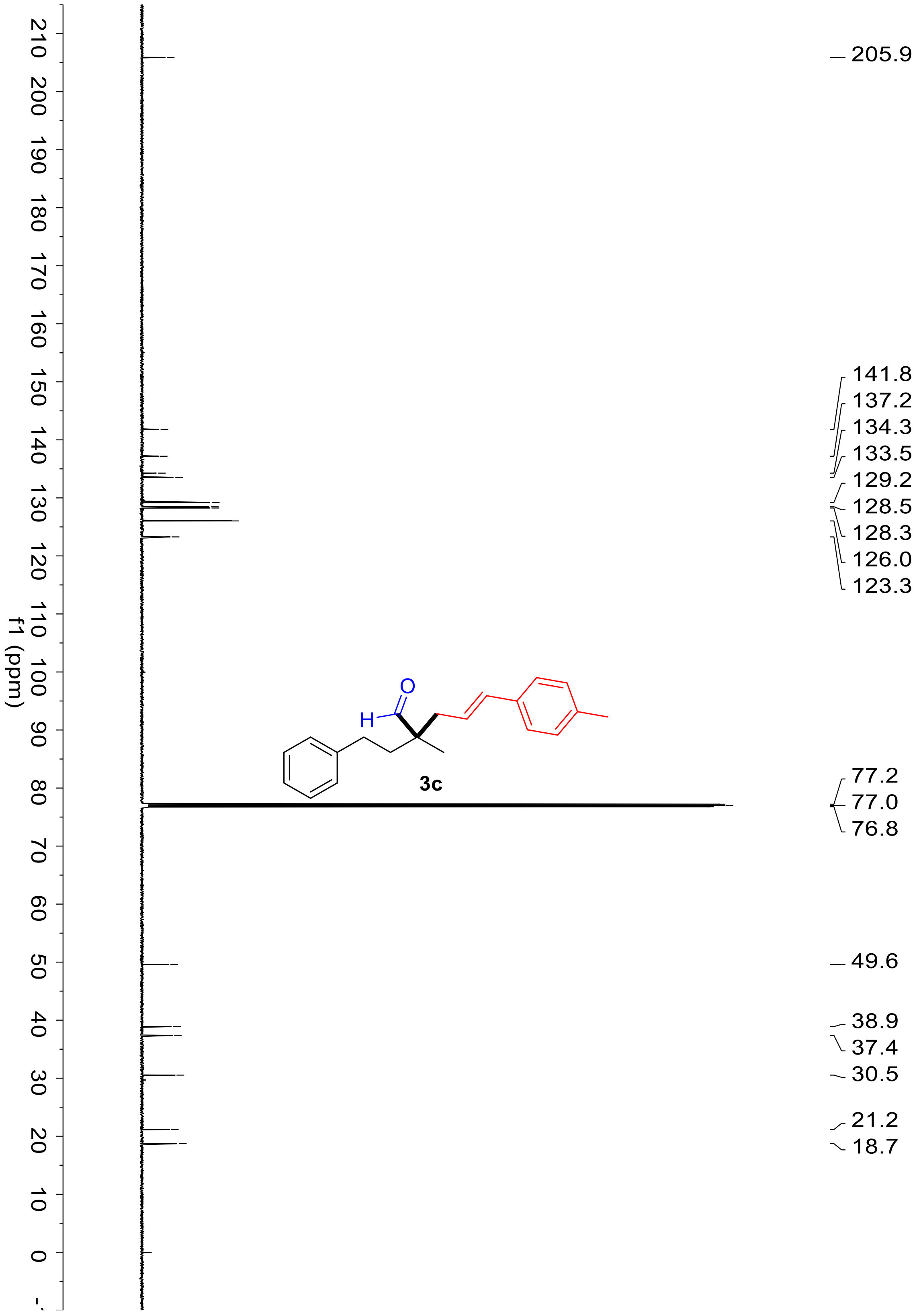
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
205.8
141.8
132.8
128.5
128.2
126.0
118.7
77.2
77.0
76.8
49.0
39.6
37.2
30.4
18.6
H
O



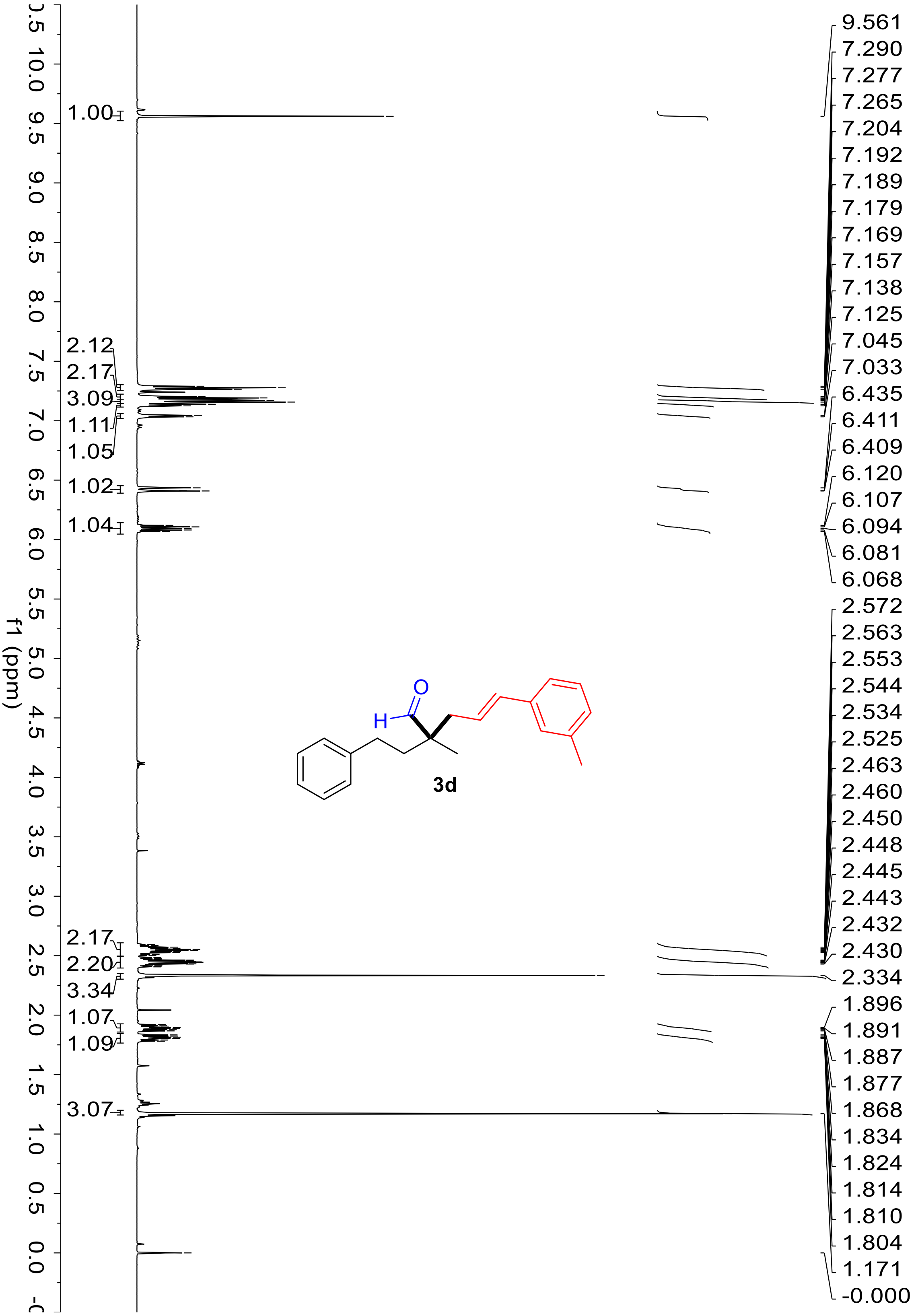
f1 (ppm)
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1.00
2.06
2.19
2.03
2.04
2.07
1.01
1.01
2.10
2.07
1.00
1.08
2.93
9.551
7.335
7.323
7.304
7.292
7.282
7.280
7.271
7.258
7.223
7.211
7.195
7.182
7.163
7.151
6.461
6.435
6.133
6.120
6.107
6.094
6.081
2.580
2.567
2.557
2.548
2.541
2.531
2.522
2.509
2.500
2.486
2.473
2.461
2.447
2.432
2.422
2.409
1.913
1.903
1.889
1.883
1.879
1.870
1.860
1.829
1.819
1.810
1.806
1.799
1.786
1.776
1.166
0.000
O
H
3b

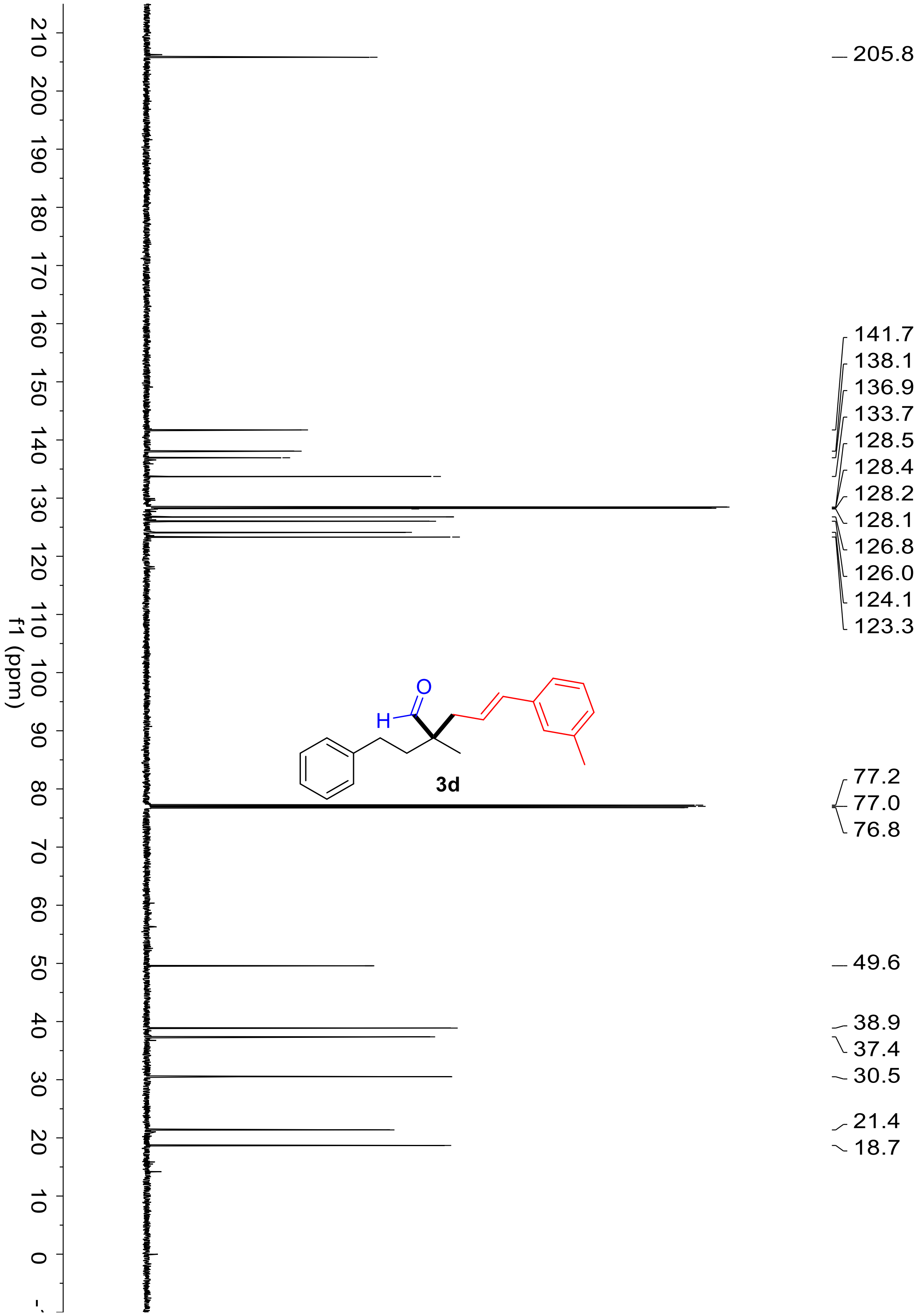

205.7
141.7
137.0
133.6
128.5
128.4
128.2
127.3
126.1
126.0
124.4
77.2
77.0
76.8
49.5
38.8
37.4
30.5
18.7
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
O
H
3b


9.564
7.290
7.277
7.265
7.238
7.225
7.202
7.190
7.178
7.168
7.157
7.118
7.104
6.437
6.413
6.411
6.081
6.069
6.056
6.043
6.030
2.573
2.564
2.554
2.545
2.535
2.526
2.459
2.457
2.447
2.445
2.443
2.432
2.430
2.329
1.894
1.889
1.885
1.875
1.865
1.833
1.823
1.814
1.810
1.804
1.801
1.790
1.170
-0.000
1.00
2.11
2.04
1.15
1.95
1.98
1.02
1.00
2.02
2.07
3.15
0.98
1.02
3.01
O
H
3c
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)

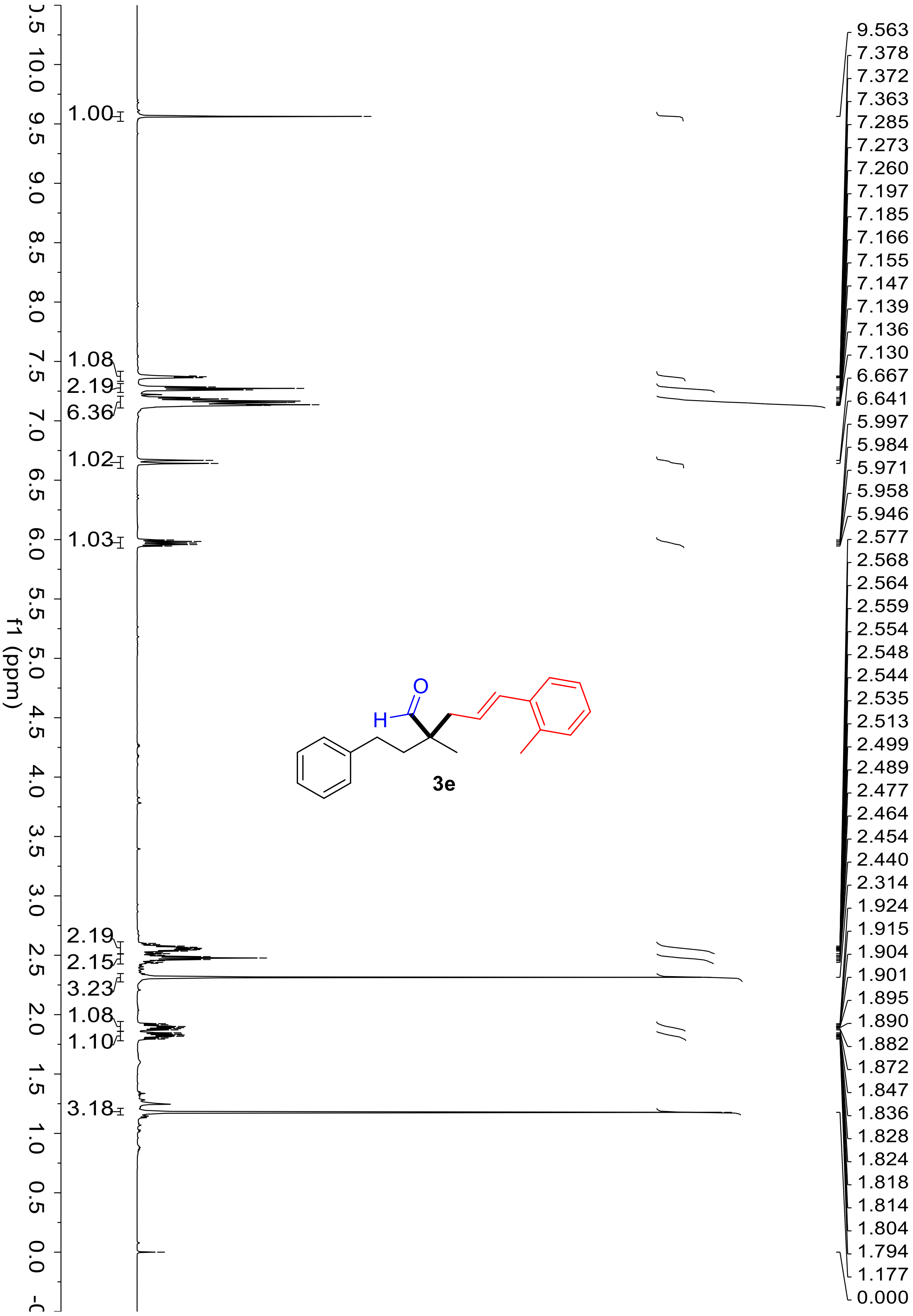

205.9
141.8
137.2
134.3
133.5
129.2
128.5
128.3
126.0
123.3
77.2
77.0
76.8
49.6
38.9
37.4
30.5
21.2
18.7
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
H

3c


3d
O
H
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
1.00
2.12
2.17
3.09
1.11
1.05
1.02
1.04
2.17
2.20
3.34
1.07
1.09
3.07
9.561
7.290
7.277
7.265
7.204
7.192
7.189
7.179
7.169
7.157
7.138
7.125
7.045
7.033
6.435
6.411
6.409
6.120
6.107
6.094
6.081
6.068
2.572
2.563
2.553
2.544
2.534
2.525
2.463
2.460
2.450
2.448
2.445
2.443
2.432
2.430
2.334
1.896
1.891
1.887
1.877
1.868
1.834
1.824
1.814
1.810
1.804
1.171
-0.000


3d

205.8
141.7
138.1
136.9
133.7
128.5
128.4
128.2
128.1
126.8
126.0
124.1
123.3
77.2
77.0
76.8
49.6
38.9
37.4
30.5
21.4
18.7
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
H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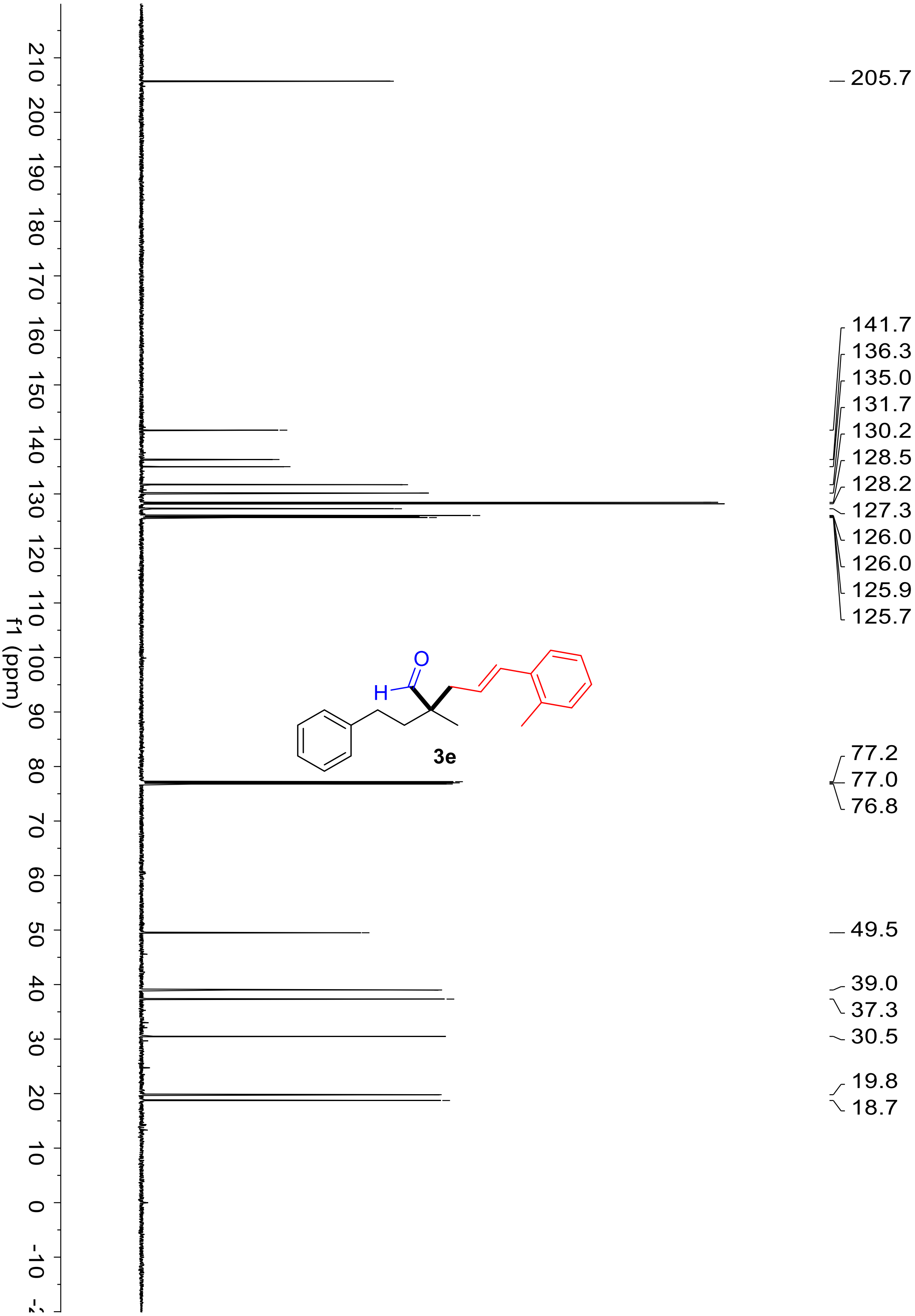
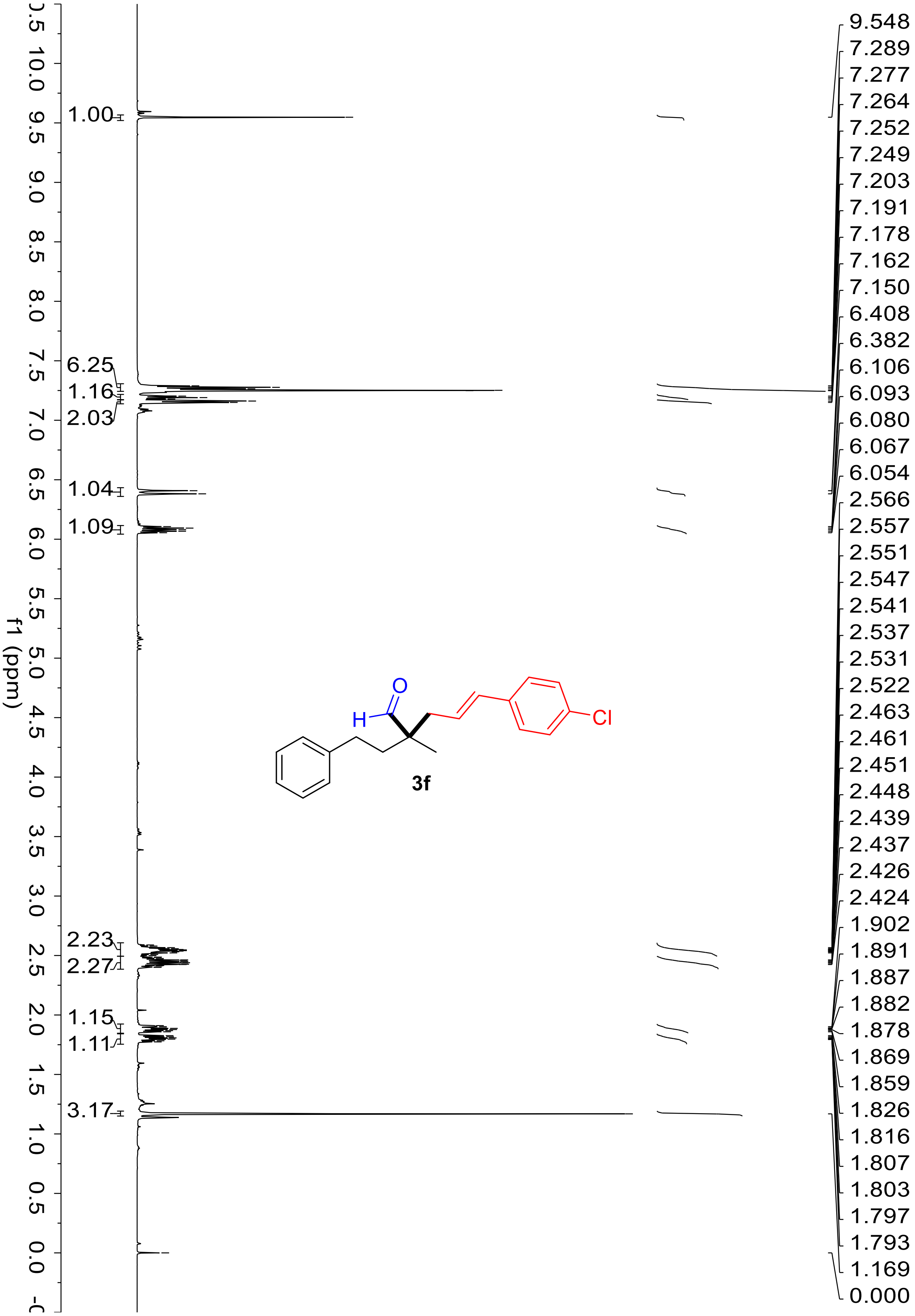
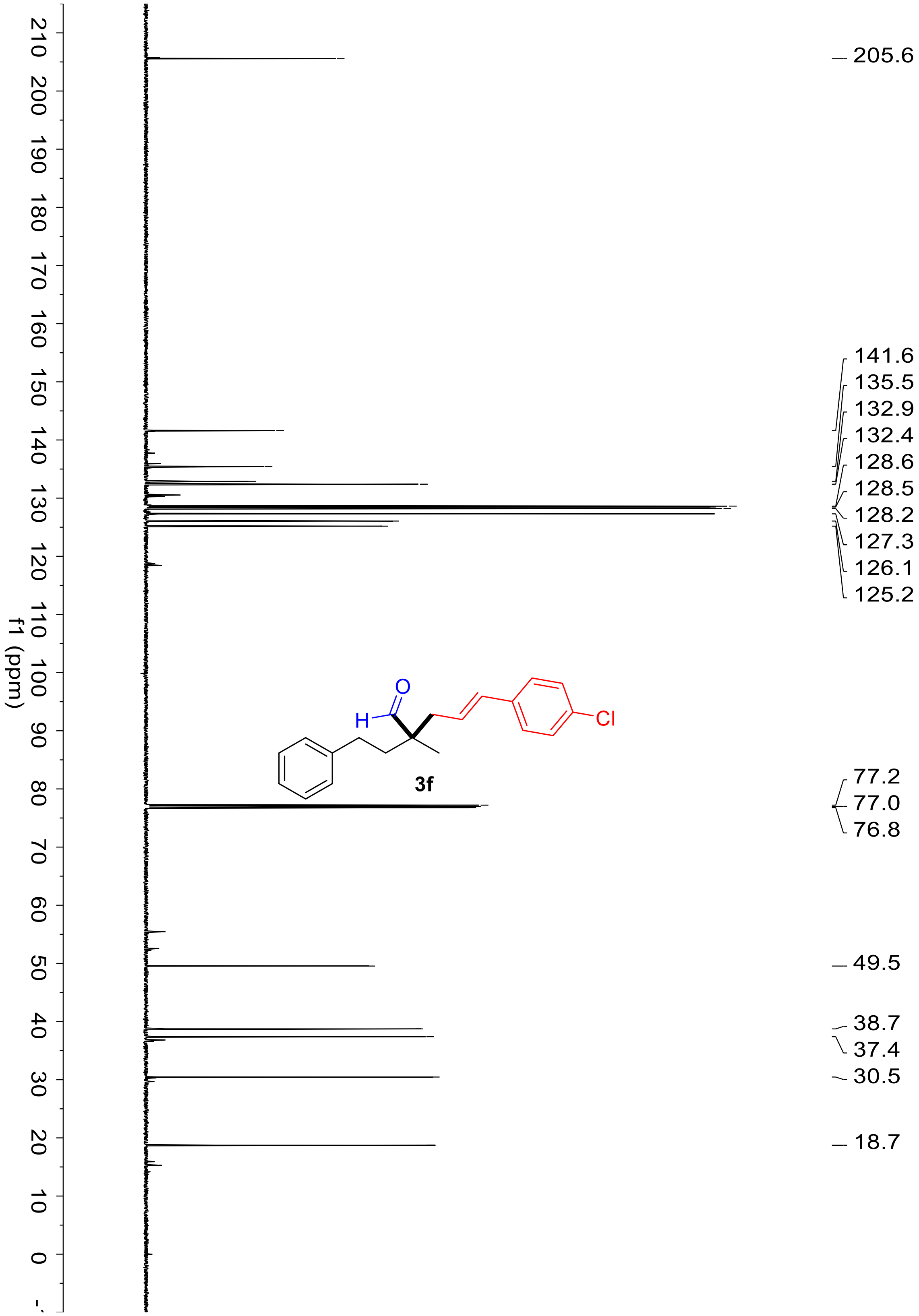
7.372
7.363
7.285
7.273
7.260
7.197
7.185
7.166
7.155
7.147
7.139
7.136
7.130
6.667
6.641
5.997
5.984
5.971
5.958
5.946
2.577
2.568
2.564
2.559
2.554
2.548
2.544
2.535
2.513
2.499
2.489
2.477
2.464
2.454
2.440
2.314
1.924
1.915
1.904
1.901
1.895
1.890
1.882
1.872
1.847
1.836
1.828
1.824
1.818
1.814
1.804
1.794
1.177
0.000
1.00
1.08
2.19
6.36
1.02
1.03
2.19
2.15
3.23
1.08
1.10
3.18
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)
O
H
3e



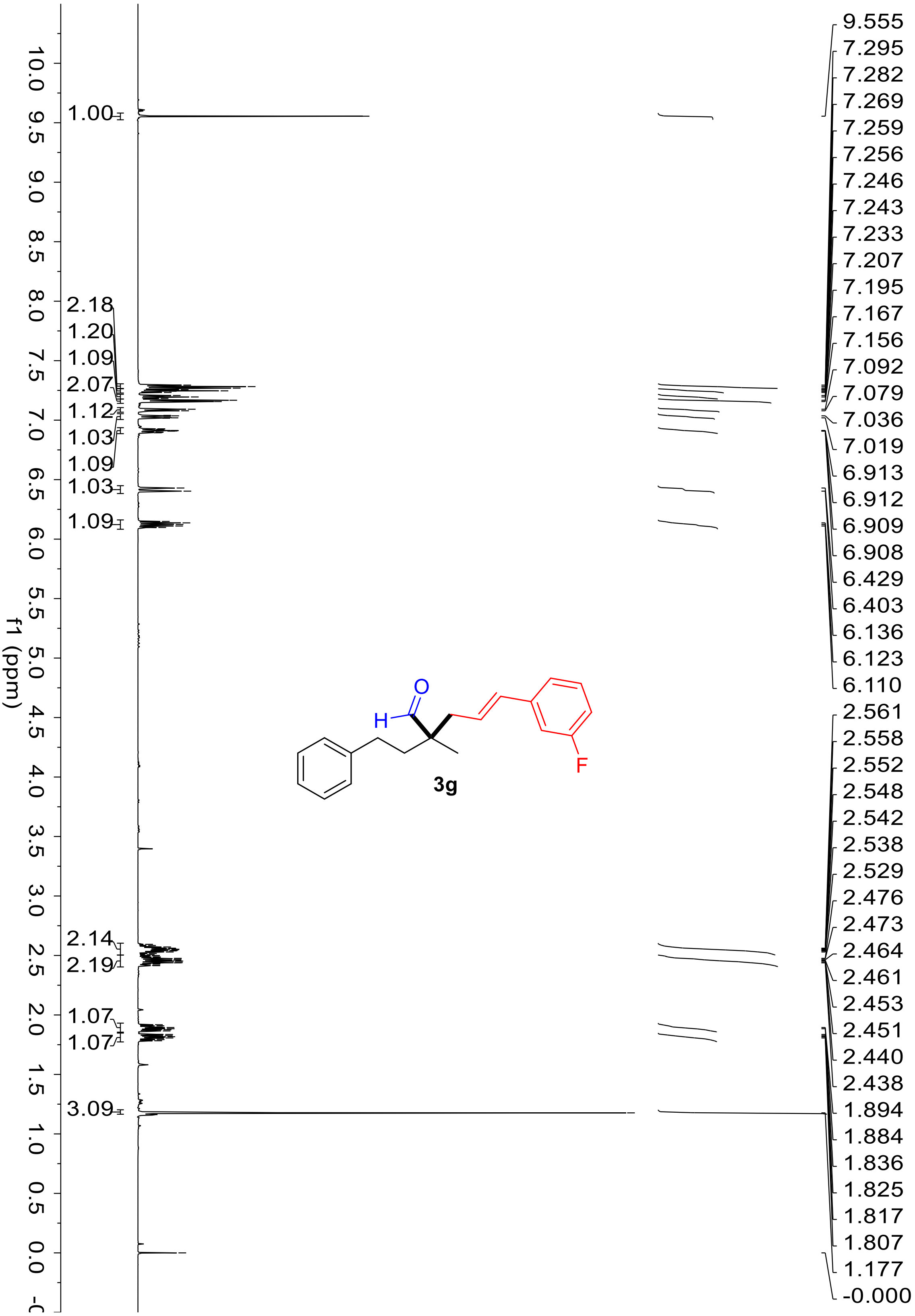
205.7
141.7
136.3
135.0
131.7
130.2
128.5
128.2
127.3
126.0
126.0
125.9
125.7
77.2
77.0
76.8
49.5
39.0
37.3
30.5
19.8
18.7
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
O
H
3e



9.548
7.289
7.277
7.264
7.252
7.249
7.203
7.191
7.178
7.162
7.150
6.408
6.382
6.106
6.093
6.080
6.067
6.054
2.566
2.557
2.551
2.547
2.541
2.537
2.531
2.522
2.463
2.461
2.451
2.448
2.439
2.437
2.426
2.424
1.902
1.891
1.887
1.882
1.878
1.869
1.859
1.826
1.816
1.807
1.803
1.797
1.793
1.169
0.000
1.00
6.25
1.16
2.03
1.04
1.09
2.23
2.27
1.15
1.11
3.17
f1 (ppm)
O
H
Cl
3f


205.6
141.6
135.5
132.9
132.4
128.6
128.5
128.2
127.3
126.1
125.2
77.2
77.0
76.8
49.5
38.7
37.4
30.5
18.7
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
O
H
Cl

3f


9.555
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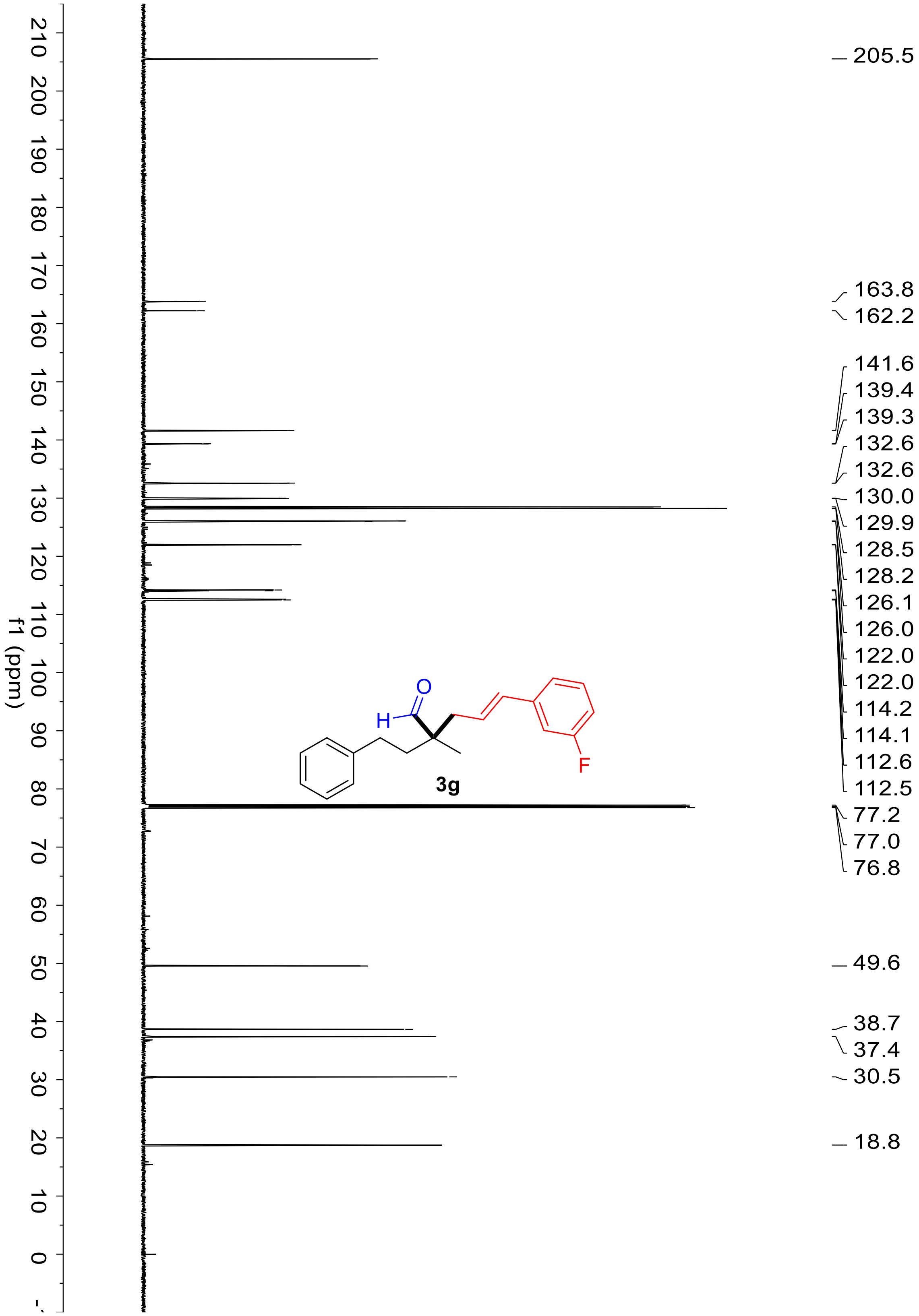
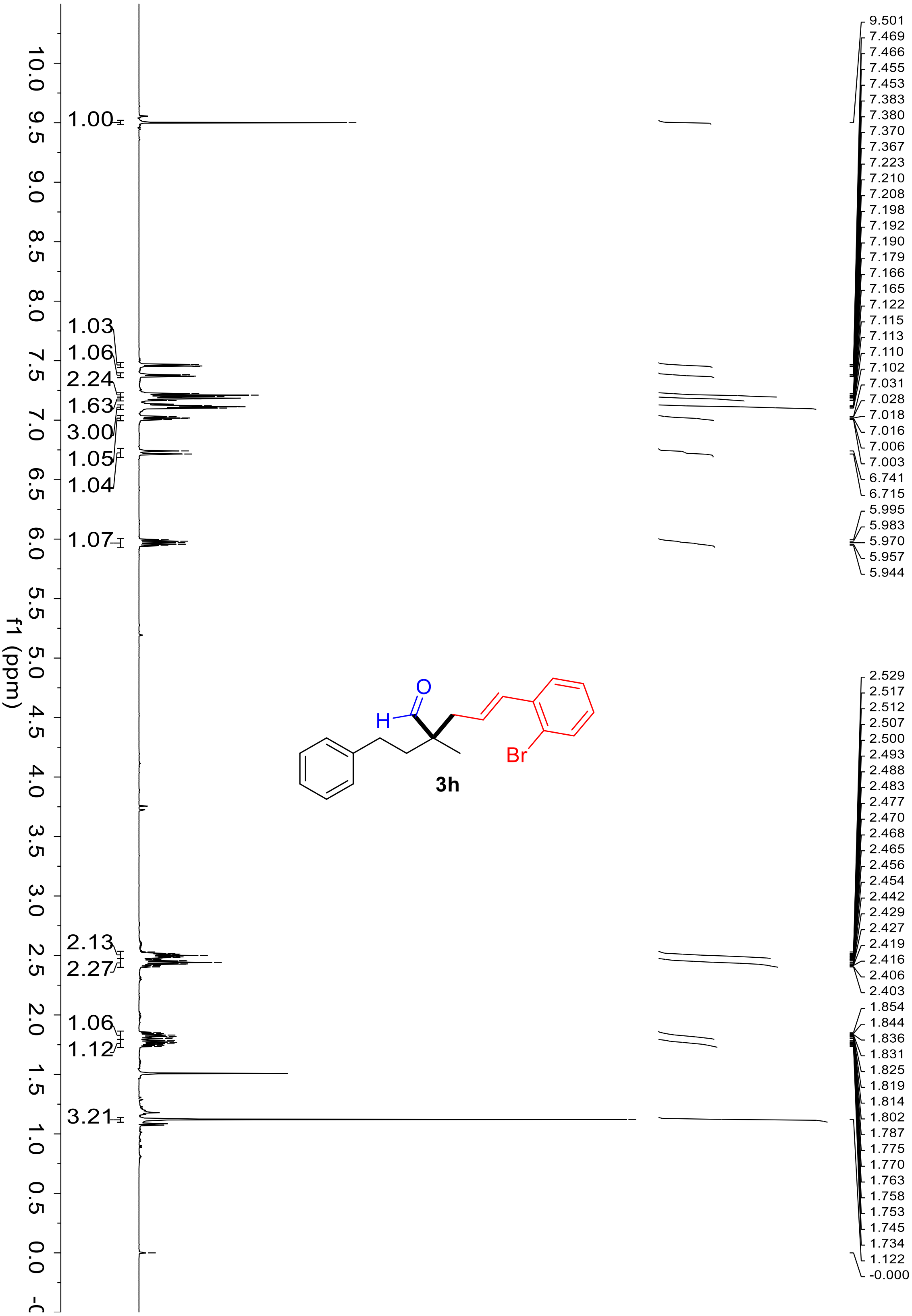
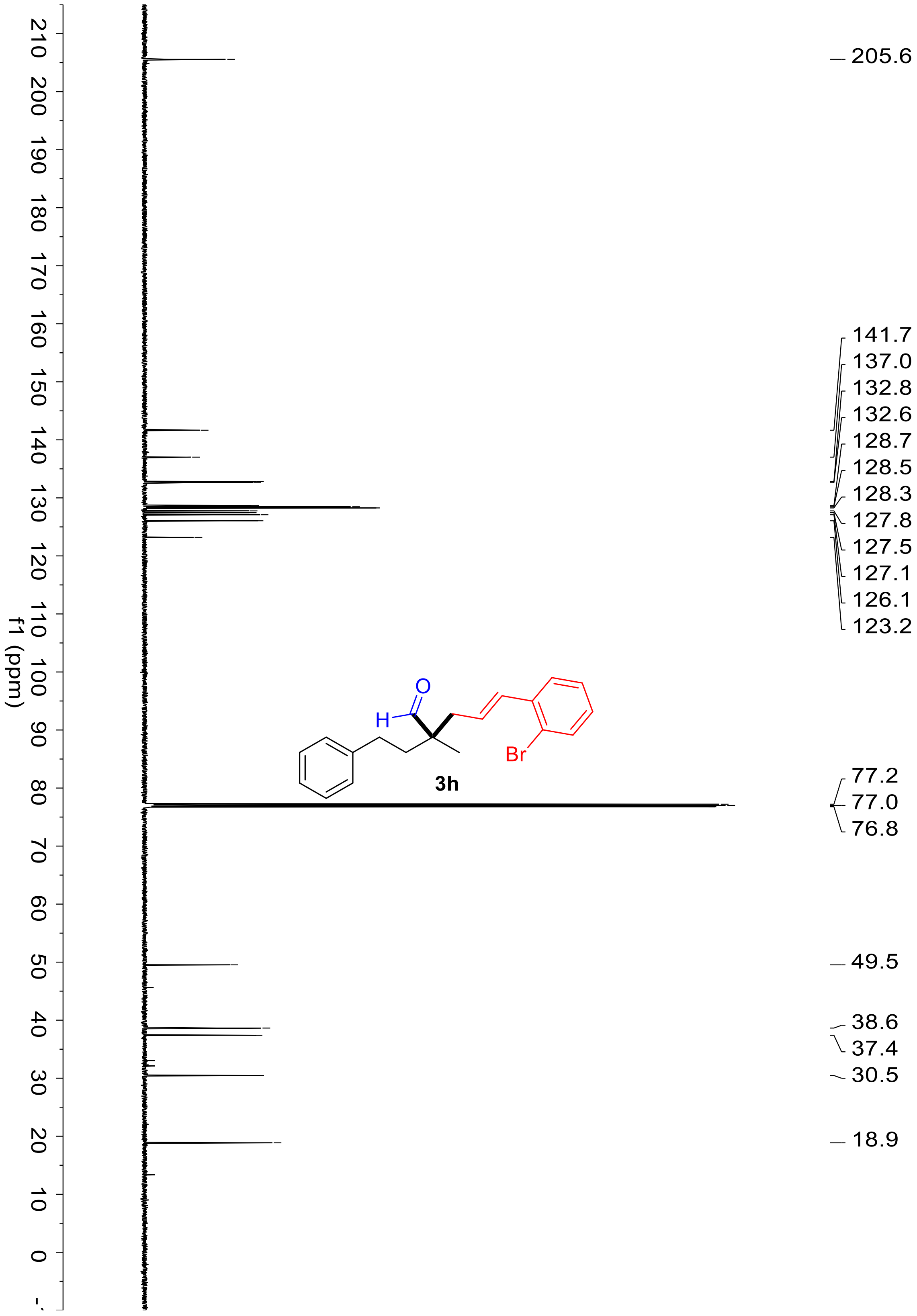
7.269
7.259
7.256
7.246
7.243
7.233
7.207
7.195
7.167
7.156
7.092
7.079
7.036
7.019
6.913
6.912
6.909
6.908
6.429
6.403
6.136
6.123
6.110
2.561
2.558
2.552
2.548
2.542
2.538
2.529
2.476
2.473
2.464
2.461
2.453
2.451
2.440
2.438
1.894
1.884
1.836
1.825
1.817
1.807
1.177
-0.000
1.00
2.18
1.20
1.09
2.07
1.12
1.03
1.09
1.03
1.09
2.14
2.19
1.07
1.07
3.09
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)
O
H
F
3g


205.5
163.8
162.2
141.6
139.4
139.3
132.6
132.6
130.0
129.9
128.5
128.2
126.1
126.0
122.0
122.0
114.2
114.1
112.6
112.5
77.2
77.0
76.8
49.6
38.7
37.4
30.5
18.8
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
O
H
F

3g



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
1.03
1.06
2.24
1.63
3.00
1.05
1.04
1.07
2.13
2.27
1.06
1.12
3.21
9.501
7.469
7.466
7.455
7.453
7.383
7.380
7.370
7.367
7.223
7.210
7.208
7.198
7.192
7.190
7.179
7.166
7.165
7.122
7.115
7.113
7.110
7.102
7.031
7.028
7.018
7.016
7.006
7.003
6.741
6.715
5.995
5.983
5.970
5.957
5.944
2.529
2.517
2.512
2.507
2.500
2.493
2.488
2.483
2.477
2.470
2.468
2.465
2.456
2.454
2.442
2.429
2.427
2.419
2.416
2.406
2.403
1.854
1.844
1.836
1.831
1.825
1.819
1.814
1.802
1.787
1.775
1.770
1.763
1.758
1.753
1.745
1.734
1.122
-0.000
O
H
Br
3h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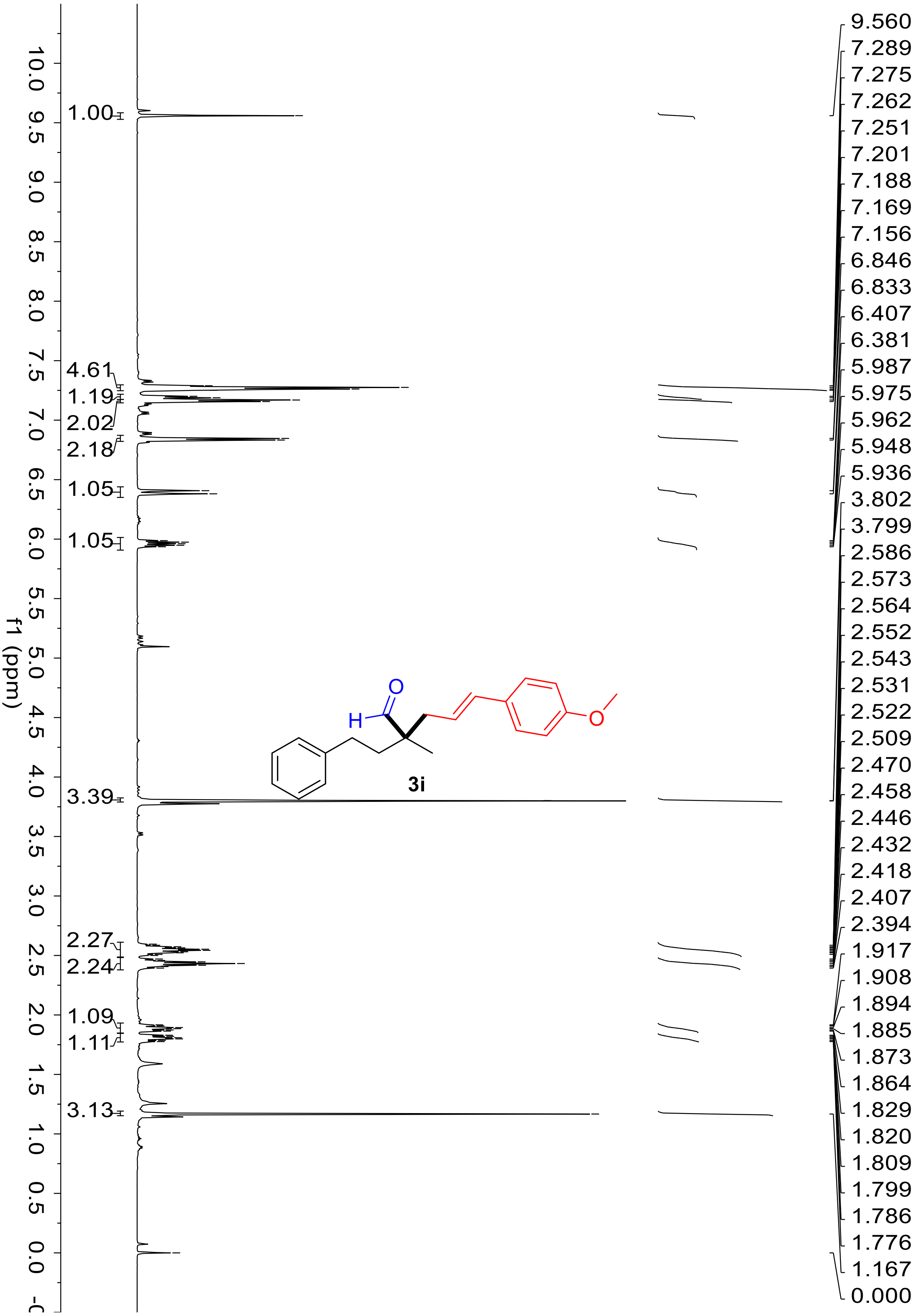
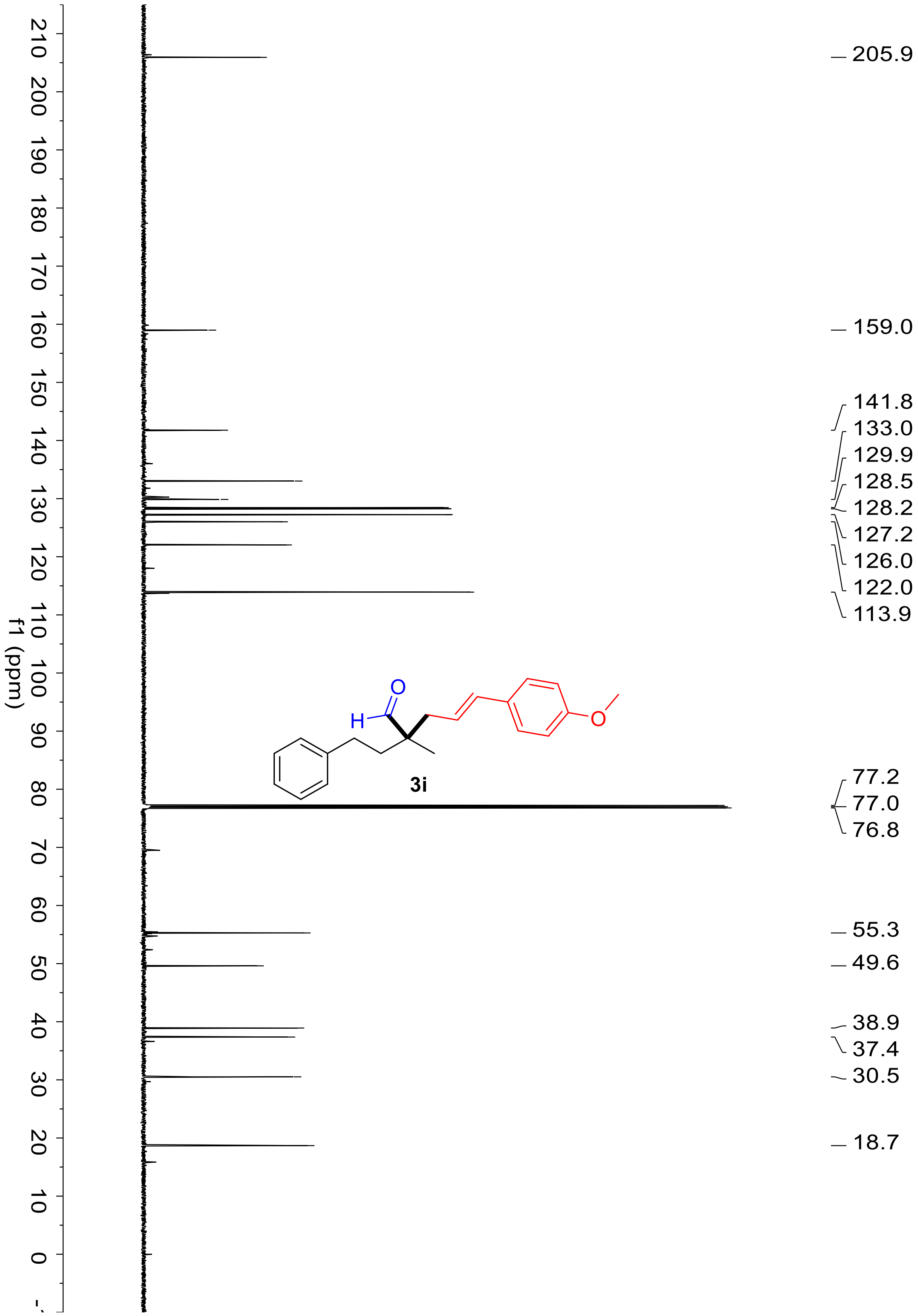
137.0
132.8
132.6
128.7
128.5
128.3
127.8
127.5
127.1
126.1
123.2
77.2
77.0
76.8
49.5
38.6
37.4
30.5
18.9
O
H
Br
3h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


3i
O
H
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
1.00
4.61
1.19
2.02
2.18
1.05
1.05
3.39
2.27
2.24
1.09
1.11
3.13
9.560
7.289
7.275
7.262
7.251
7.201
7.188
7.169
7.156
6.846
6.833
6.407
6.381
5.987
5.975
5.962
5.948
5.936
3.802
3.799
2.586
2.573
2.564
2.552
2.543
2.531
2.522
2.509
2.470
2.458
2.446
2.432
2.418
2.407
2.394
1.917
1.908
1.894
1.885
1.873
1.864
1.829
1.820
1.809
1.799
1.786
1.776
1.167
0.000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159.0
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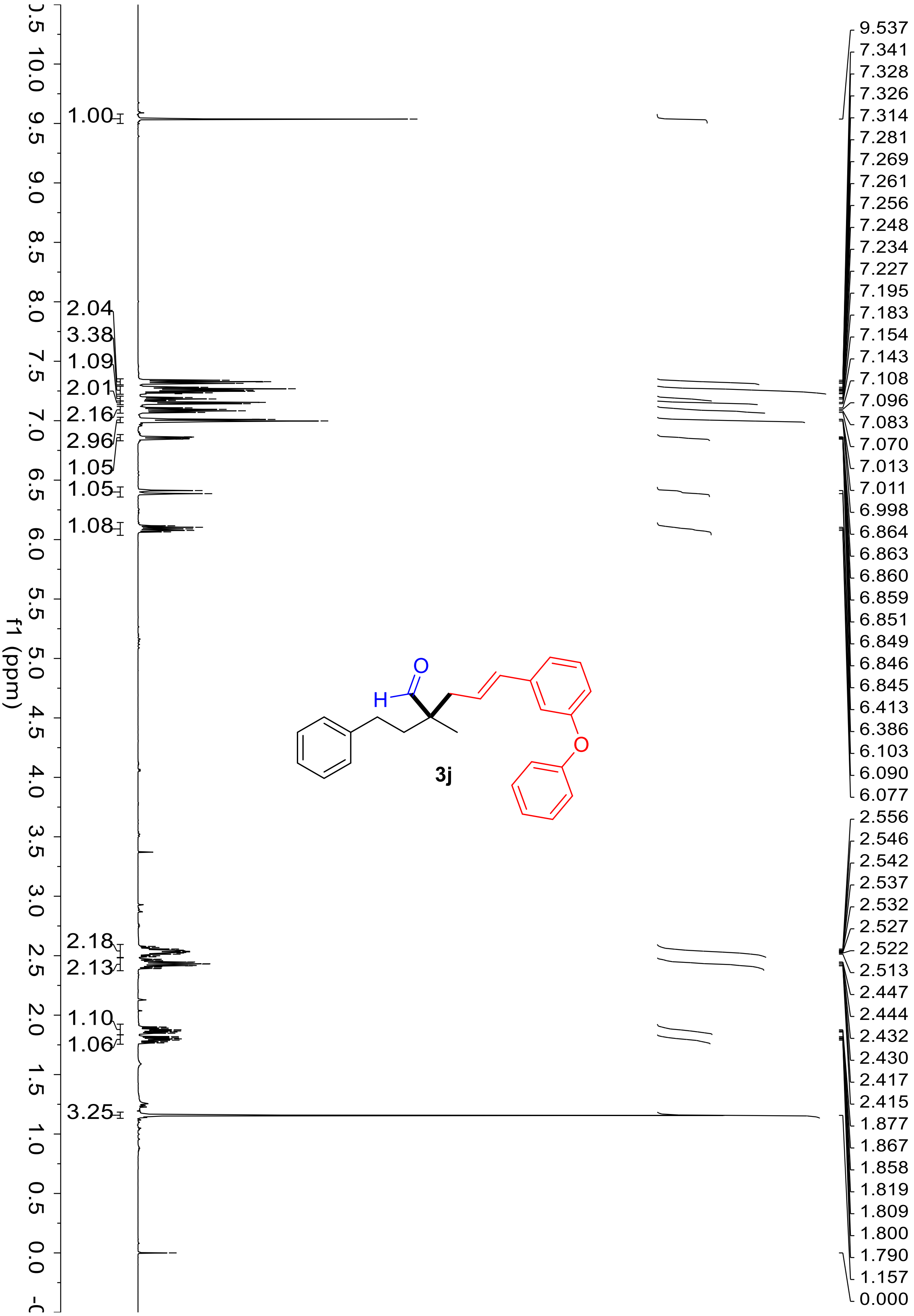
133.0
129.9
128.5
128.2
127.2
126.0
122.0
113.9
77.2
77.0
76.8
55.3
49.6
38.9
37.4
30.5
18.7
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
O
H
O
3i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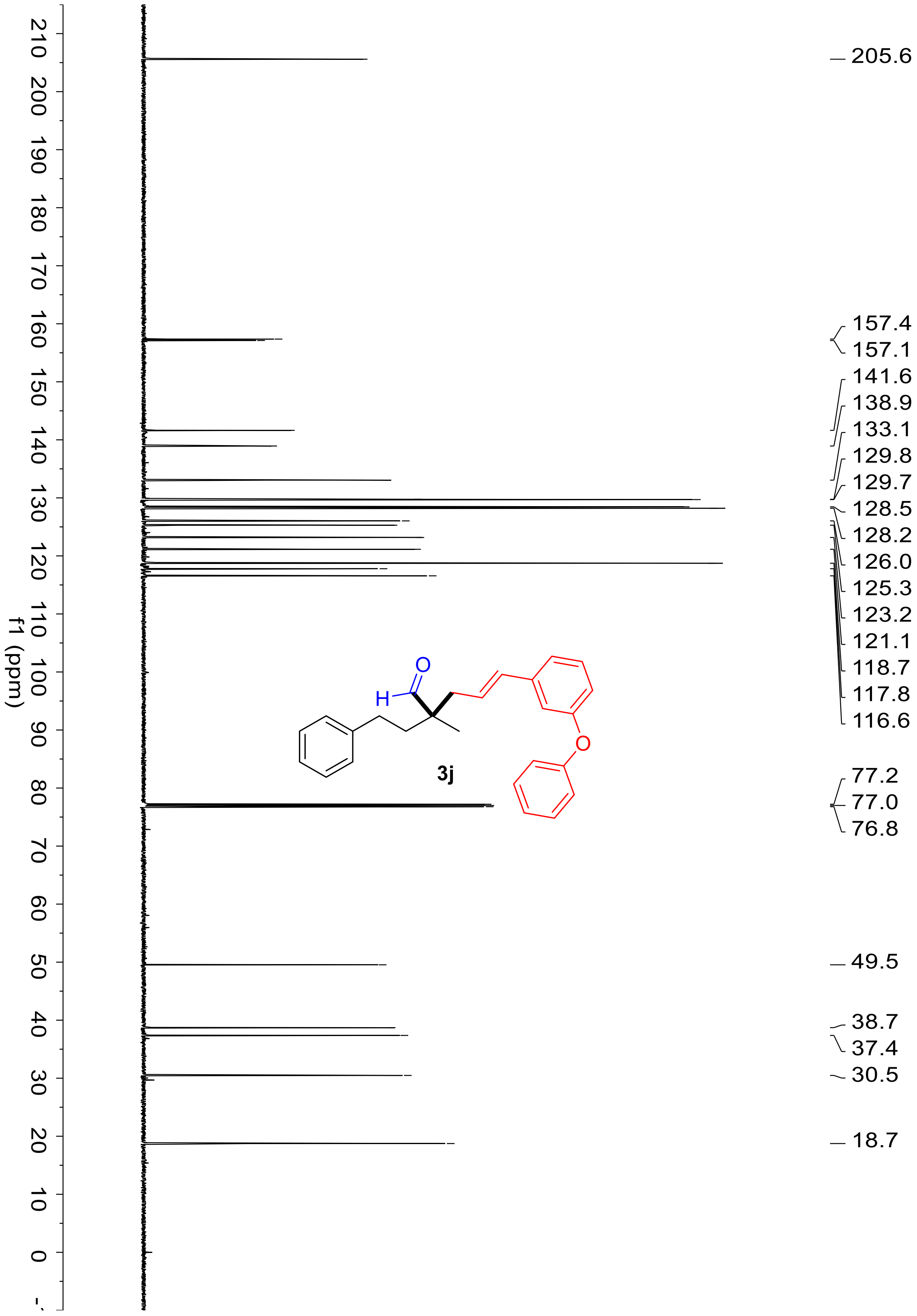
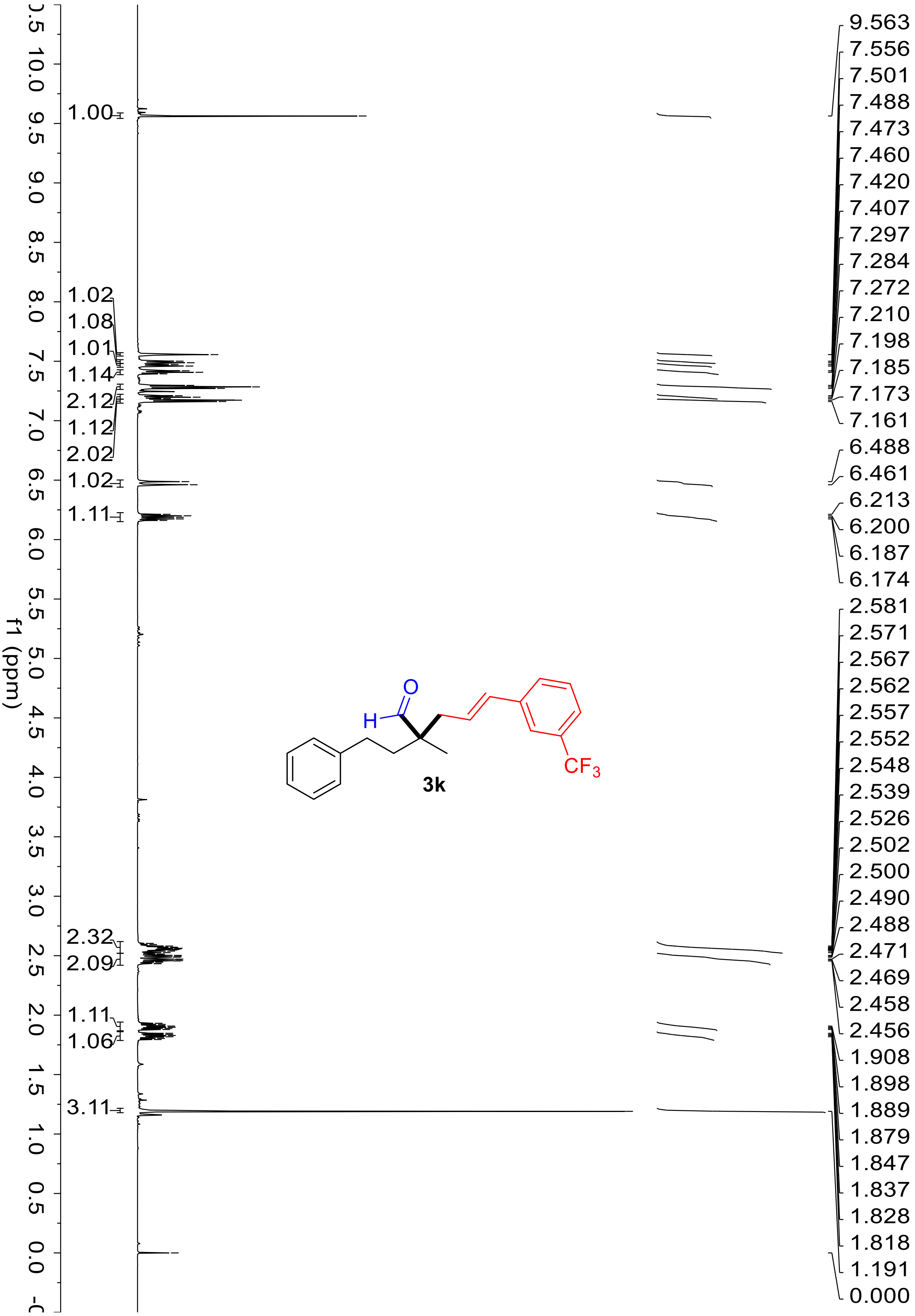
7.326
7.314
7.281
7.269
7.261
7.256
7.248
7.234
7.227
7.195
7.183
7.154
7.143
7.108
7.096
7.083
7.070
7.013
7.011
6.998
6.864
6.863
6.860
6.859
6.851
6.849
6.846
6.845
6.413
6.386
6.103
6.090
6.077
2.556
2.546
2.542
2.537
2.532
2.527
2.522
2.513
2.447
2.444
2.432
2.430
2.417
2.415
1.877
1.867
1.858
1.819
1.809
1.800
1.790
1.157
0.000
1.00
2.04
3.38
1.09
2.01
2.16
2.96
1.05
1.05
1.08
2.18
2.13
1.10
1.06
3.25
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)
O
H
O

3j


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
205.6
157.4
157.1
141.6
138.9
133.1
129.8
129.7
128.5
128.2
126.0
125.3
123.2
121.1
118.7
117.8
116.6
77.2
77.0
76.8
49.5
38.7
37.4
30.5
18.7
O
H
O

3j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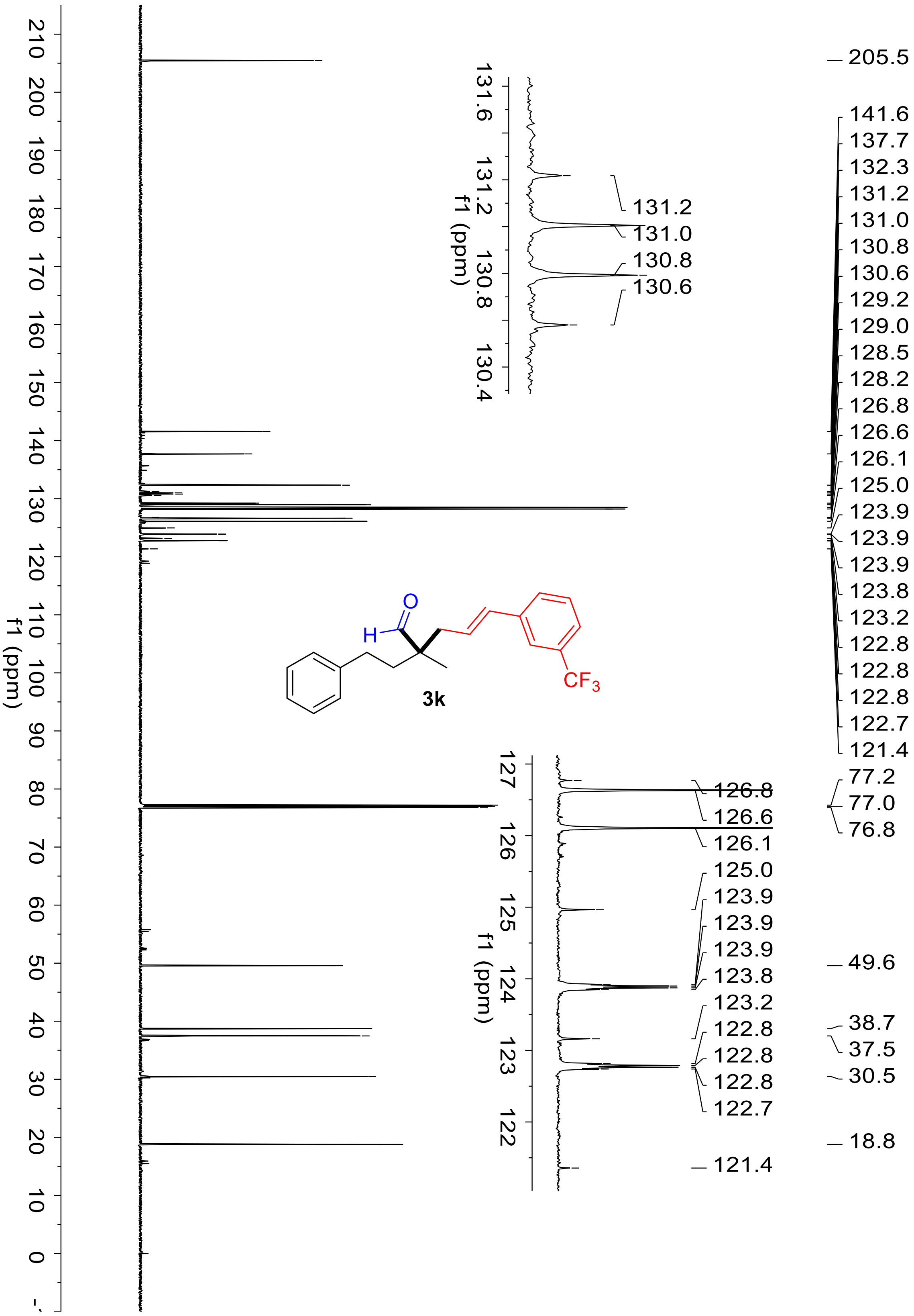
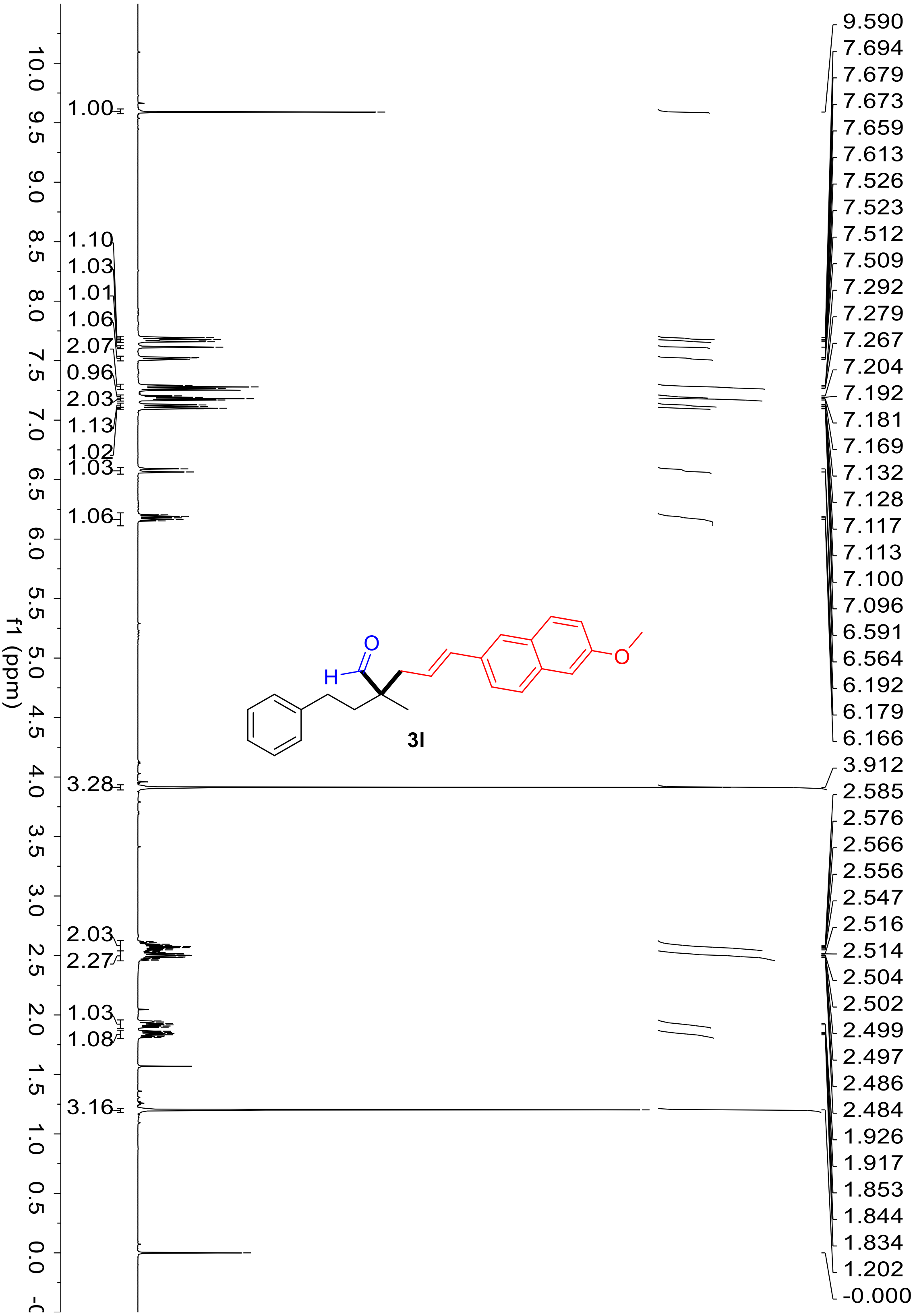
7.501
7.488
7.473
7.460
7.420
7.407
7.297
7.284
7.272
7.210
7.198
7.185
7.173
7.161
6.488
6.461
6.213
6.200
6.187
6.174
2.581
2.571
2.567
2.562
2.557
2.552
2.548
2.539
2.526
2.502
2.500
2.490
2.488
2.471
2.469
2.458
2.456
1.908
1.898
1.889
1.879
1.847
1.837
1.828
1.818
1.191
0.000
1.00
1.02
1.08
1.01
1.14
2.12
1.12
2.02
1.02
1.11
2.32
2.09
1.11
1.06
3.11
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)
O
H
CF_3

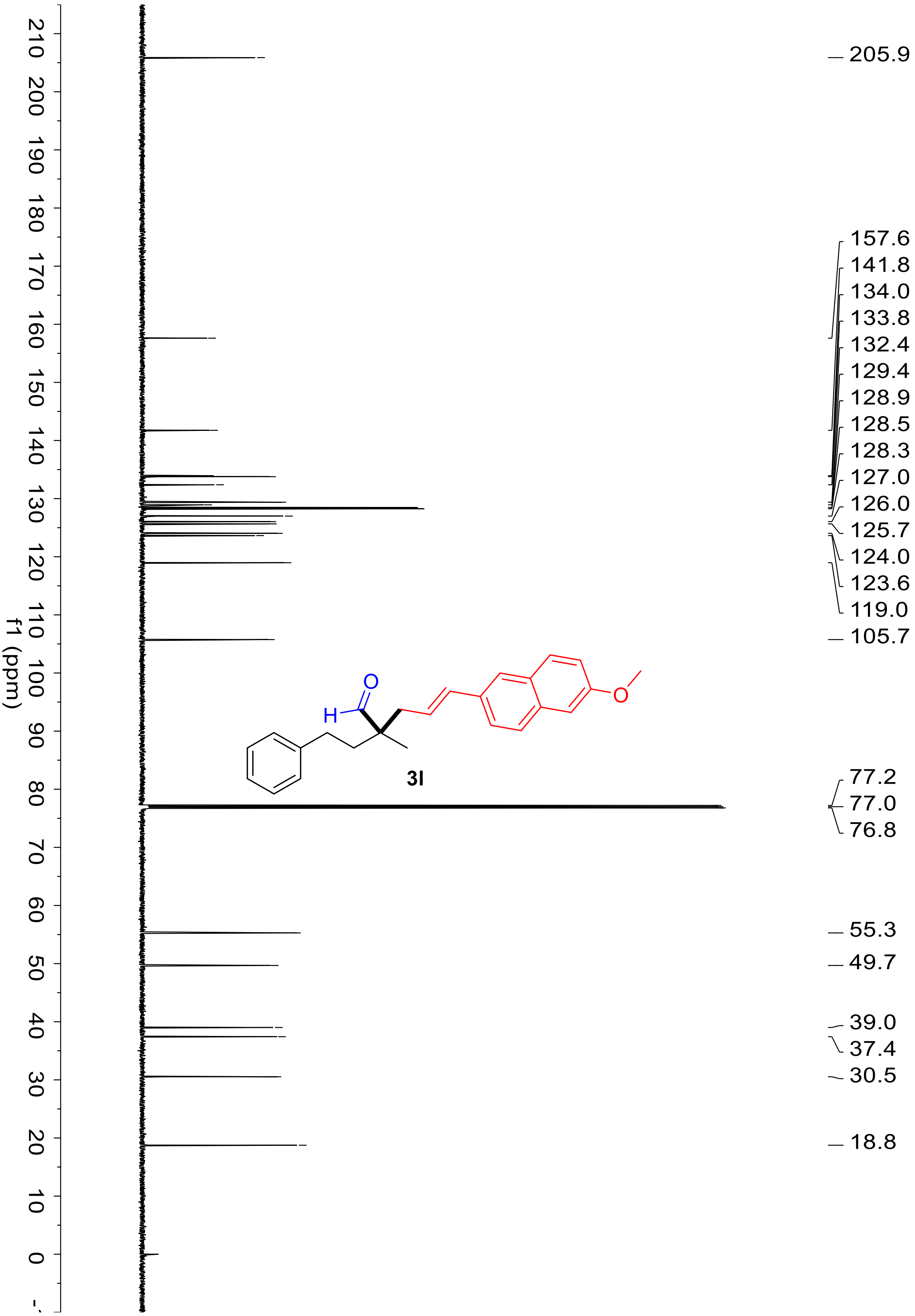
3k


3k

205.5
141.6
137.7
132.3
131.2
131.0
130.8
130.6
129.2
129.0
128.5
128.2
126.8
126.6
126.1
125.0
123.9
123.9
123.9
123.8
123.2
122.8
122.8
122.8
122.7
121.4
77.2
77.0
76.8
49.6
38.7
37.5
30.5
18.8
131.2
131.0
130.8
130.6
131.6
131.2
130.8
130.4
f1 (ppm)
126.8
126.6
126.1
125.0
123.9
123.9
123.9
123.8
123.2
122.8
122.8
122.8
122.7
121.4
127
126
125
124
123
122
f1 (ppm)
O
H
CF_3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



9.590
7.694
7.679
7.673
7.659
7.613
7.526
7.523
7.512
7.509
7.292
7.279
7.267
7.204
7.192
7.181
7.169
7.132
7.128
7.117
7.113
7.100
7.096
6.591
6.564
6.192
6.179
6.166
3.912
2.585
2.576
2.566
2.556
2.547
2.516
2.514
2.504
2.502
2.499
2.497
2.486
2.484
1.926
1.917
1.853
1.844
1.834
1.202
-0.000
1.00
1.10
1.03
1.01
1.06
2.07
0.96
2.03
1.13
1.02
1.03
1.06
3.28
2.03
2.27
1.03
1.08
3.16
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)
H
O
O
3l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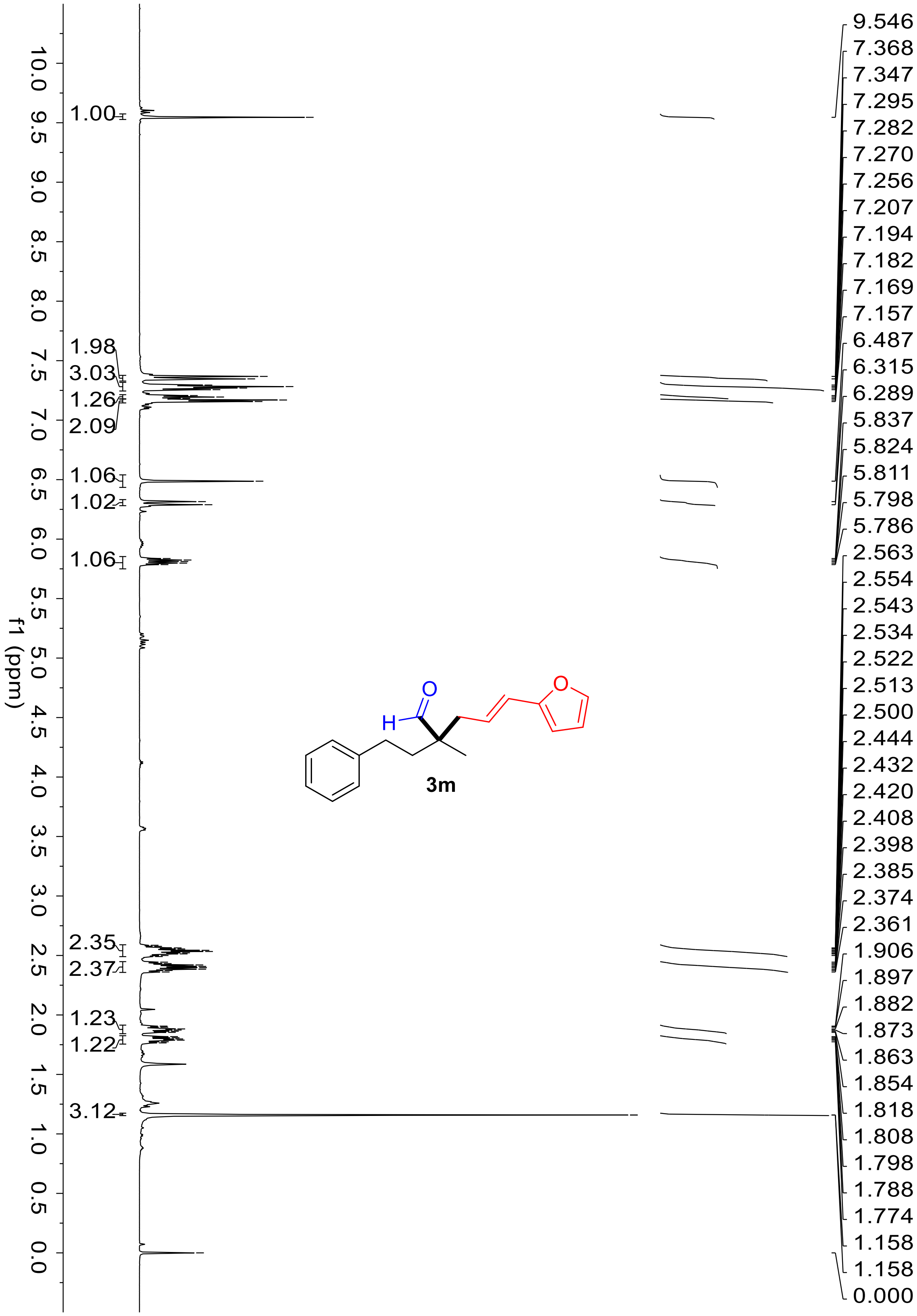
141.8
134.0
133.8
132.4
129.4
128.9
128.5
128.3
127.0
126.0
125.7
124.0
123.6
119.0
105.7
77.2
77.0
76.8
55.3
49.7
39.0
37.4
30.5
18.8
3l
O
H
O
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0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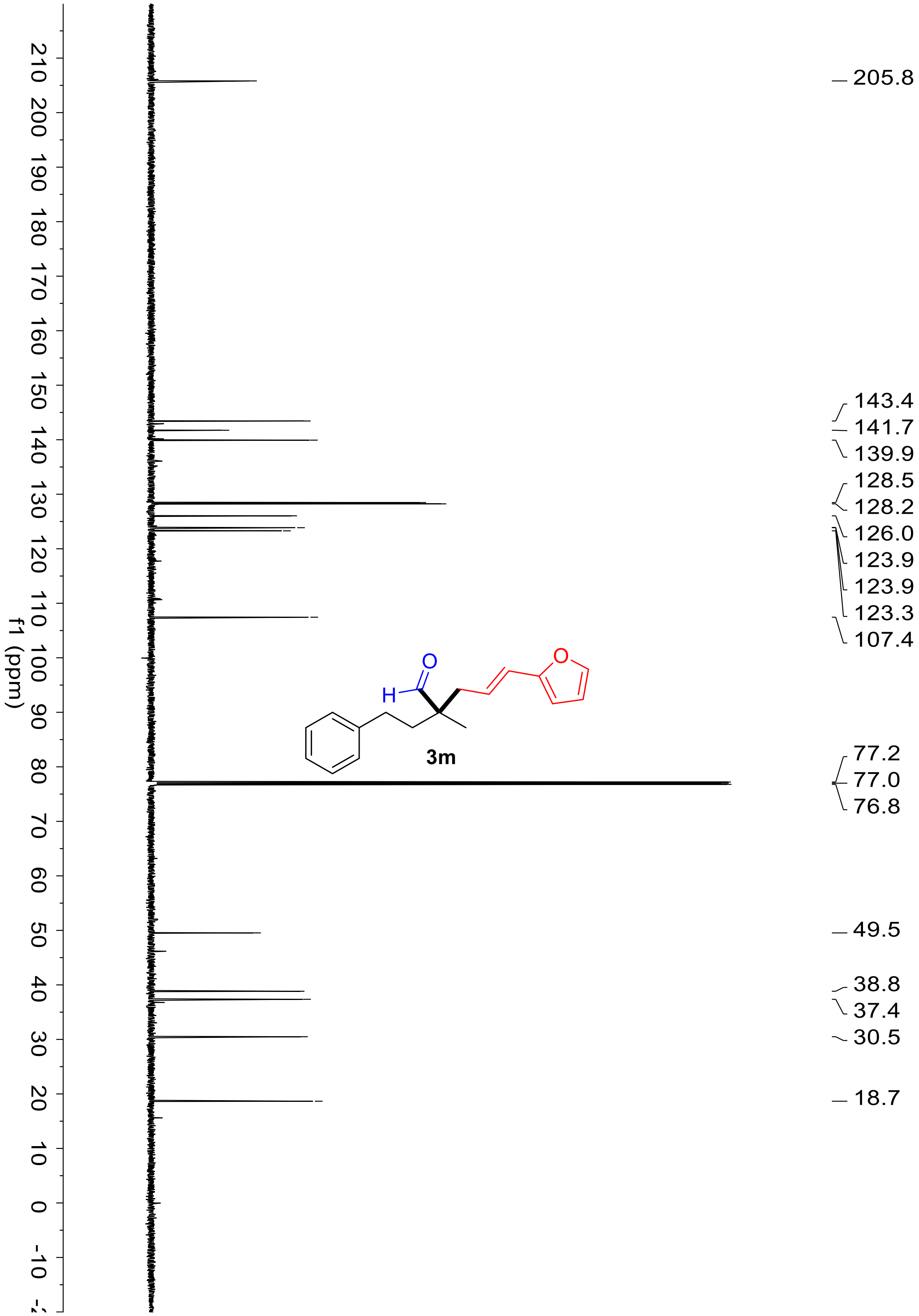
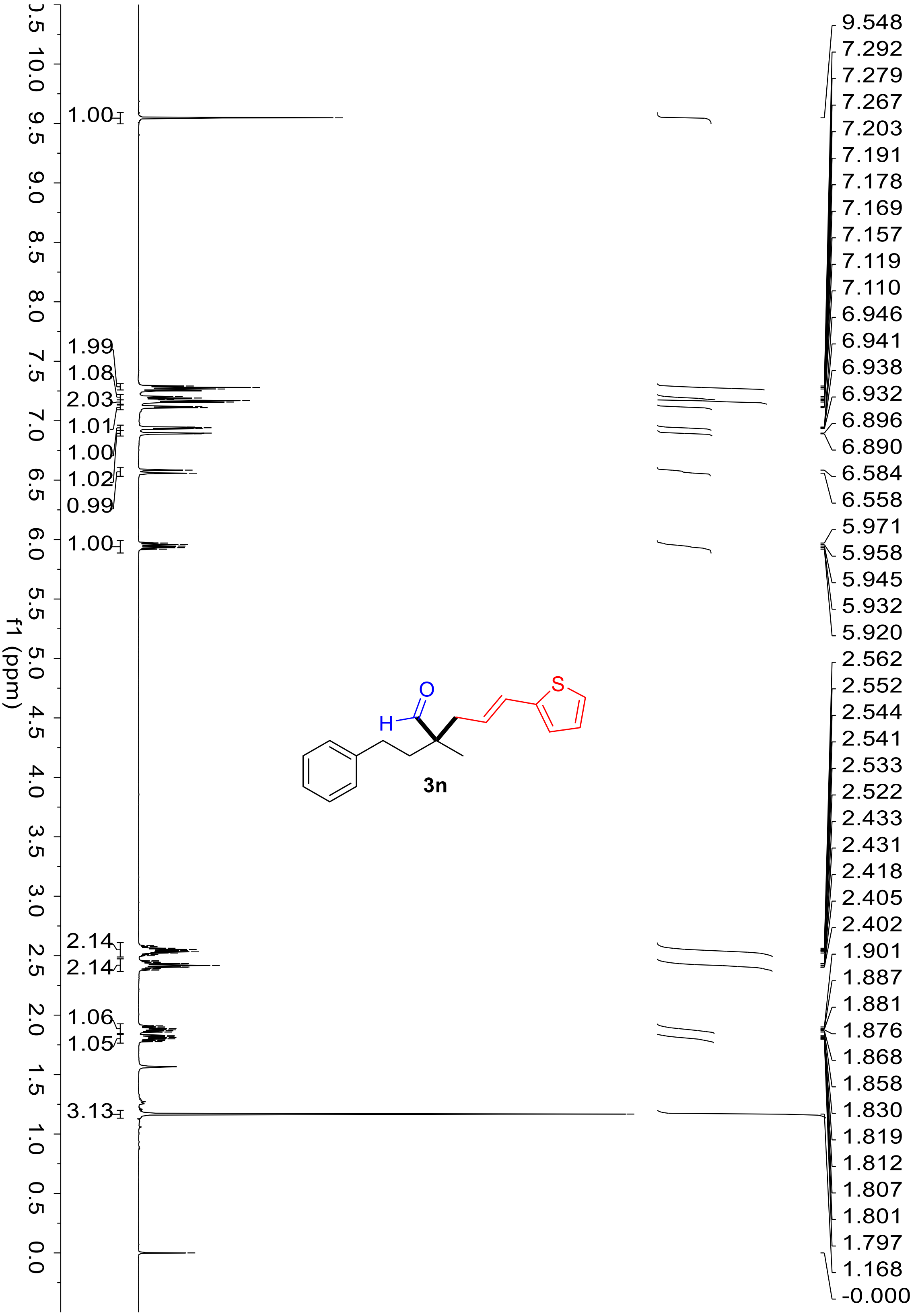
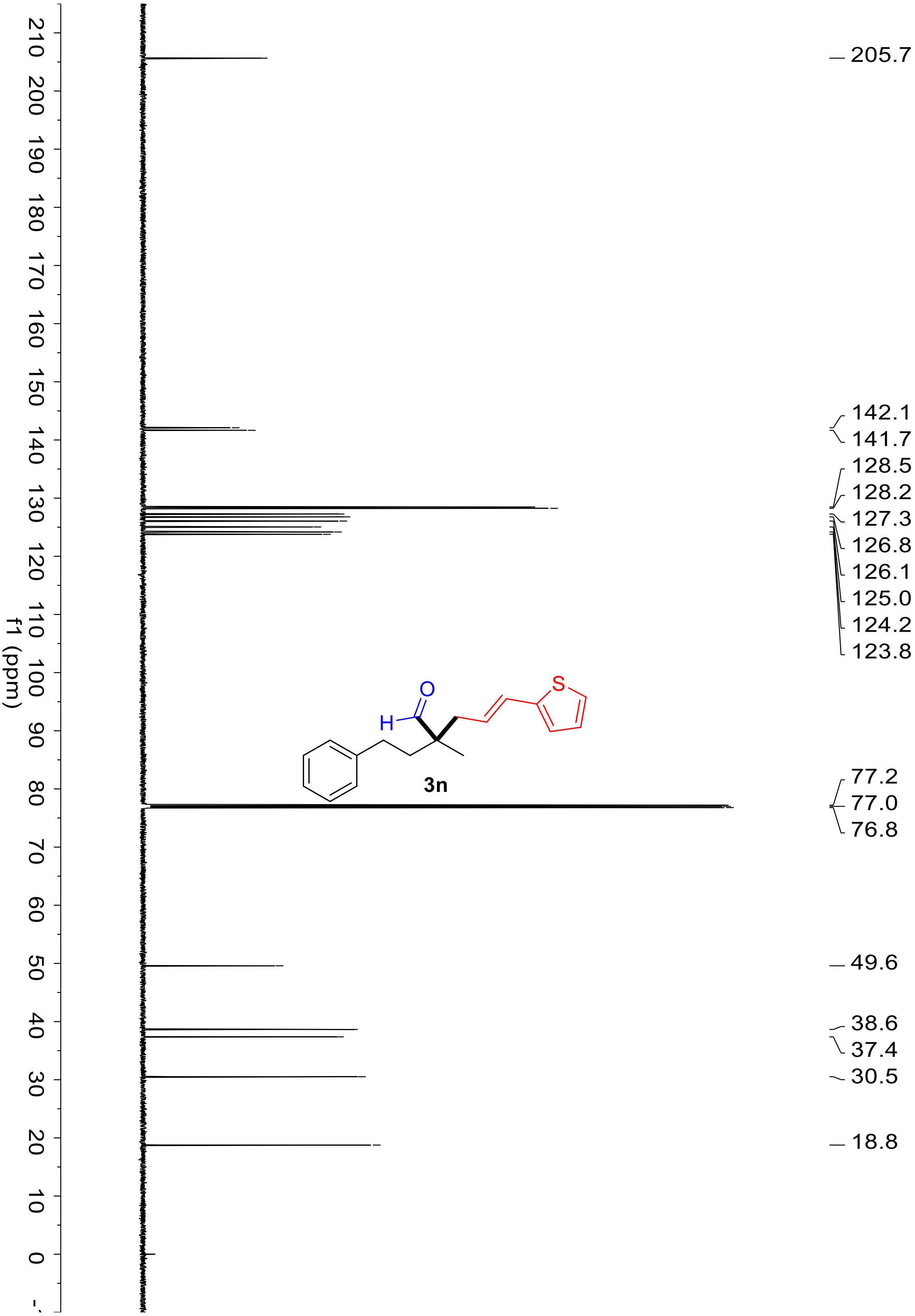
7.295
7.282
7.270
7.256
7.207
7.194
7.182
7.169
7.157
6.487
6.315
6.289
5.837
5.824
5.811
5.798
5.786
2.563
2.554
2.543
2.534
2.522
2.513
2.500
2.444
2.432
2.420
2.408
2.398
2.385
2.374
2.361
1.906
1.897
1.882
1.873
1.863
1.854
1.818
1.808
1.798
1.788
1.774
1.158
1.158
0.000
1.00
1.98
3.03
1.26
2.09
1.06
1.02
1.06
2.35
2.37
1.23
1.22
3.12
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)
O
H
O
3m


205.8
143.4
141.7
139.9
128.5
128.2
126.0
123.9
123.9
123.3
107.4
77.2
77.0
76.8
49.5
38.8
37.4
30.5
18.7
3m
H
O
O
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)



3n

9.548
7.292
7.279
7.267
7.203
7.191
7.178
7.169
7.157
7.119
7.110
6.946
6.941
6.938
6.932
6.896
6.890
6.584
6.558
5.971
5.958
5.945
5.932
5.920
2.562
2.552
2.544
2.541
2.533
2.522
2.433
2.431
2.418
2.405
2.402
1.901
1.887
1.881
1.876
1.868
1.858
1.830
1.819
1.812
1.807
1.801
1.797
1.168
-0.000
1.00
1.99
1.08
2.03
1.01
1.00
1.02
0.99
1.00
2.14
2.14
1.06
1.05
3.13
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
O
H
S



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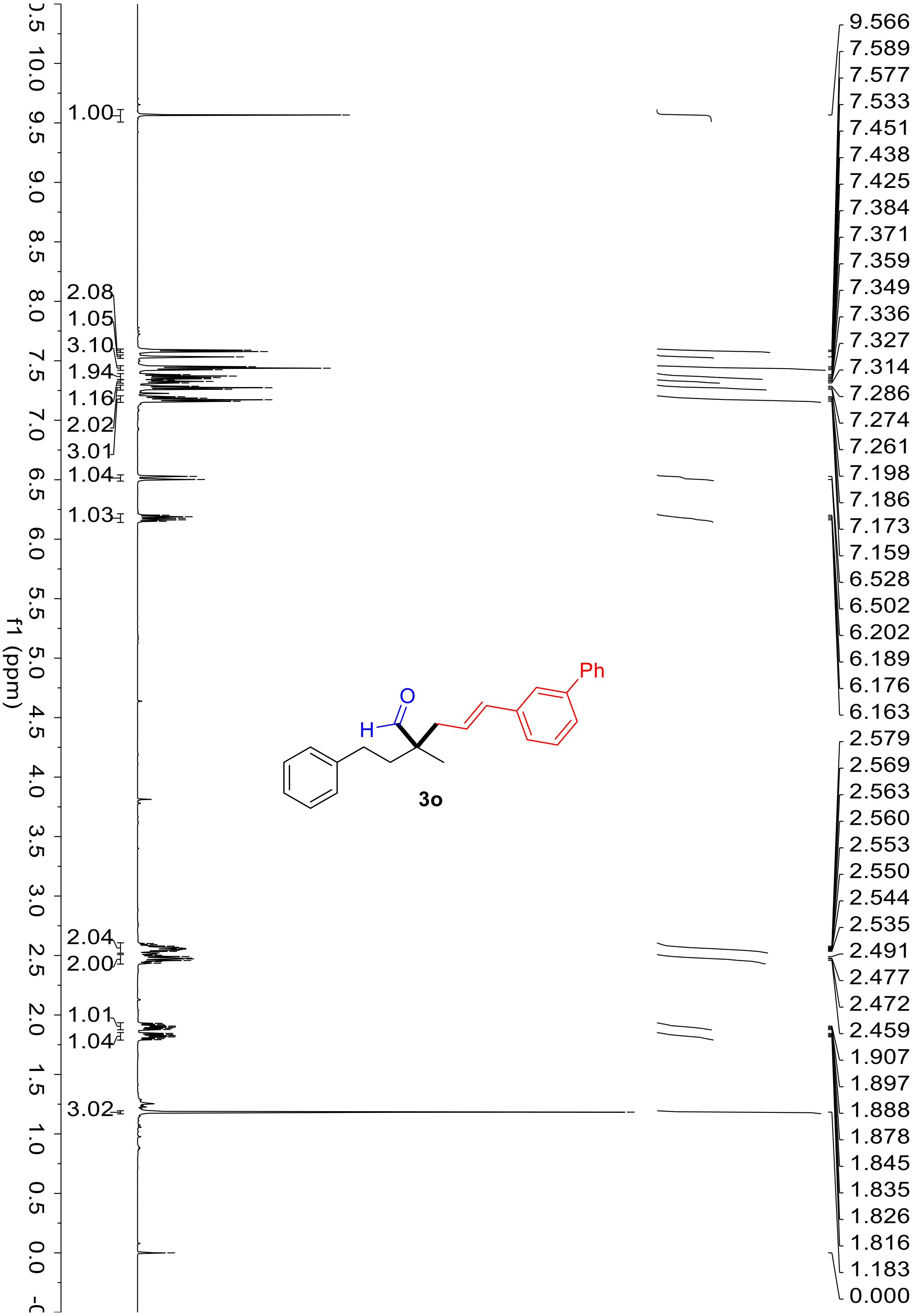
142.1
141.7
128.5
128.2
127.3
126.8
126.1
125.0
124.2
123.8
77.2
77.0
76.8
49.6
38.6
37.4
30.5
18.8
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
O
H
S
3n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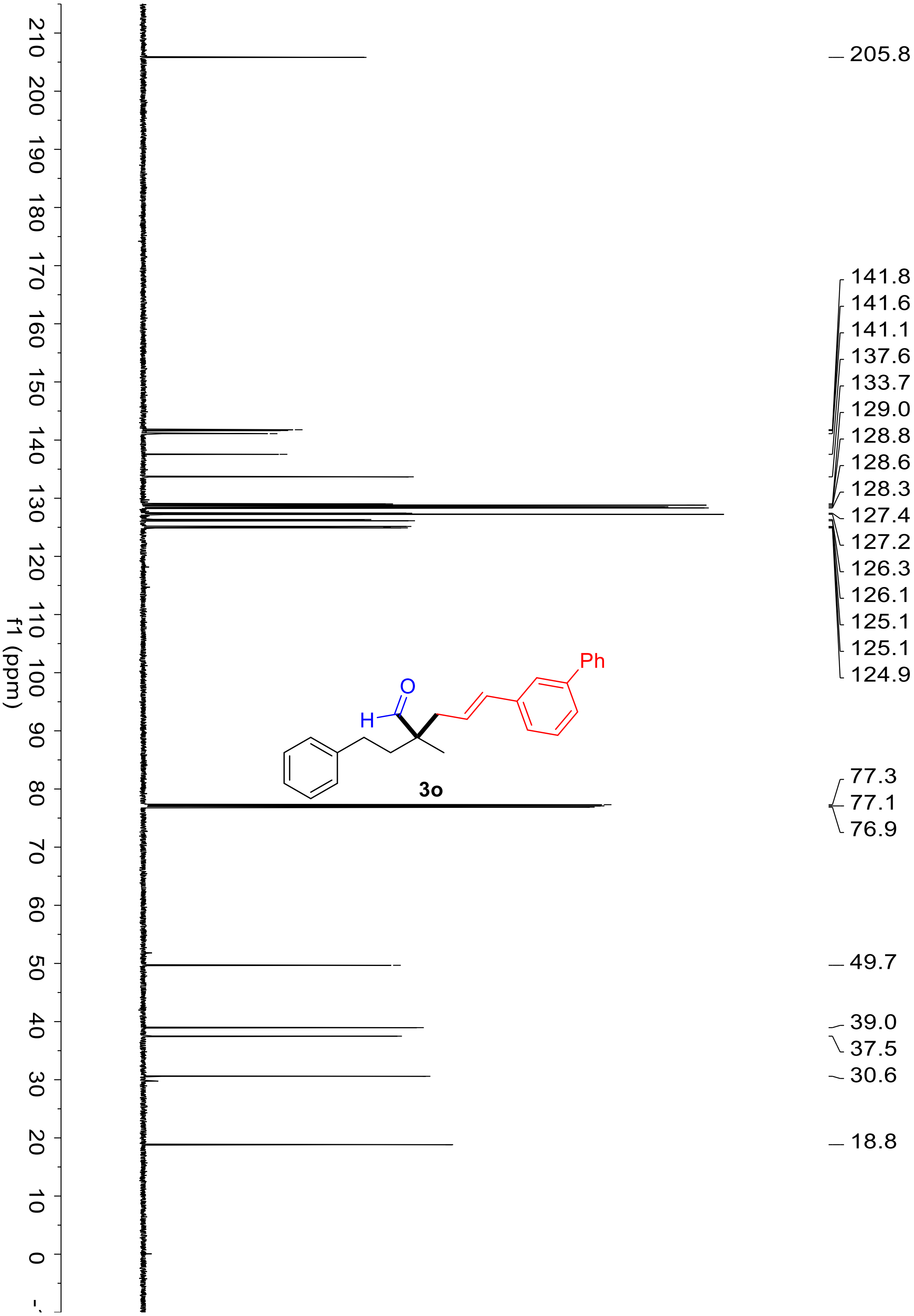
7.425
7.384
7.371
7.359
7.349
7.336
7.327
7.314
7.286
7.274
7.261
7.198
7.186
7.173
7.159
6.528
6.502
6.202
6.189
6.176
6.163
2.579
2.569
2.563
2.560
2.553
2.550
2.544
2.535
2.491
2.477
2.472
2.459
1.907
1.897
1.888
1.878
1.845
1.835
1.826
1.816
1.183
0.000
1.00
2.08
1.05
3.10
1.94
1.16
2.02
3.01
1.04
1.03
2.04
2.00
1.01
1.04
3.02
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
-0
f1 (ppm)
O
H
Ph
3o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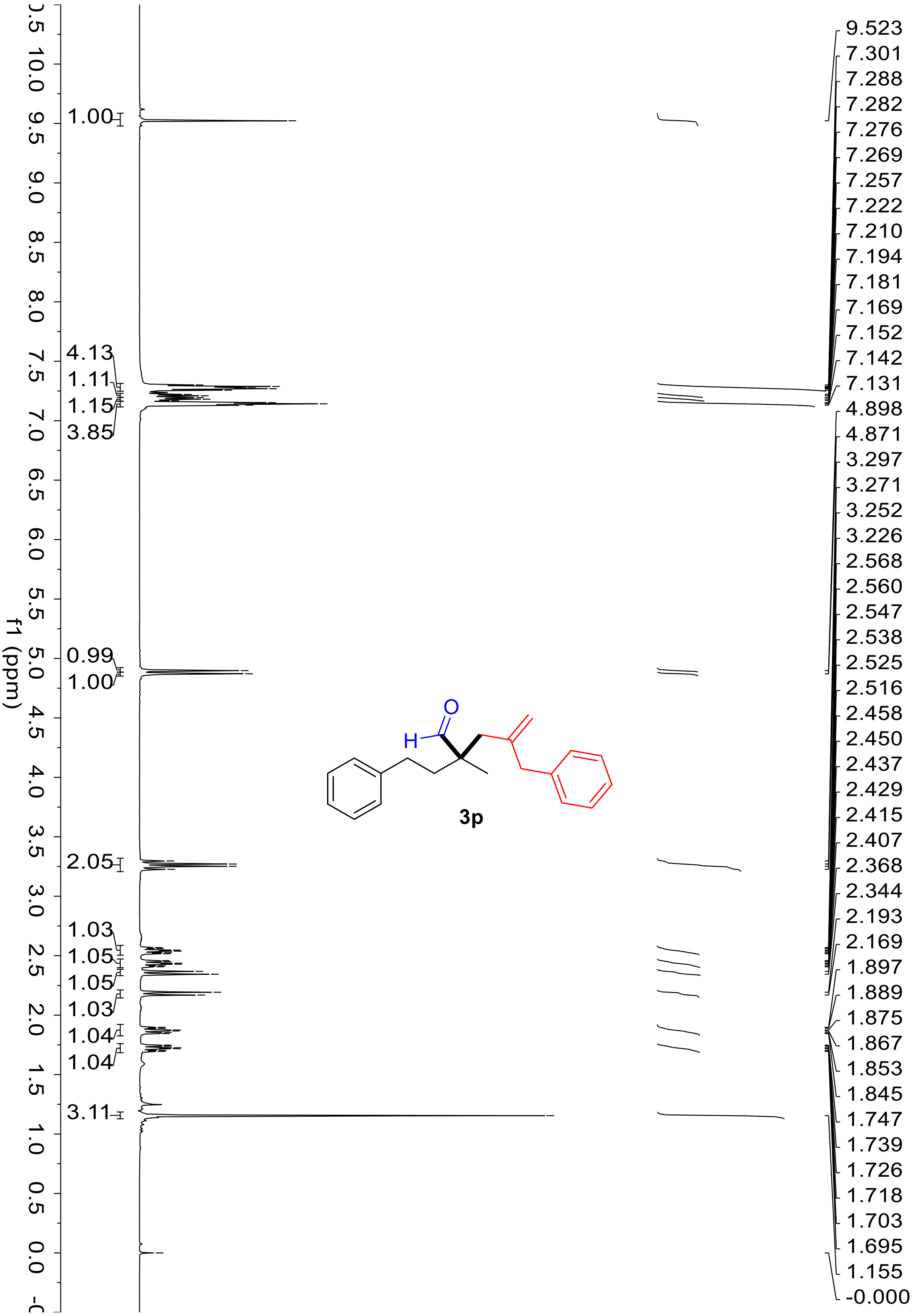
141.8
141.6
141.1
137.6
133.7
129.0
128.8
128.6
128.3
127.4
127.2
126.3
126.1
125.1
125.1
124.9
77.3
77.1
76.9
49.7
39.0
37.5
30.6
18.8
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
H
O
Ph
3o


3p
H
O
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7.269
7.257
7.222
7.210
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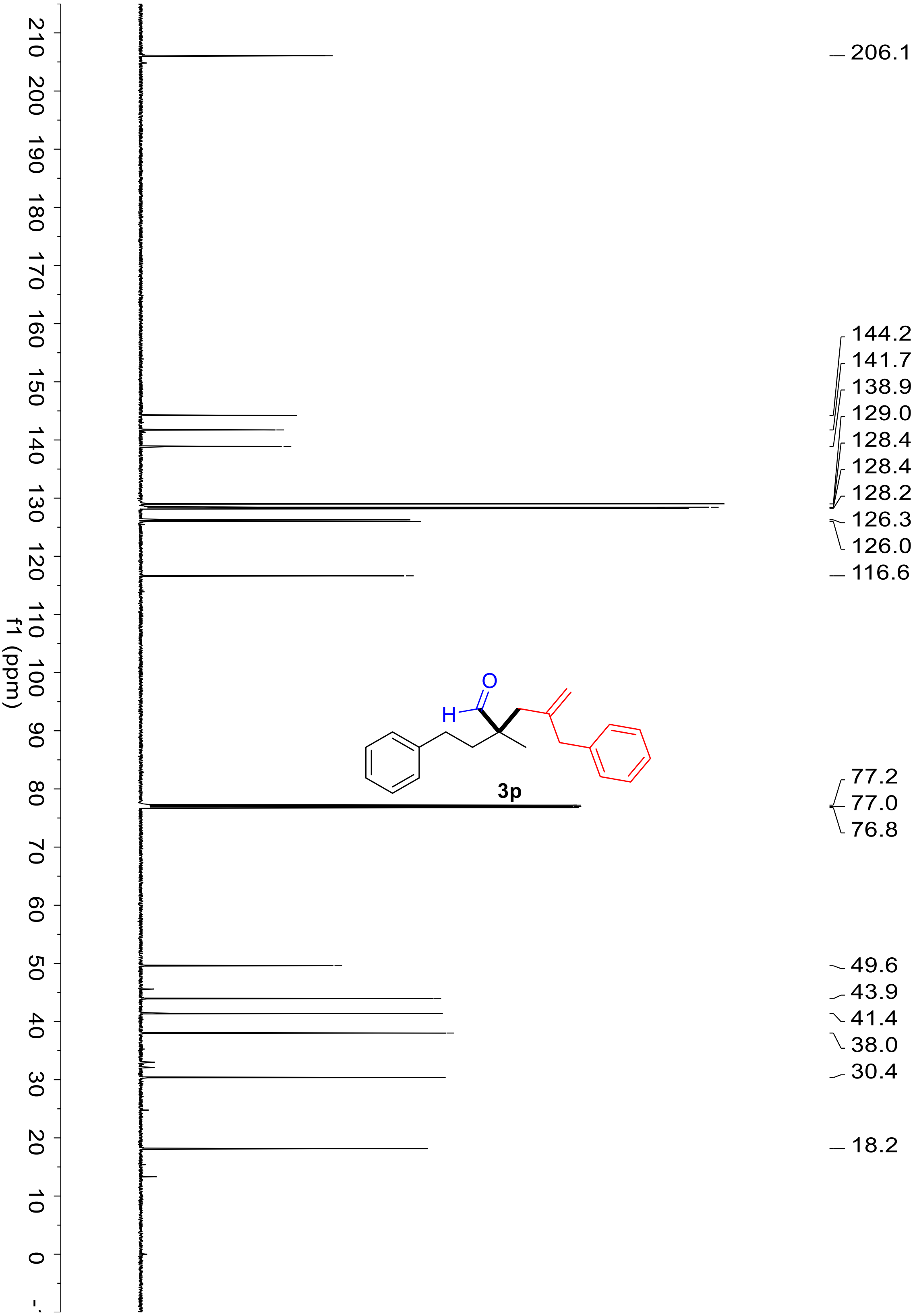
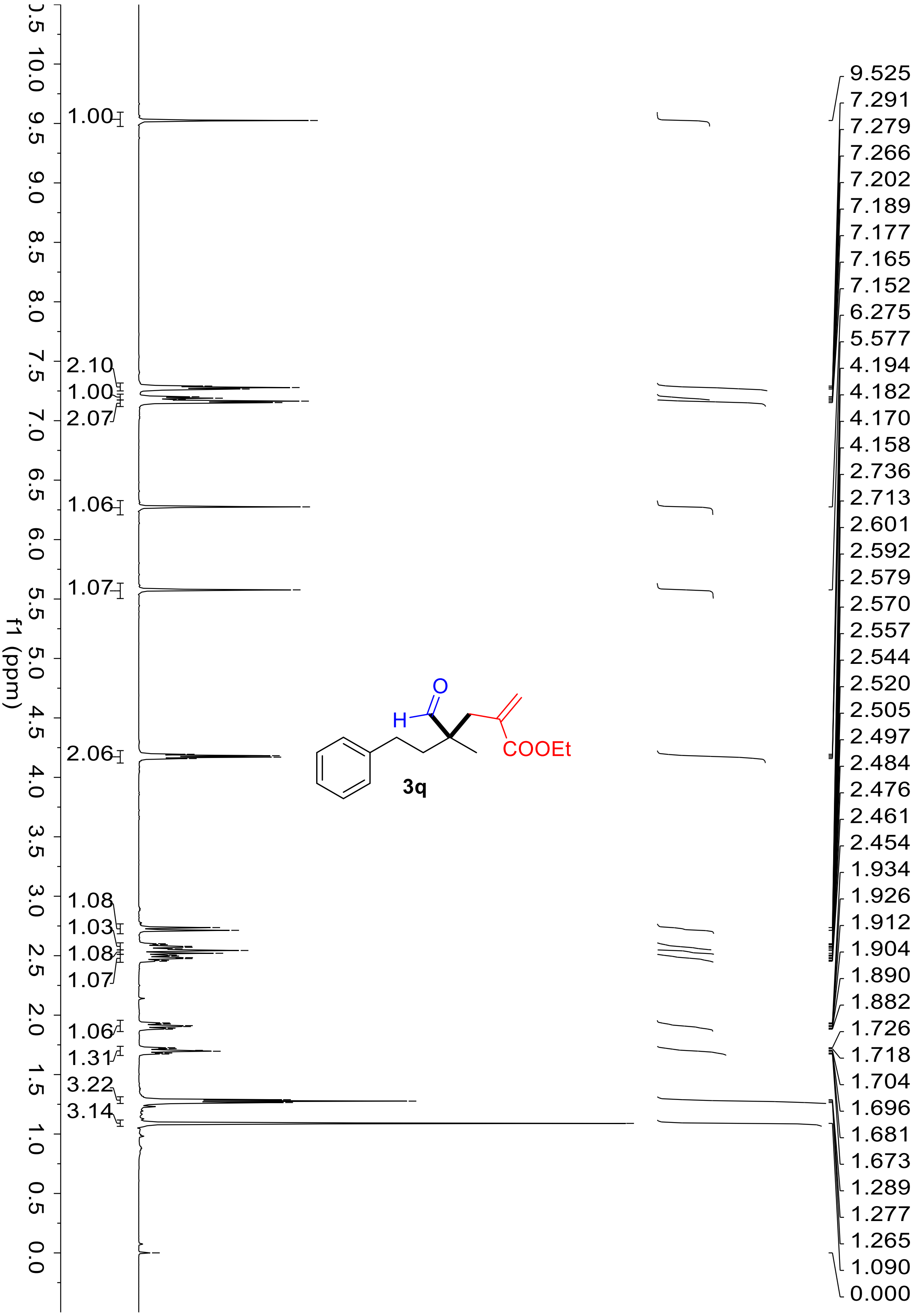
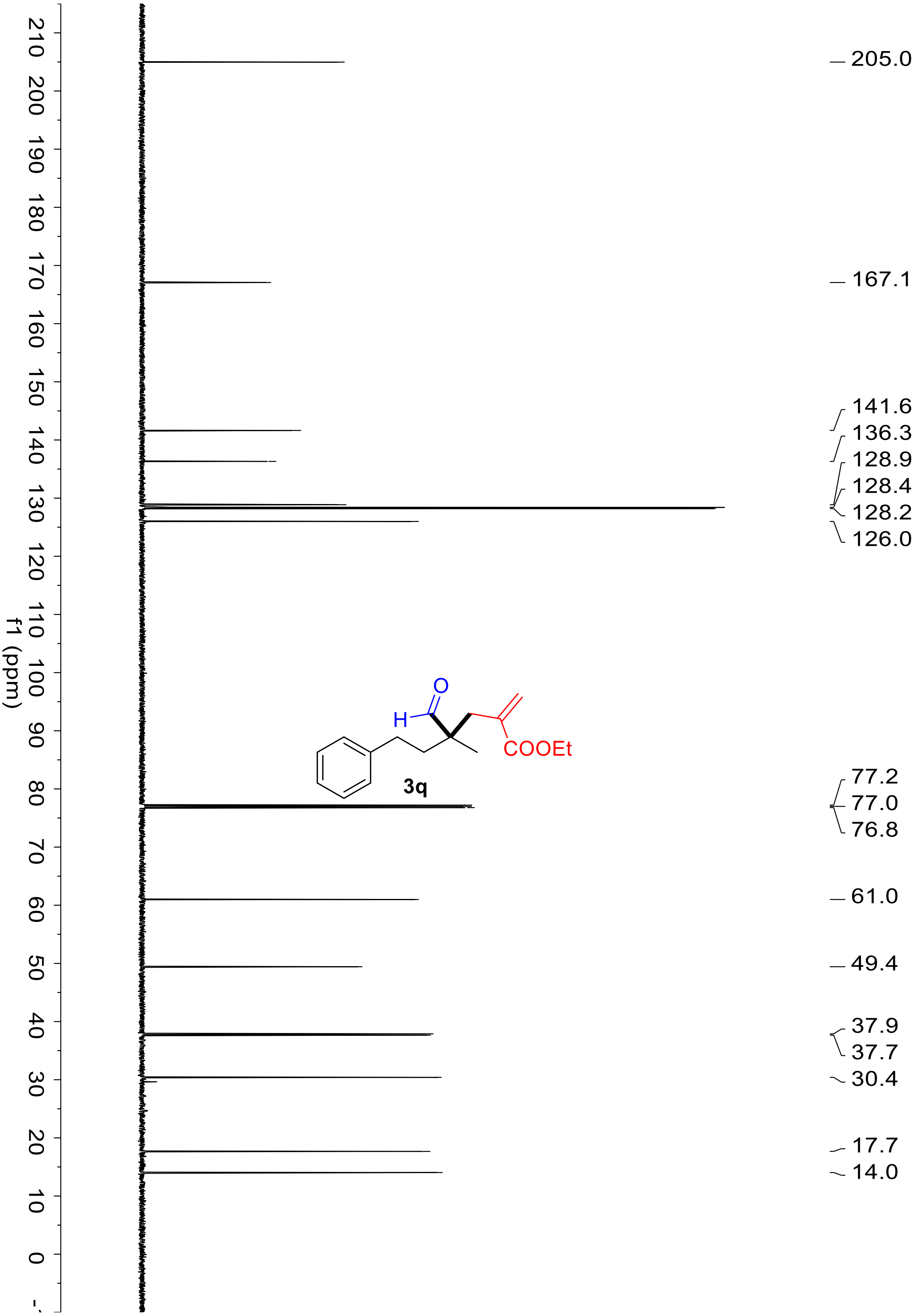
7.181
7.169
7.152
7.142
7.131
4.898
4.871
3.297
3.271
3.252
3.226
2.568
2.560
2.547
2.538
2.525
2.516
2.458
2.450
2.437
2.429
2.415
2.407
2.368
2.344
2.193
2.169
1.897
1.889
1.875
1.867
1.853
1.845
1.747
1.739
1.726
1.718
1.703
1.695
1.155
-0.000
1.00
4.13
1.11
1.15
3.85
0.99
1.00
2.05
1.03
1.05
1.05
1.03
1.04
1.04
3.11
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


206.1
144.2
141.7
138.9
129.0
128.4
128.4
128.2
126.3
126.0
116.6
77.2
77.0
76.8
49.6
43.9
41.4
38.0
30.4
18.2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
H

3p



9.525
7.291
7.279
7.266
7.202
7.189
7.177
7.165
7.152
6.275
5.577
4.194
4.182
4.170
4.158
2.736
2.713
2.601
2.592
2.579
2.570
2.557
2.544
2.520
2.505
2.497
2.484
2.476
2.461
2.454
1.934
1.926
1.912
1.904
1.890
1.882
1.726
1.718
1.704
1.696
1.681
1.673
1.289
1.277
1.265
1.090
0.000
1.00
2.10
1.00
2.07
1.06
1.07
2.06
1.08
1.03
1.08
1.07
1.06
1.31
3.22
3.14
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)
O
H
COOEt
3q


3q
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167.1
141.6
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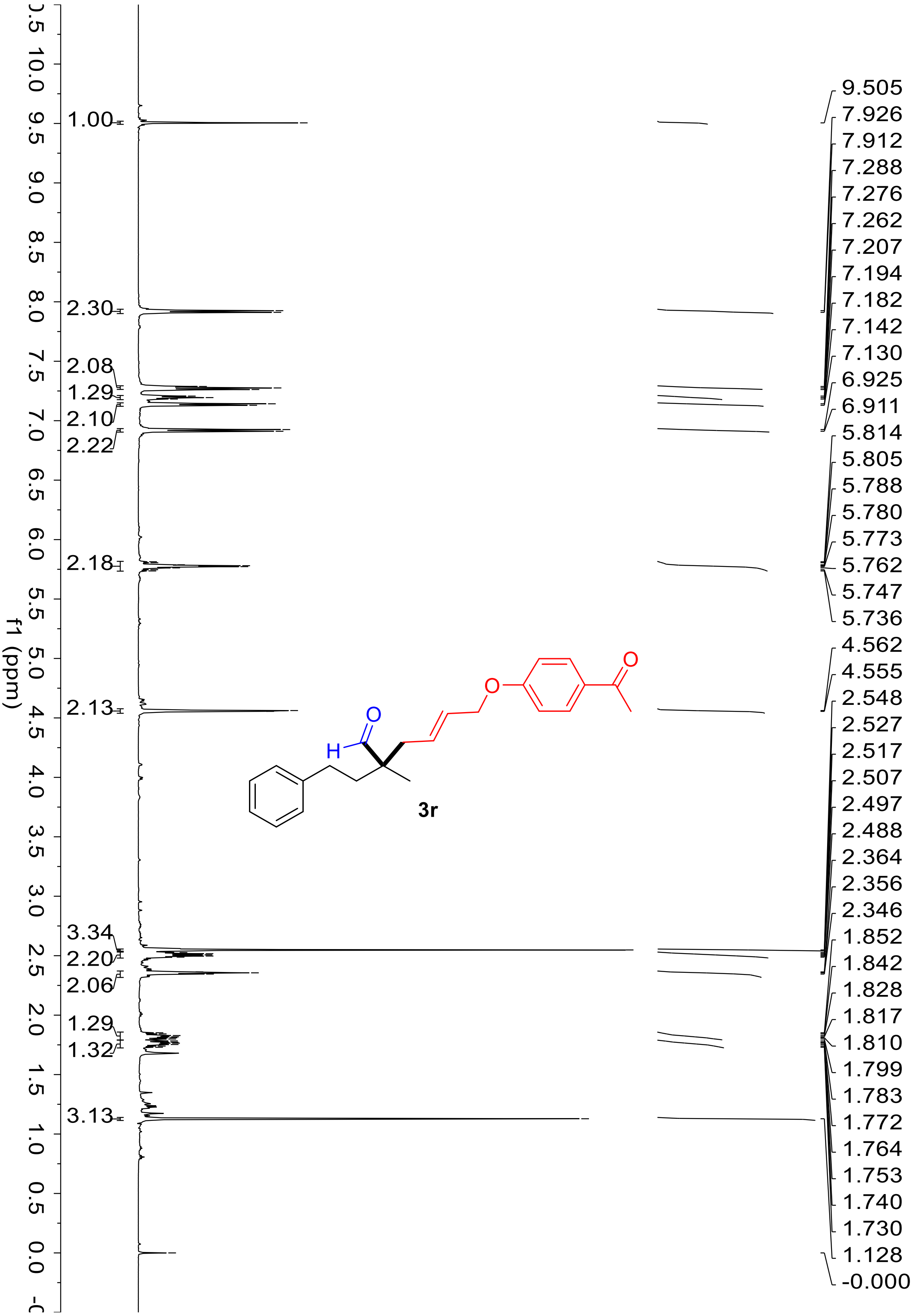
128.9
128.4
128.2
126.0
77.2
77.0
76.8
61.0
49.4
37.9
37.7
30.4
17.7
14.0
O
H
COOEt
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0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7.194
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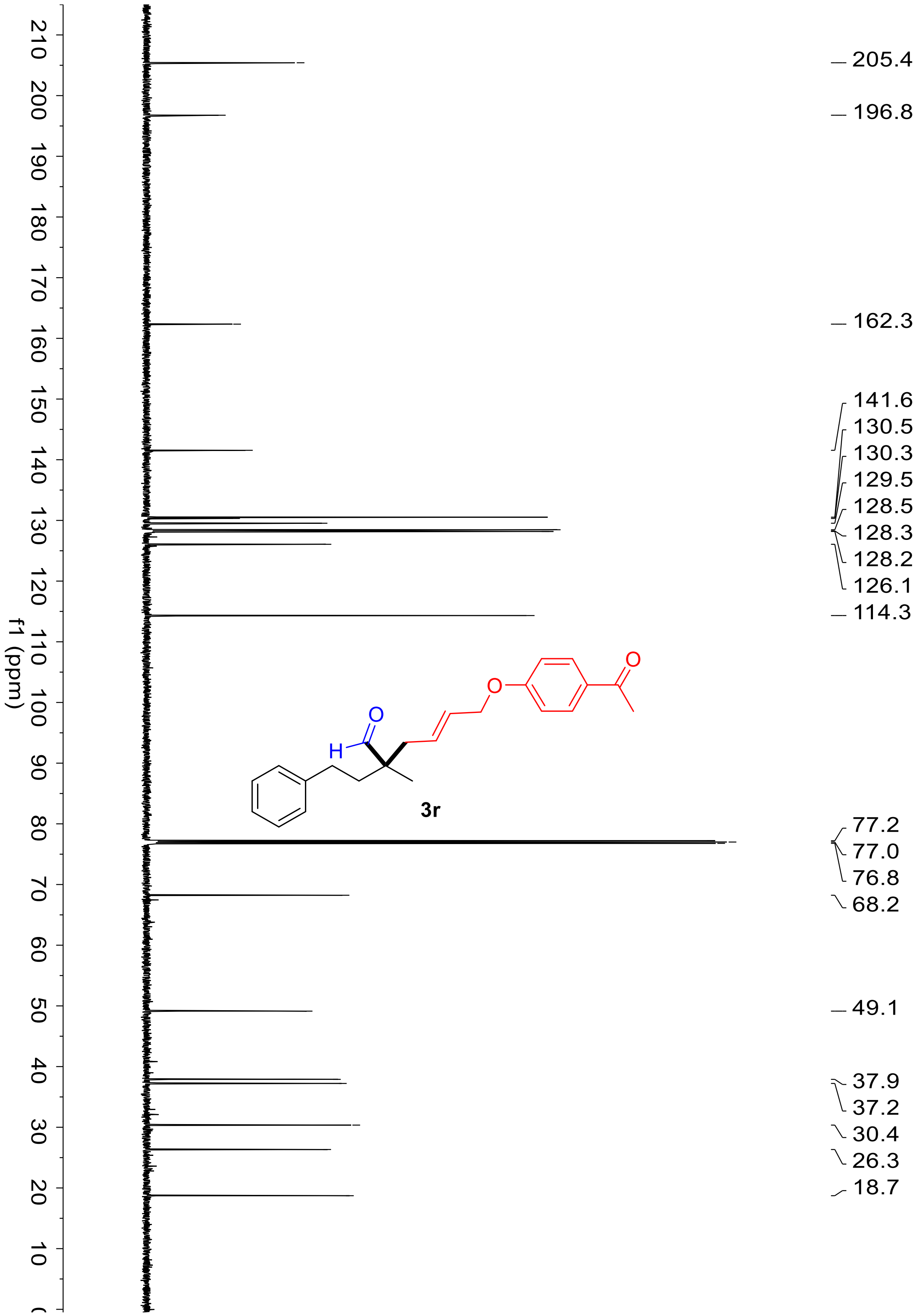
7.142
7.130
6.925
6.911
5.814
5.805
5.788
5.780
5.773
5.762
5.747
5.736
4.562
4.555
2.548
2.527
2.517
2.507
2.497
2.488
2.364
2.356
2.346
1.852
1.842
1.828
1.817
1.810
1.799
1.783
1.772
1.764
1.753
1.740
1.730
1.128
-0.000
1.00
2.30
2.08
1.29
2.10
2.22
2.18
2.13
3.34
2.20
2.06
1.29
1.32
3.13
f1 (ppm)
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
O
H
O
O

3r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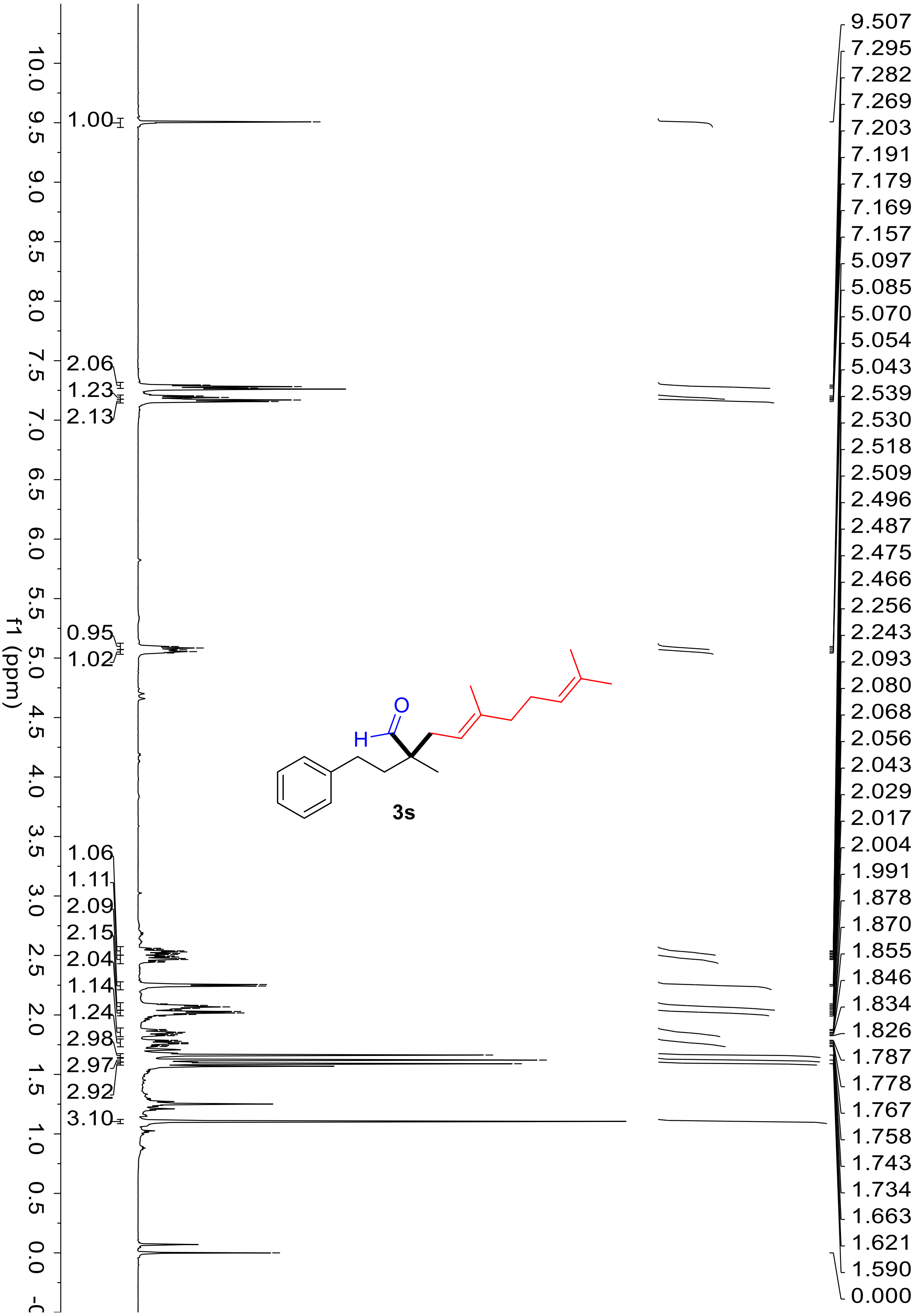
130.3
129.5
128.5
128.3
128.2
126.1
114.3
77.2
77.0
76.8
68.2
49.1
37.9
37.2
30.4
26.3
18.7
O
H
O
O
3r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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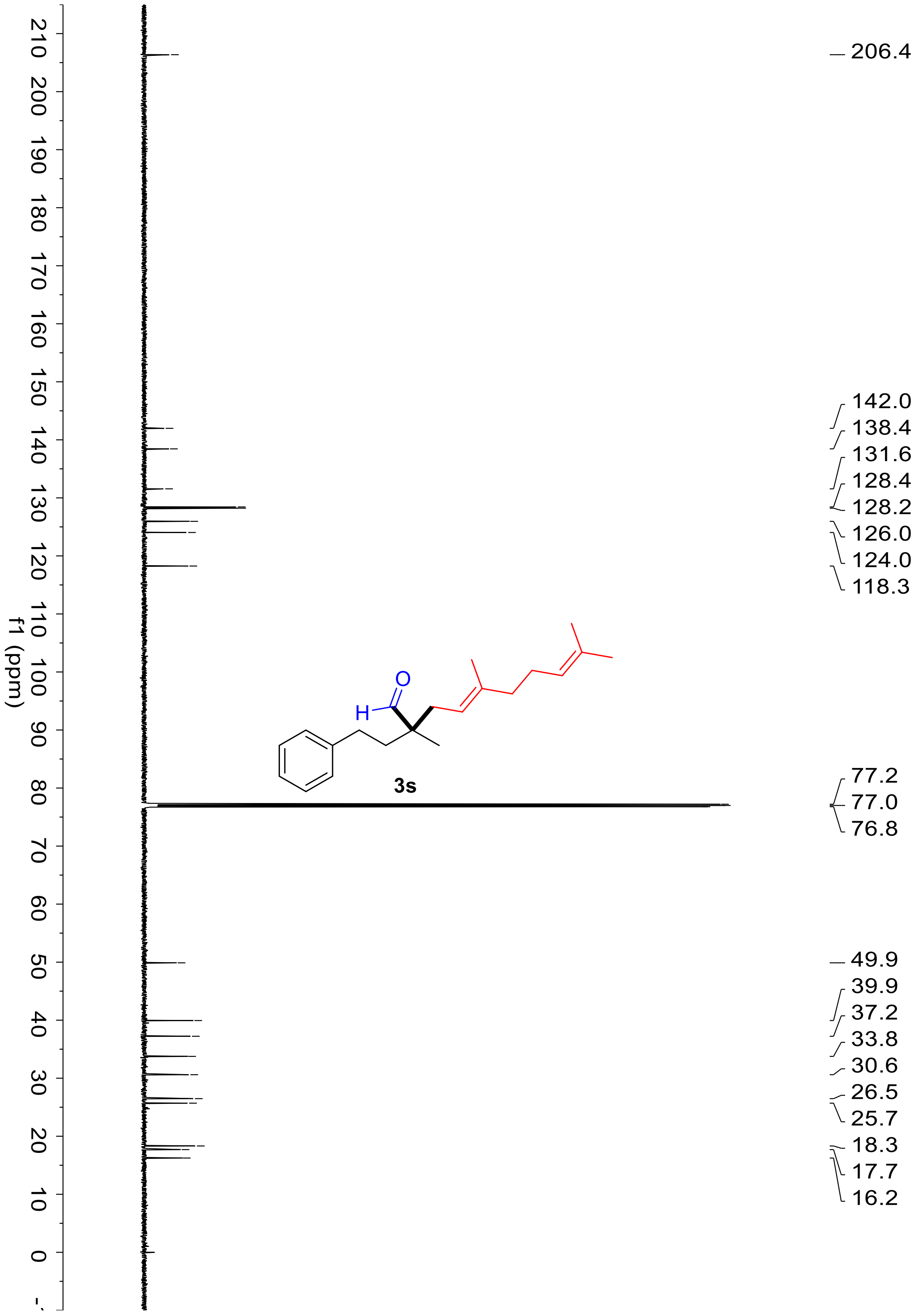
5.085
5.070
5.054
5.043
2.539
2.530
2.518
2.509
2.496
2.487
2.475
2.466
2.256
2.243
2.093
2.080
2.068
2.056
2.043
2.029
2.017
2.004
1.991
1.878
1.870
1.855
1.846
1.834
1.826
1.787
1.778
1.767
1.758
1.743
1.734
1.663
1.621
1.590
0.000
1.00
2.06
1.23
2.13
0.95
1.02
1.06
1.11
2.09
2.15
2.04
1.14
1.24
2.98
2.97
2.92
3.10
O
H
3s
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.4
128.2
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124.0
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77.2
77.0
76.8
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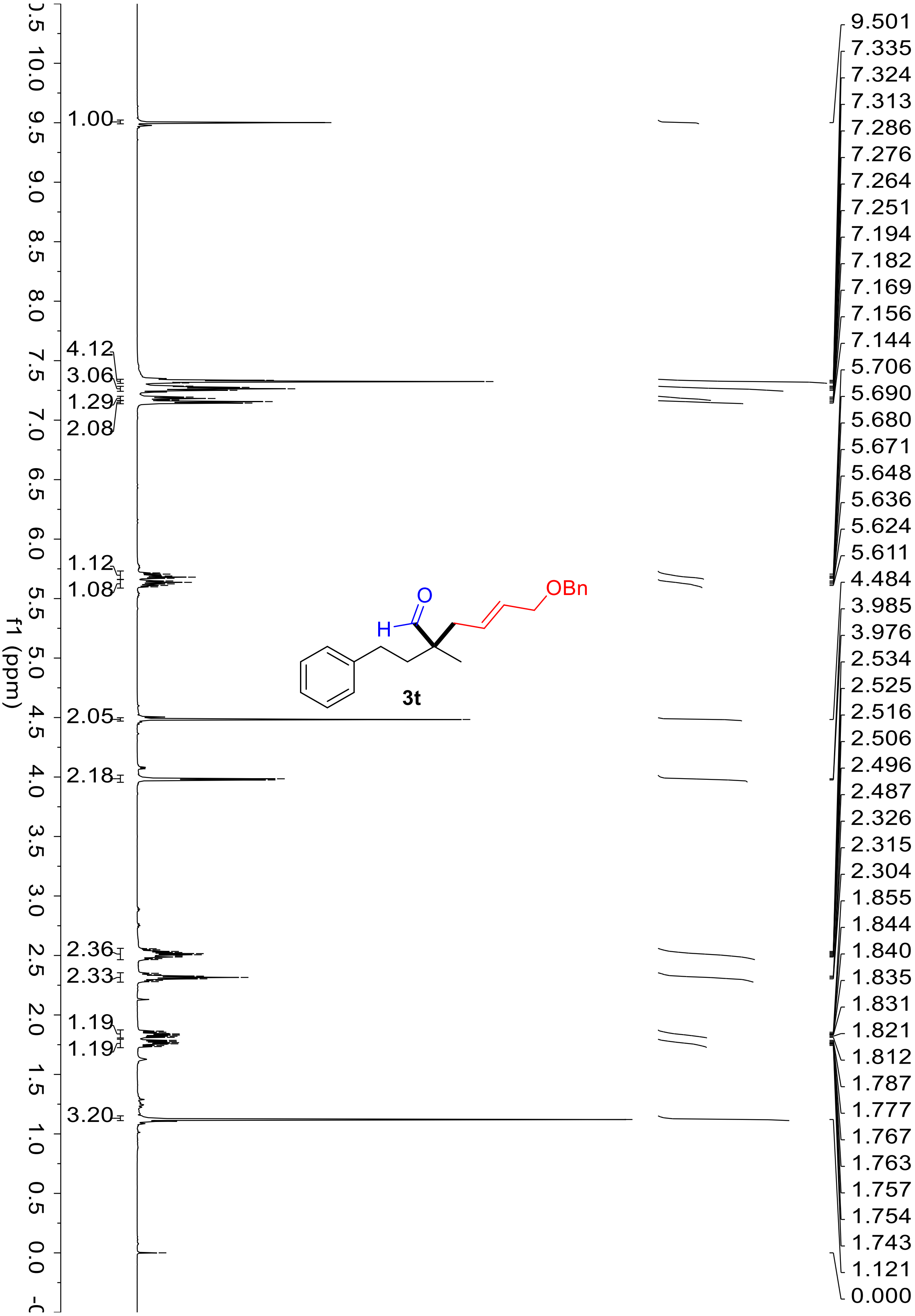
39.9
37.2
33.8
30.6
26.5
25.7
18.3
17.7
16.2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
H

3s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7.324
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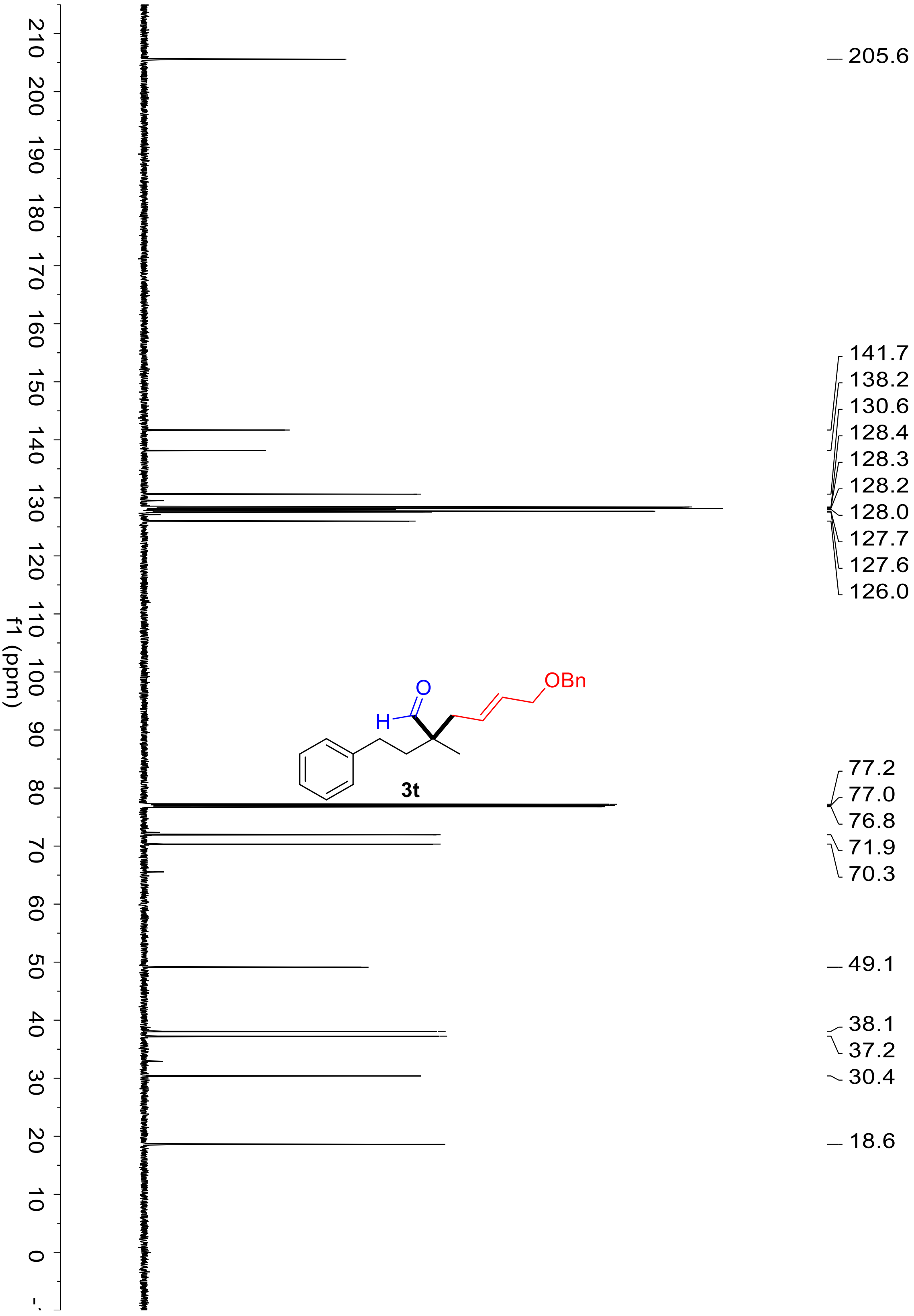
7.276
7.264
7.251
7.194
7.182
7.169
7.156
7.144
5.706
5.690
5.680
5.671
5.648
5.636
5.624
5.611
4.484
3.985
3.976
2.534
2.525
2.516
2.506
2.496
2.487
2.326
2.315
2.304
1.855
1.844
1.840
1.835
1.831
1.821
1.812
1.787
1.777
1.767
1.763
1.757
1.754
1.743
1.121
0.000
1.00
4.12
3.06
1.29
2.08
1.12
1.08
2.05
2.18
2.36
2.33
1.19
1.19
3.20
O
H
OBn
3t
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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141.7
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130.6
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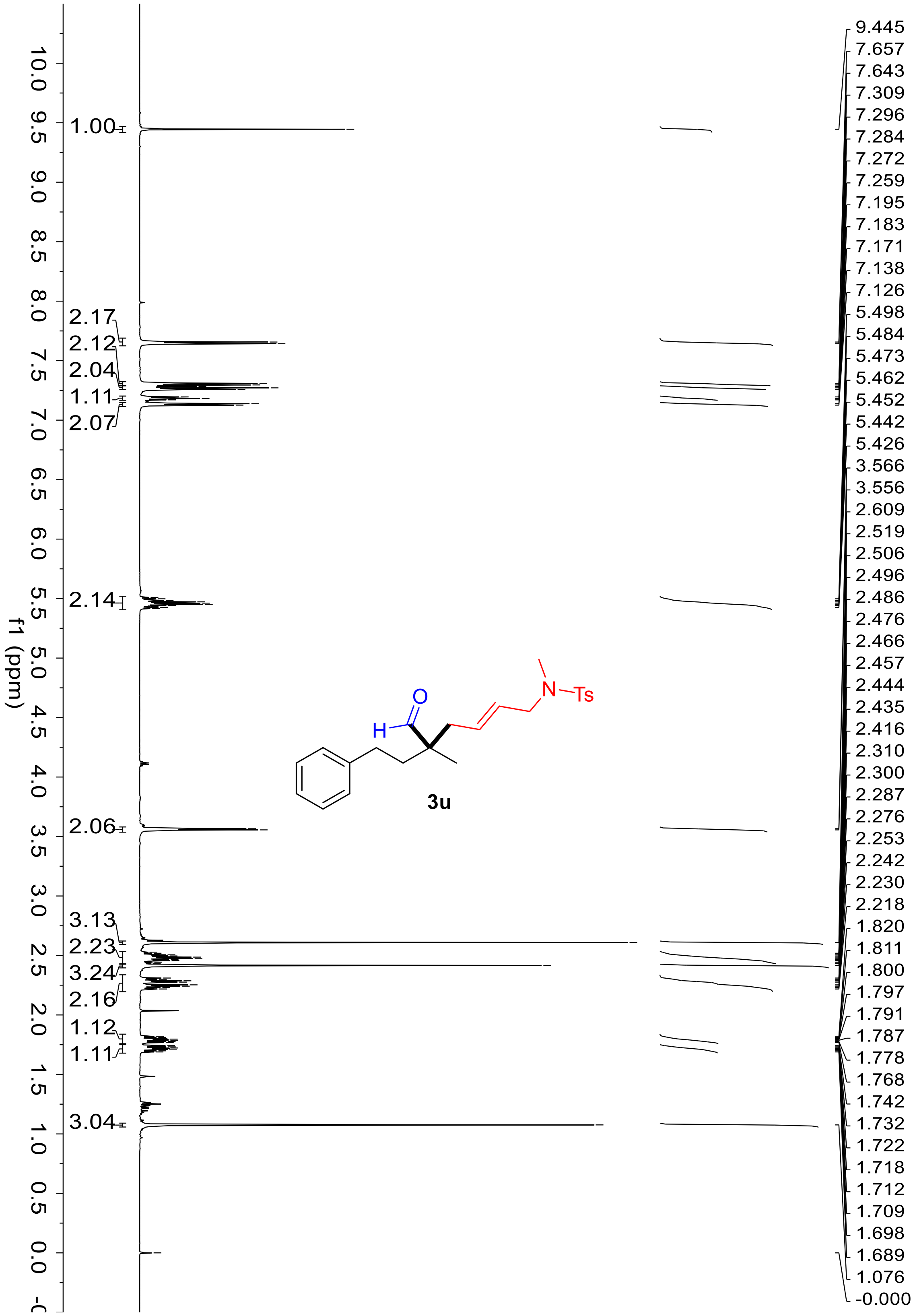
128.3
128.2
128.0
127.7
127.6
126.0
77.2
77.0
76.8
71.9
70.3
49.1
38.1
37.2
30.4
18.6
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
H
OBn

3t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7.284
7.272
7.259
7.195
7.183
7.171
7.138
7.126
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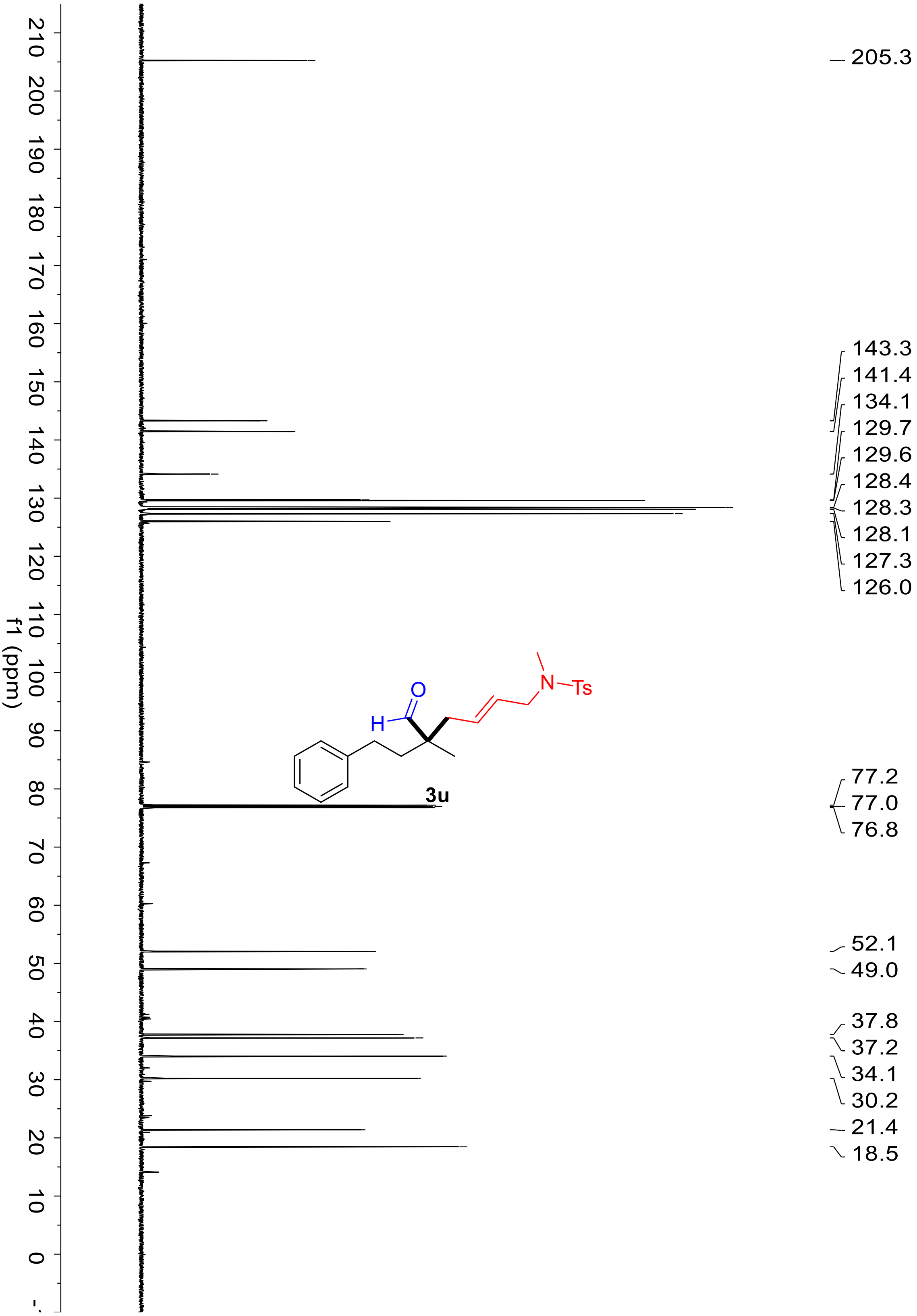
5.484
5.473
5.462
5.452
5.442
5.426
3.566
3.556
2.609
2.519
2.506
2.496
2.486
2.476
2.466
2.457
2.444
2.435
2.416
2.310
2.300
2.287
2.276
2.253
2.242
2.230
2.218
1.820
1.811
1.800
1.797
1.791
1.787
1.778
1.768
1.742
1.732
1.722
1.718
1.712
1.709
1.698
1.689
1.076
-0.000
1.00
2.17
2.12
2.04
1.11
2.07
2.14
2.06
3.13
2.23
3.24
2.16
1.12
1.11
3.04
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)
H
O
N
Ts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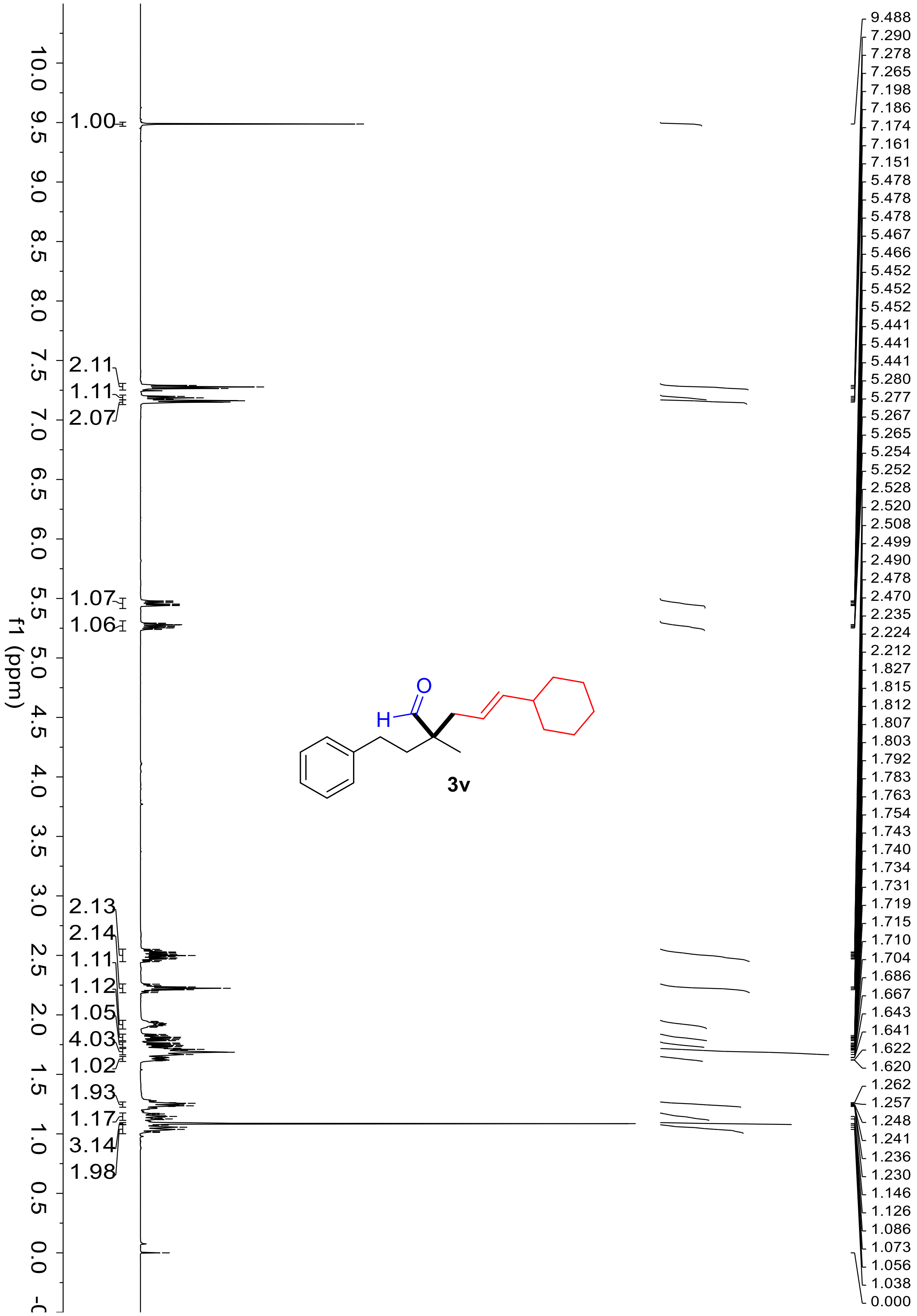
143.3
141.4
134.1
129.7
129.6
128.4
128.3
128.1
127.3
126.0
77.2
77.0
76.8
52.1
49.0
37.8
37.2
34.1
30.2
21.4
18.5
O
H
N
Ts
3u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



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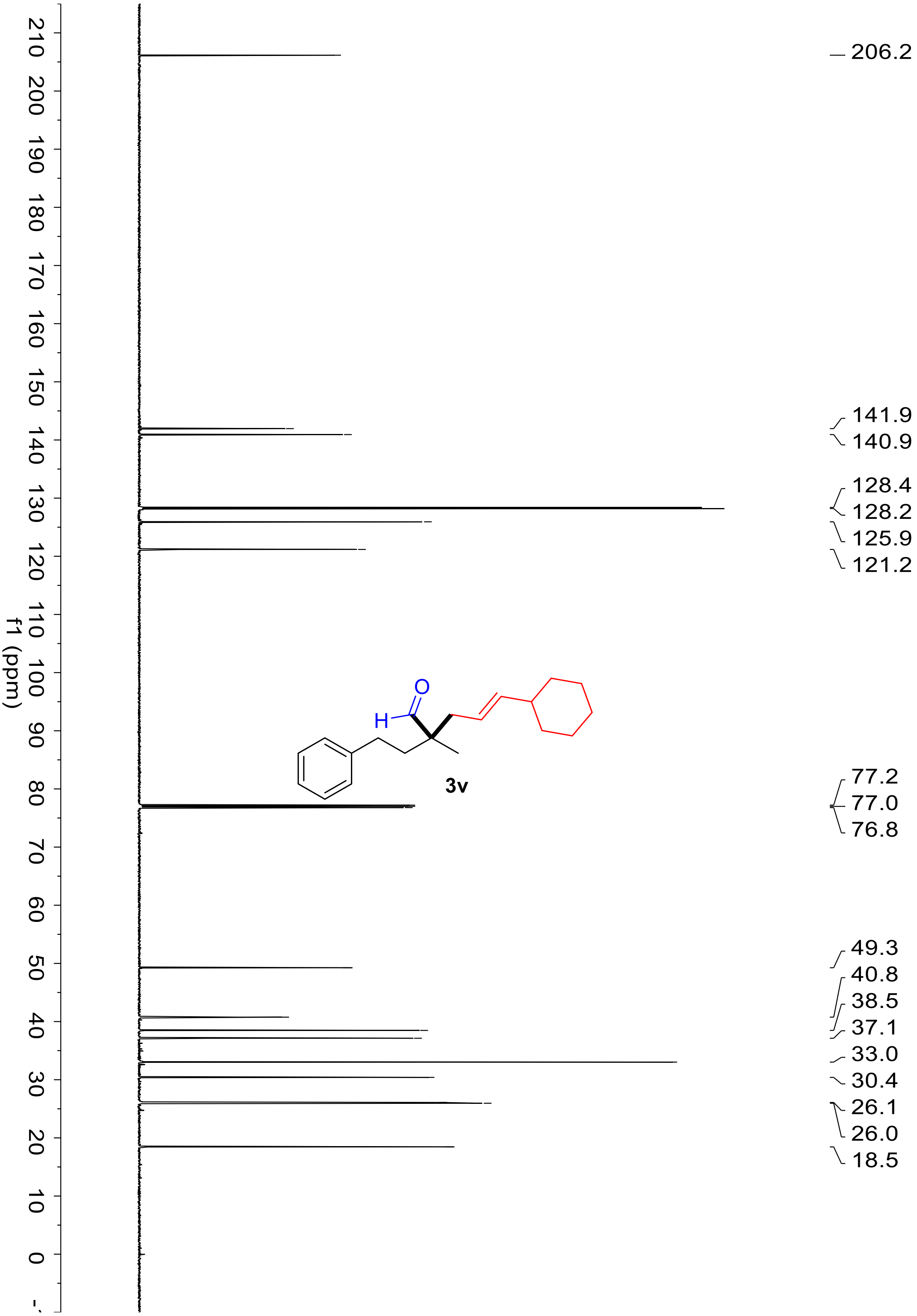
7.278
7.265
7.198
7.186
7.174
7.161
7.151
5.478
5.478
5.478
5.467
5.466
5.452
5.452
5.452
5.441
5.441
5.441
5.280
5.277
5.267
5.265
5.254
5.252
2.528
2.520
2.508
2.499
2.490
2.478
2.470
2.235
2.224
2.212
1.827
1.815
1.812
1.807
1.803
1.792
1.783
1.763
1.754
1.743
1.740
1.734
1.731
1.719
1.715
1.710
1.704
1.686
1.667
1.643
1.641
1.622
1.620
1.262
1.257
1.248
1.241
1.236
1.230
1.146
1.126
1.086
1.073
1.056
1.038
0.000
1.00
2.11
1.11
2.07
1.07
1.06
2.13
2.14
1.11
1.12
1.05
4.03
1.02
1.93
1.17
3.14
1.98
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)
O
H
3v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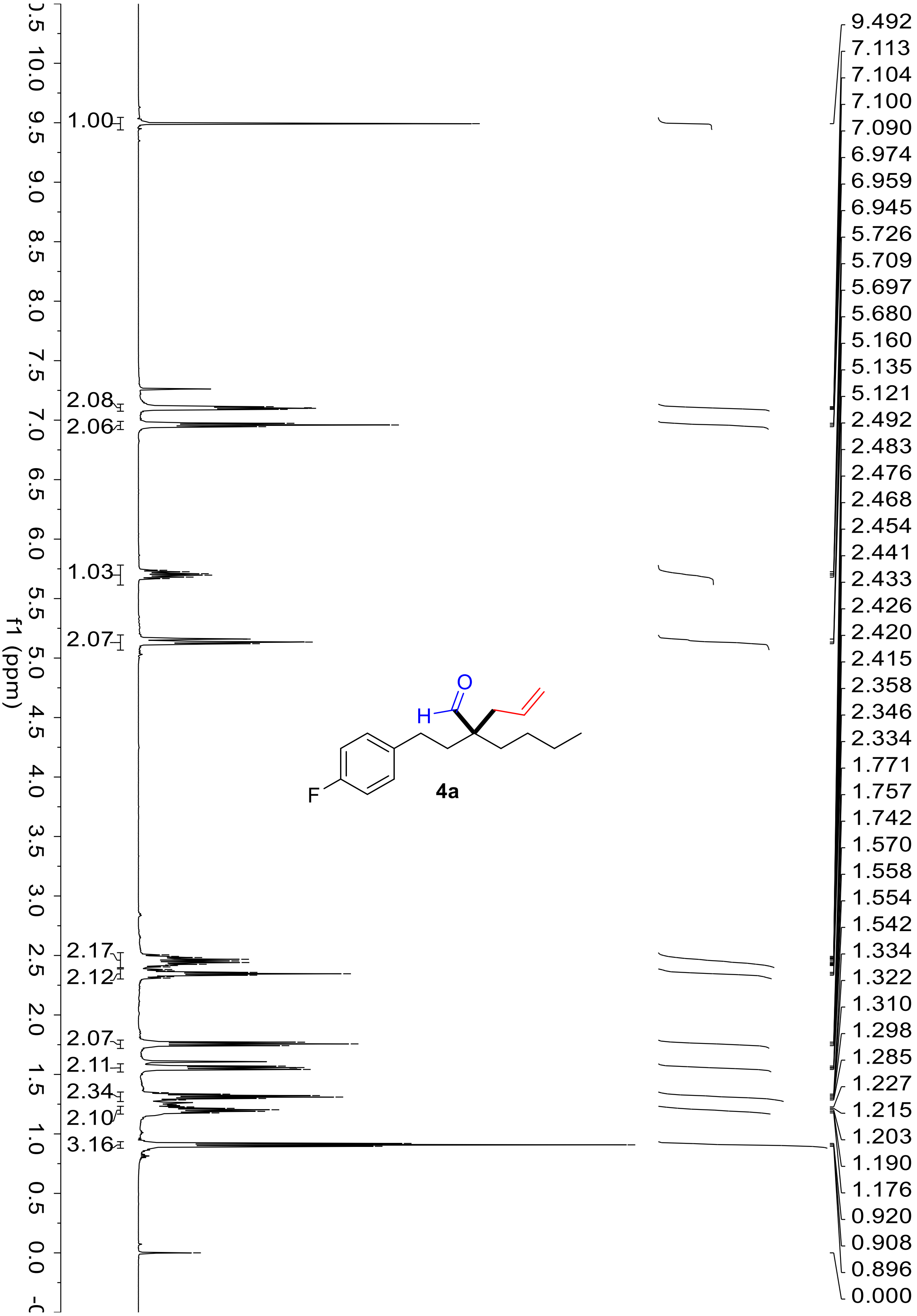
140.9
128.4
128.2
125.9
121.2
77.2
77.0
76.8
49.3
40.8
38.5
37.1
33.0
30.4
26.1
26.0
18.5
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
H
O
3v



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7.100
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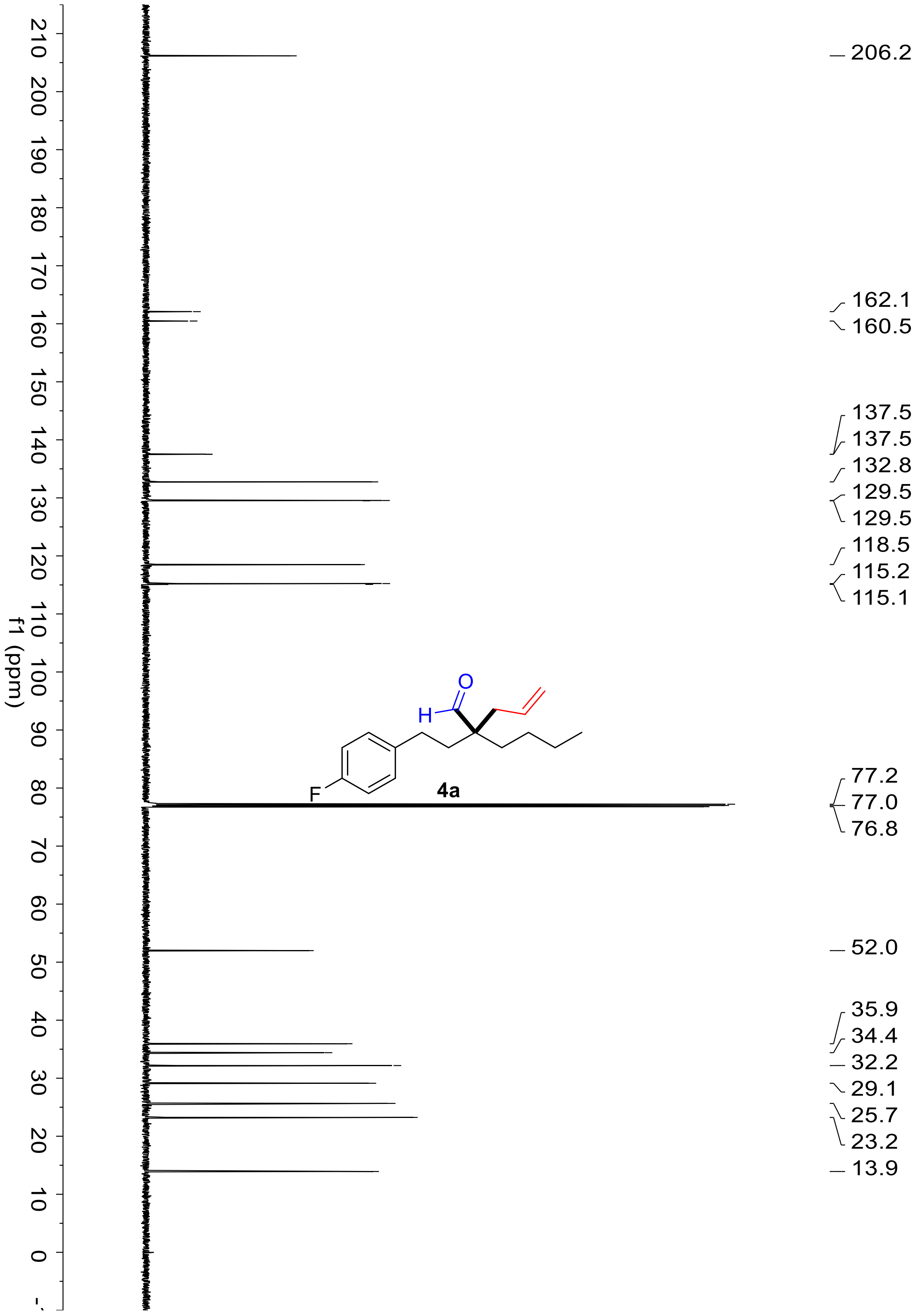
6.945
5.726
5.709
5.697
5.680
5.160
5.135
5.121
2.492
2.483
2.476
2.468
2.454
2.441
2.433
2.426
2.420
2.415
2.358
2.346
2.334
1.771
1.757
1.742
1.570
1.558
1.554
1.542
1.334
1.322
1.310
1.298
1.285
1.227
1.215
1.203
1.190
1.176
0.920
0.908
0.896
0.000
1.00
2.08
2.06
1.03
2.07
2.17
2.12
2.07
2.11
2.34
2.10
3.16
f1 (ppm)
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
-0.5
O
H
F
4a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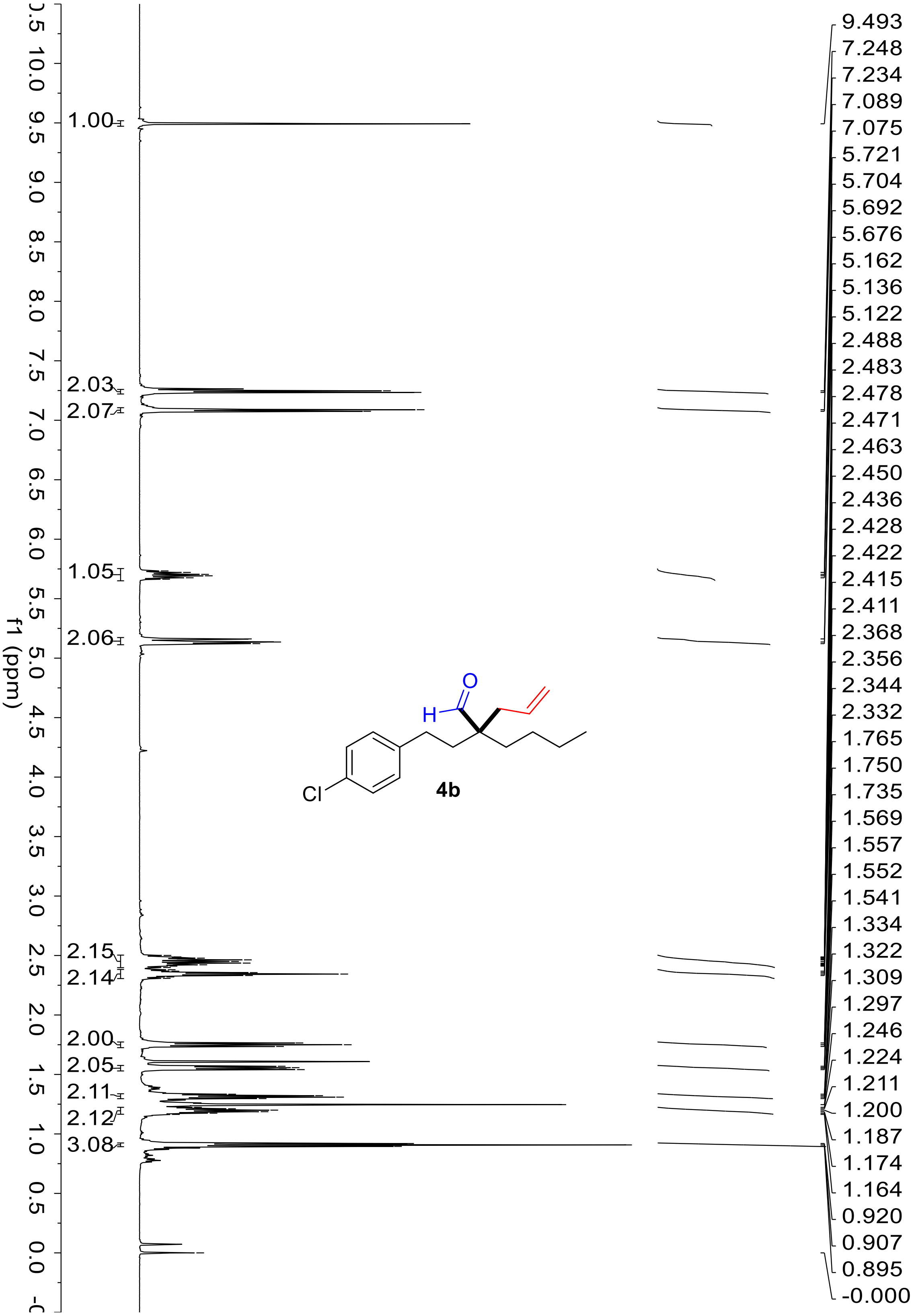
160.5
137.5
137.5
132.8
129.5
129.5
118.5
115.2
115.1
77.2
77.0
76.8
52.0
35.9
34.4
32.2
29.1
25.7
23.2
13.9
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
H
F
4a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7.234
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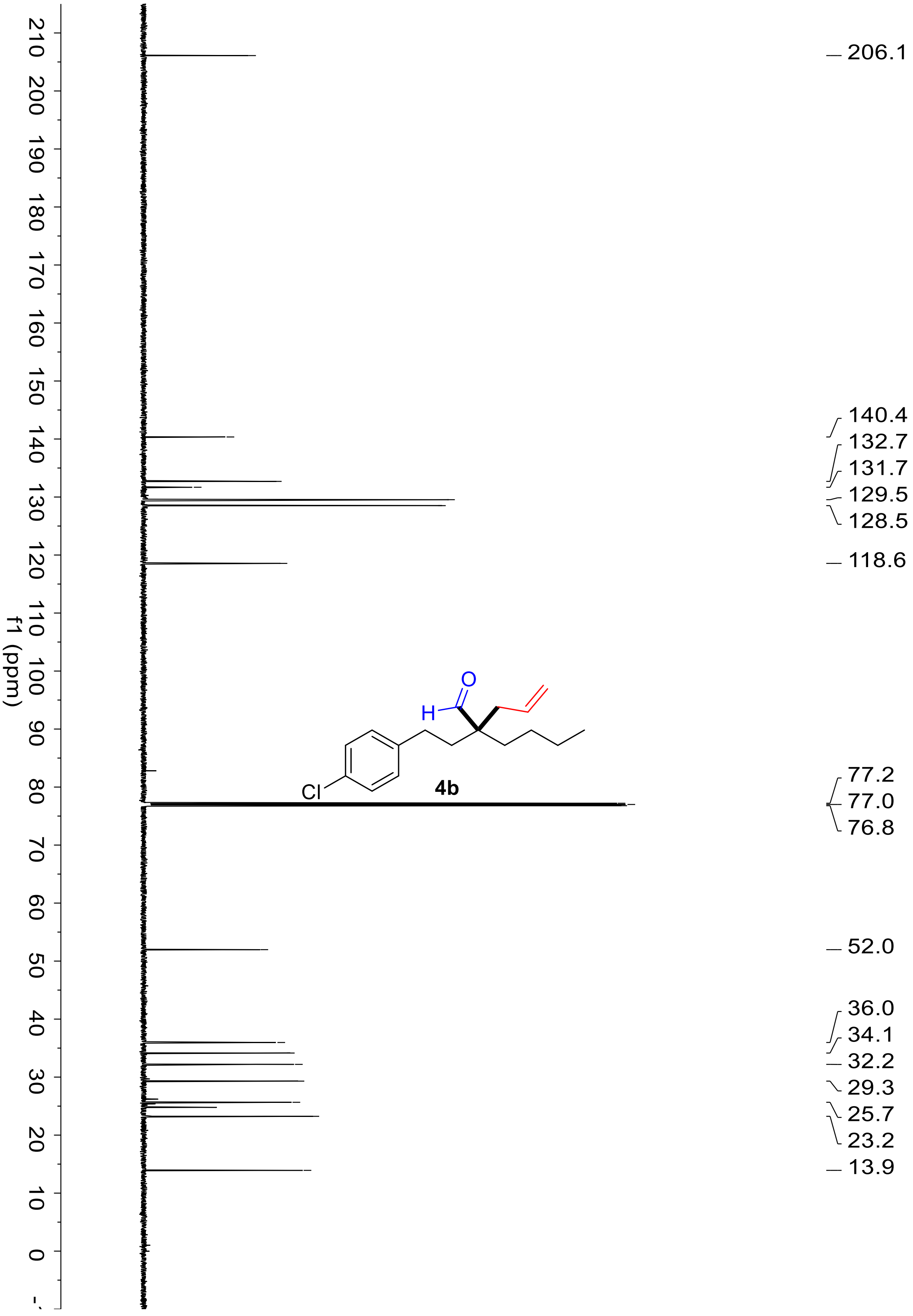
5.721
5.704
5.692
5.676
5.162
5.136
5.122
2.488
2.483
2.478
2.471
2.463
2.450
2.436
2.428
2.422
2.415
2.411
2.368
2.356
2.344
2.332
1.765
1.750
1.735
1.569
1.557
1.552
1.541
1.334
1.322
1.309
1.297
1.246
1.224
1.211
1.200
1.187
1.174
1.164
0.920
0.907
0.895
-0.000
1.00
2.03
2.07
1.05
2.06
2.15
2.14
2.00
2.05
2.11
2.12
3.08
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)
O
H
Cl

4b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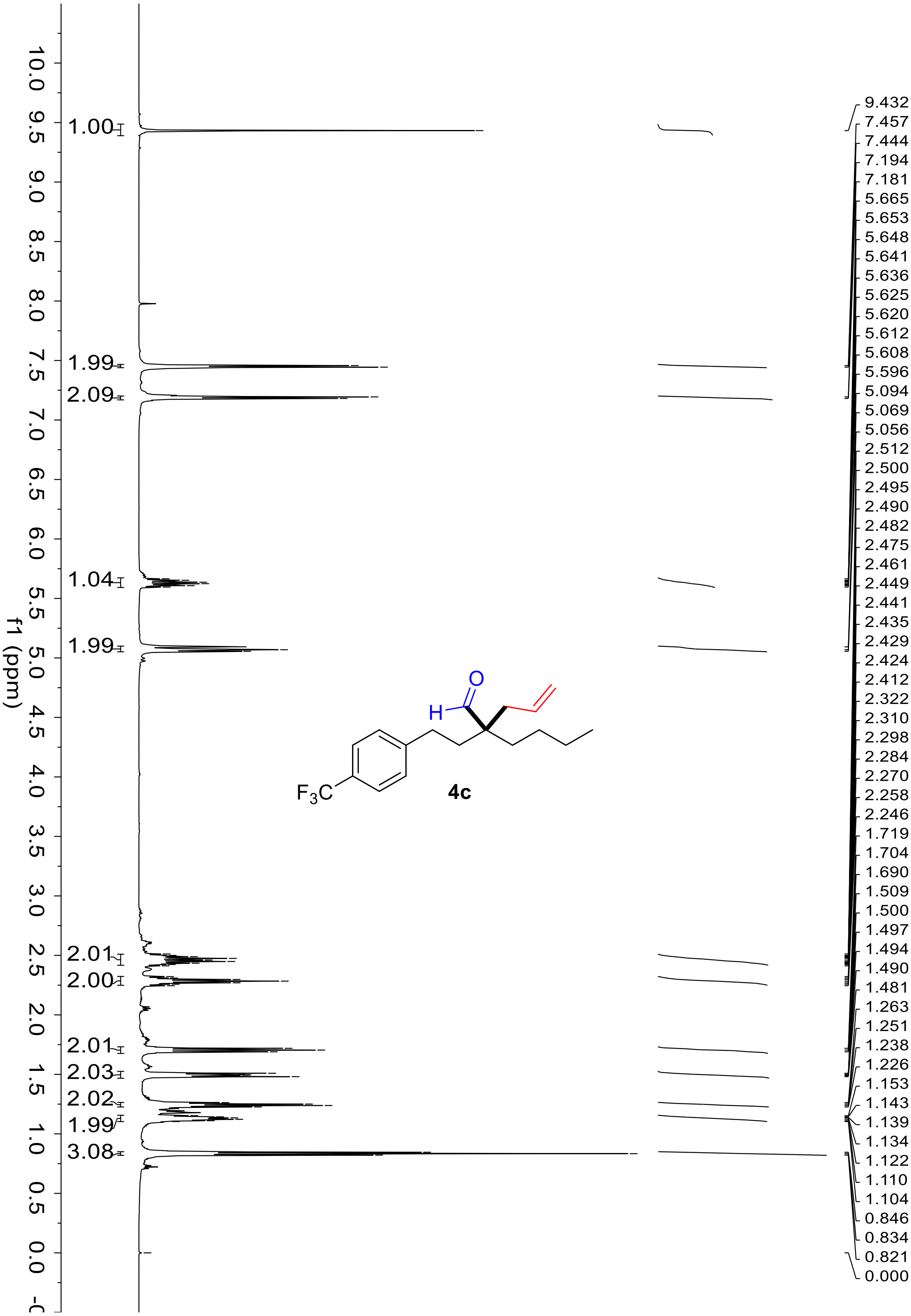
140.4
132.7
131.7
129.5
128.5
118.6
77.2
77.0
76.8
52.0
36.0
34.1
32.2
29.3
25.7
23.2
13.9
O
H
Cl
4b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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5.636
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5.620
5.612
5.608
5.596
5.094
5.069
5.056
2.512
2.500
2.495
2.490
2.482
2.475
2.461
2.449
2.441
2.435
2.429
2.424
2.412
2.322
2.310
2.298
2.284
2.270
2.258
2.246
1.719
1.704
1.690
1.509
1.500
1.497
1.494
1.490
1.481
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1.251
1.238
1.226
1.153
1.143
1.139
1.134
1.122
1.110
1.104
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0.834
0.821
0.000
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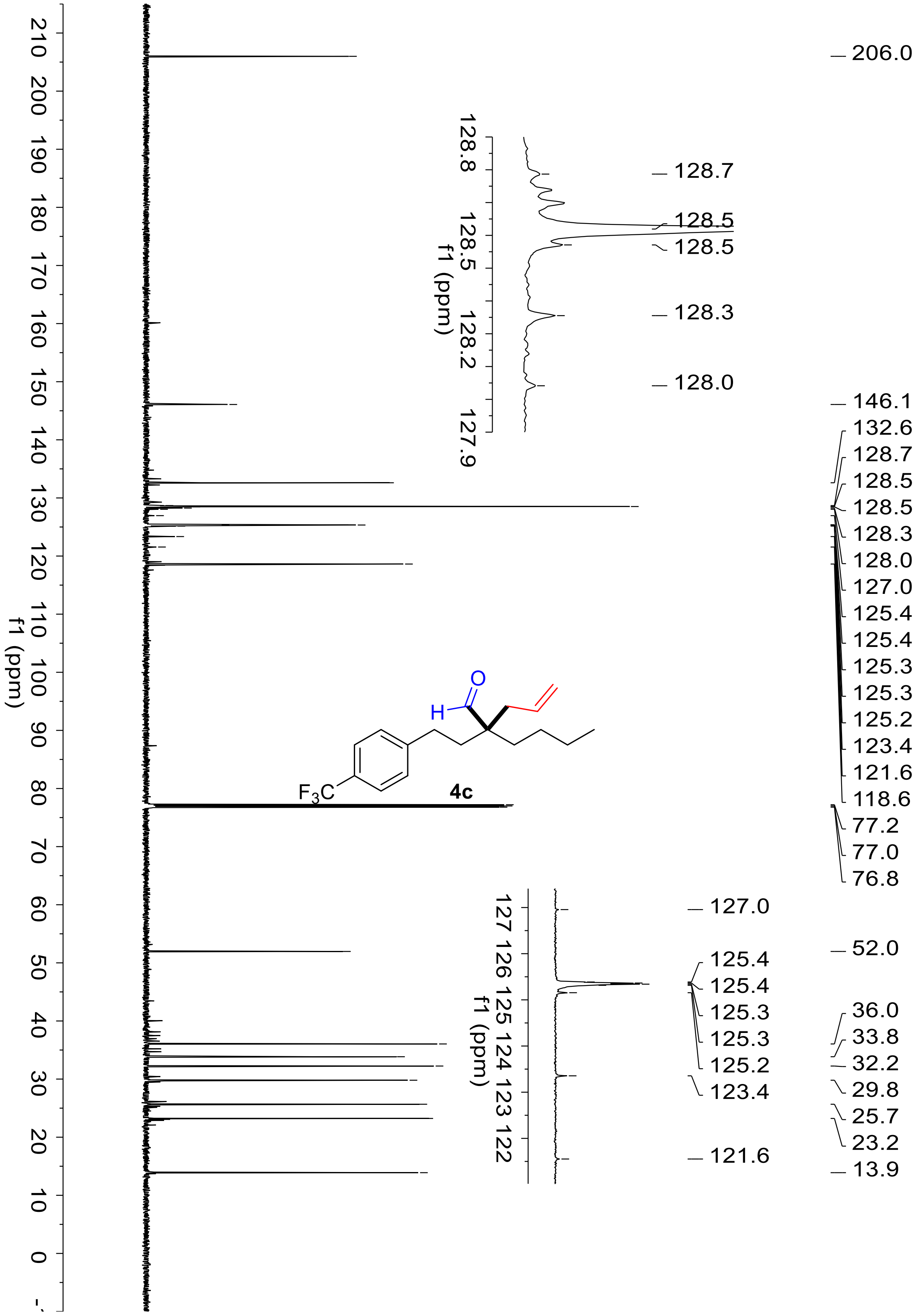
2.09
1.04
1.99
2.01
2.00
2.01
2.03
2.02
1.99
3.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-(
f1 (ppm)
O
H
F_3C

4c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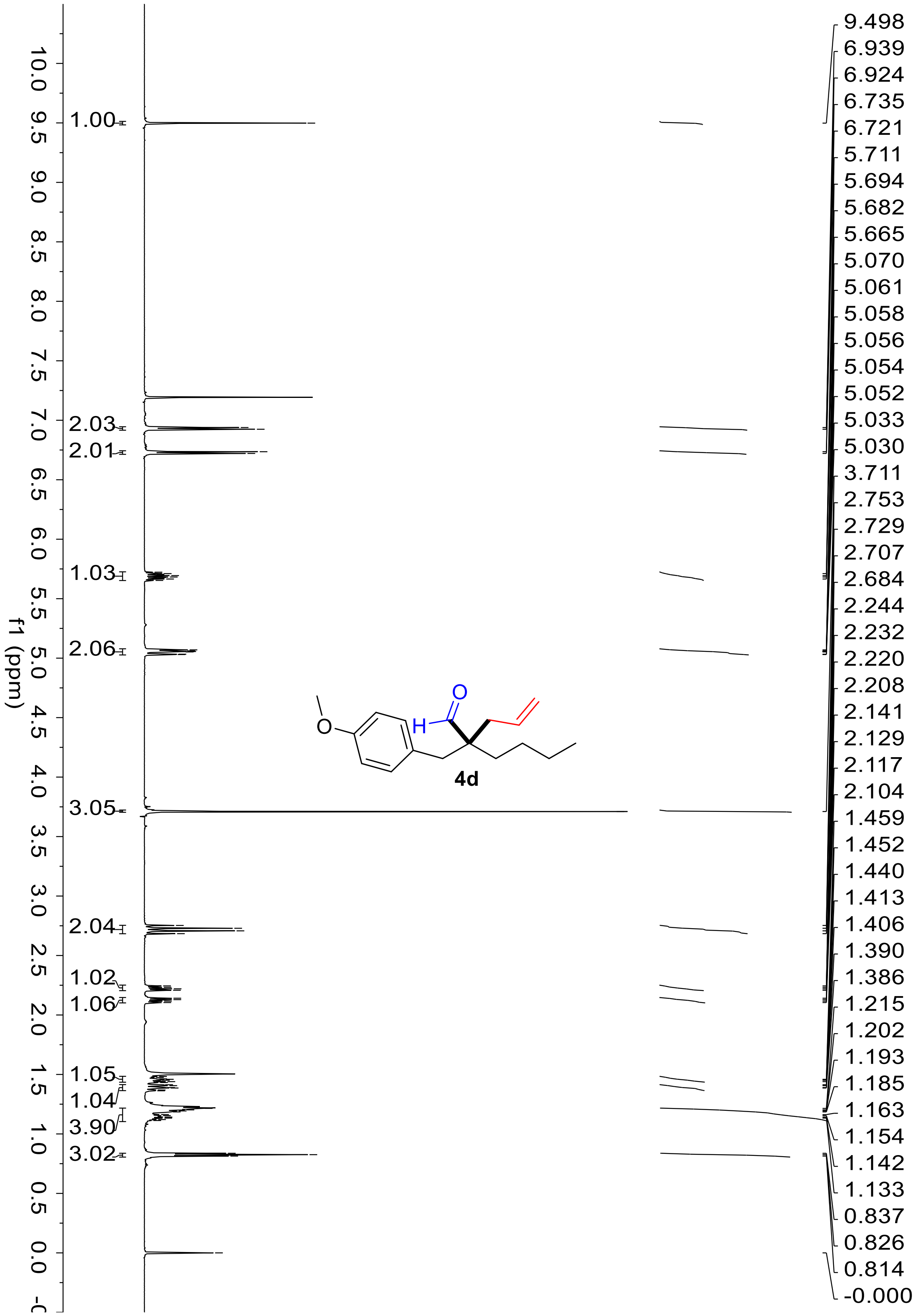
128.7
128.5
128.5
128.3
128.0
127.0
125.4
125.4
125.3
125.3
125.2
123.4
121.6
118.6
77.2
77.0
76.8
52.0
36.0
33.8
32.2
29.8
25.7
23.2
13.9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
128.8 128.5 128.2 127.9
f1 (ppm)
127 126 125 124 123 122
f1 (ppm)
O
H
F3C

4c


4d

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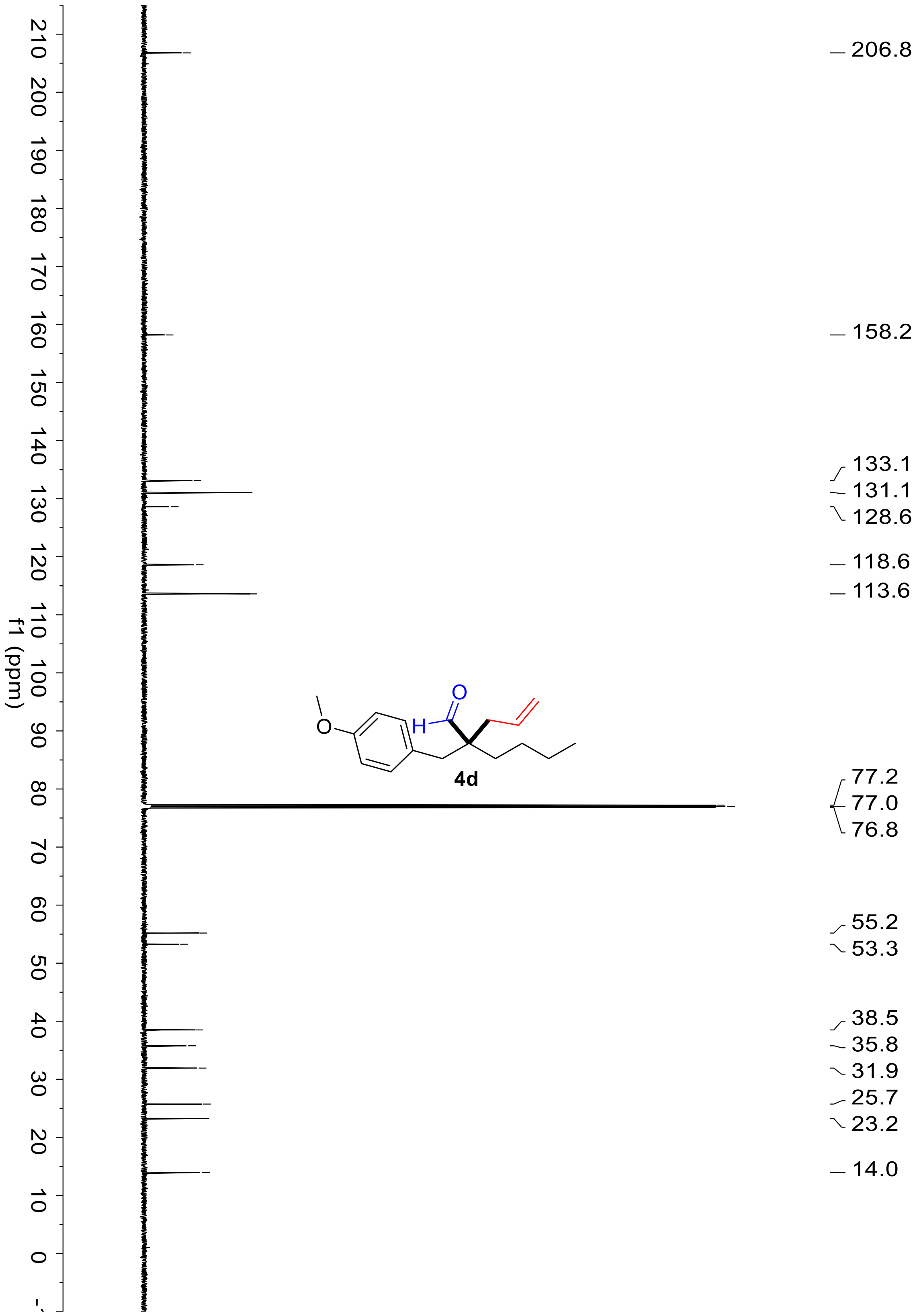
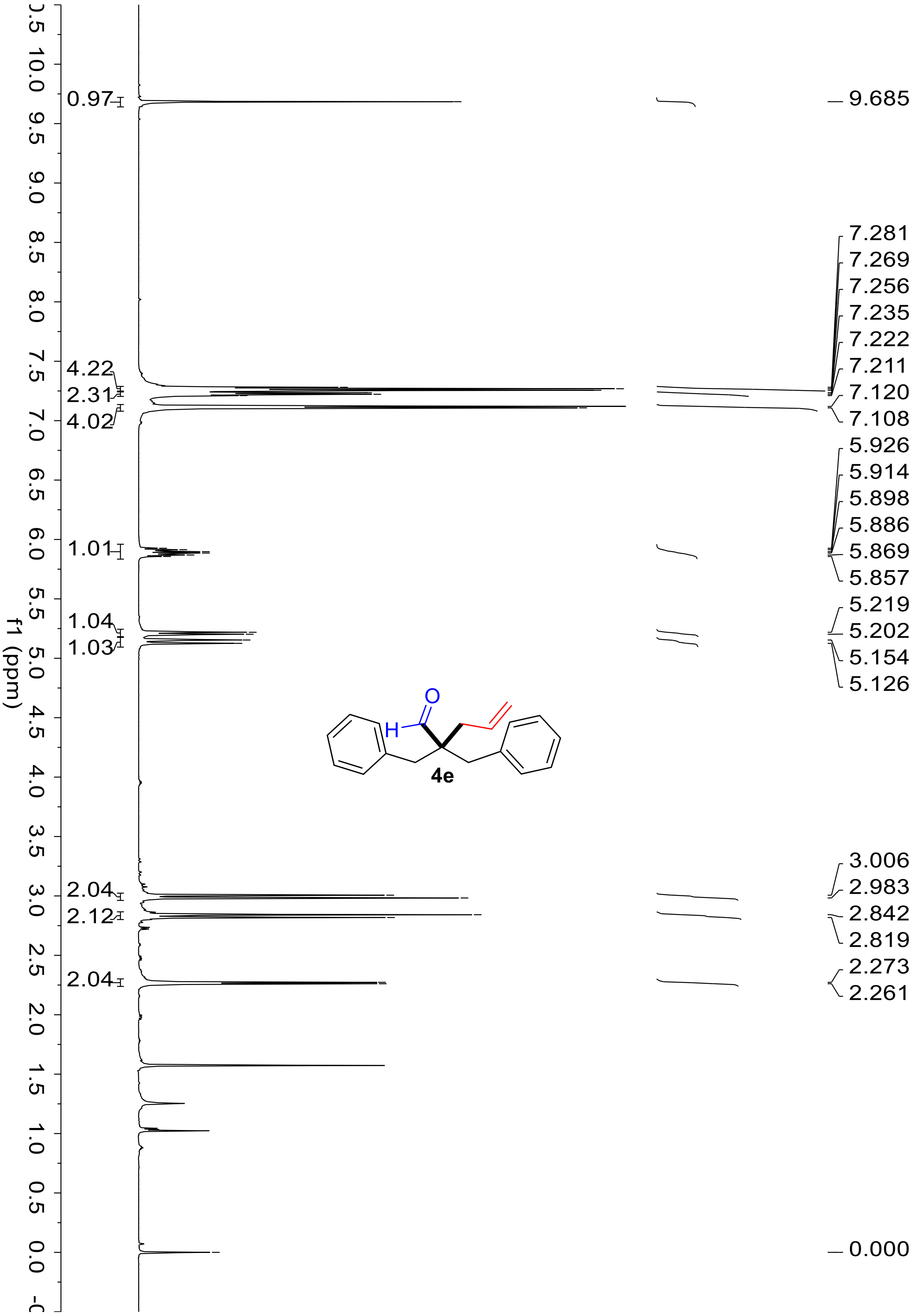
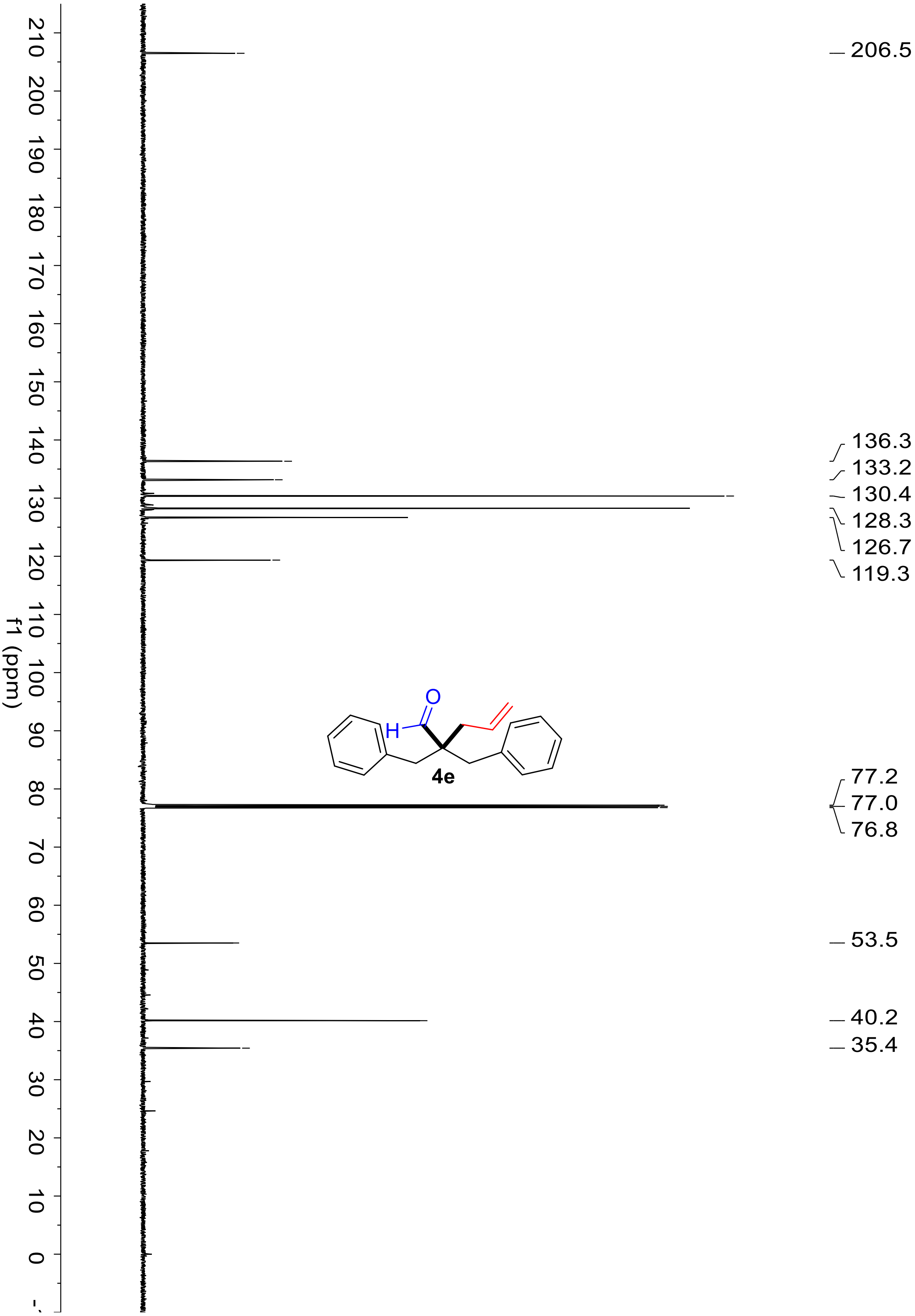
5.682
5.665
5.070
5.061
5.058
5.056
5.054
5.052
5.033
5.030
3.711
2.753
2.729
2.707
2.684
2.244
2.232
2.220
2.208
2.141
2.129
2.117
2.104
1.459
1.452
1.440
1.413
1.406
1.390
1.386
1.215
1.202
1.193
1.185
1.163
1.154
1.142
1.133
0.837
0.826
0.814
-0.000
1.00
2.03
2.01
1.03
2.06
3.05
2.04
1.02
1.06
1.05
1.04
3.90
3.02
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)
O
H
O

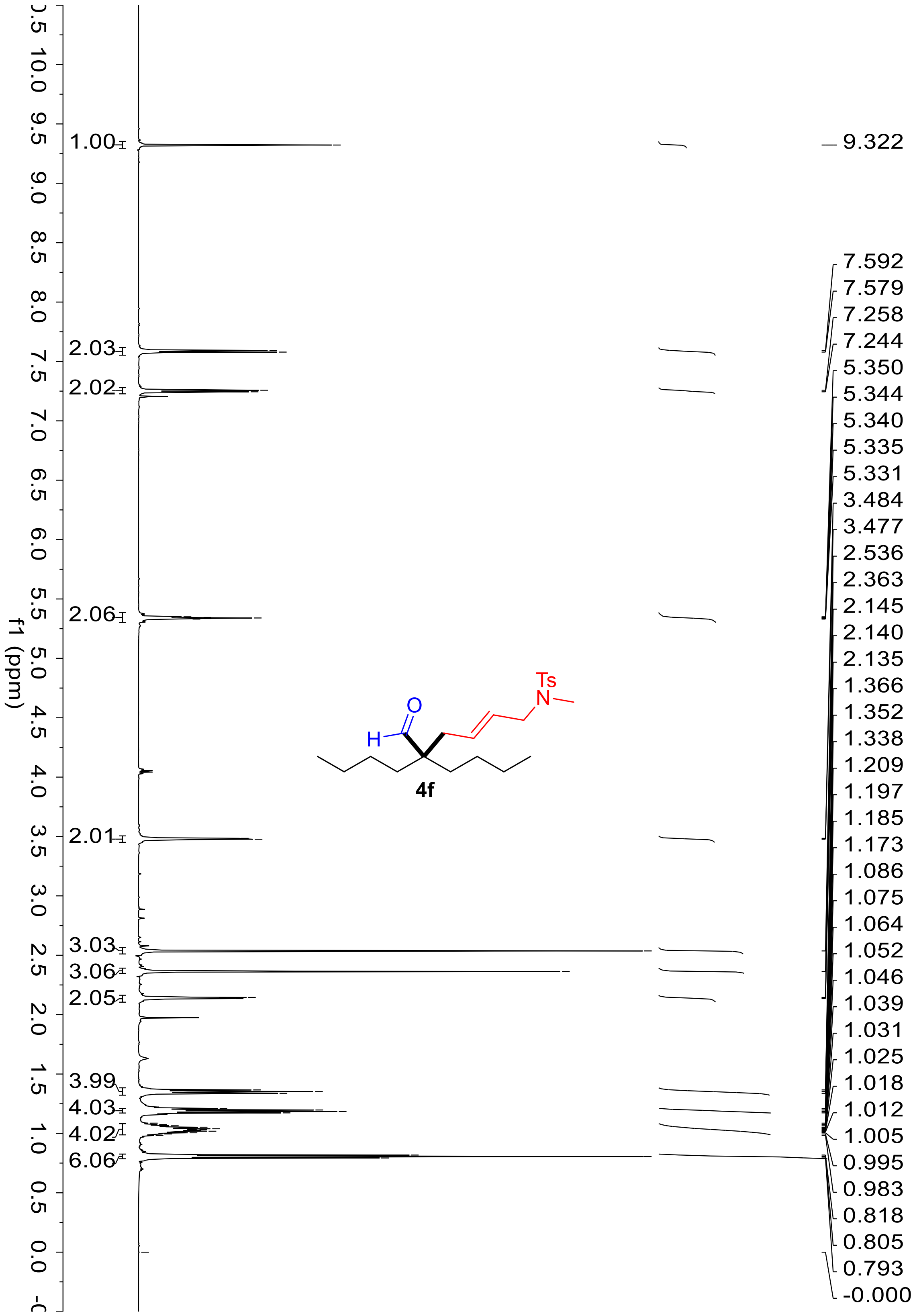

206.8
158.2
133.1
131.1
128.6
118.6
113.6
77.2
77.0
76.8
55.2
53.3
38.5
35.8
31.9
25.7
23.2
14.0
O
H
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -
f1 (ppm)

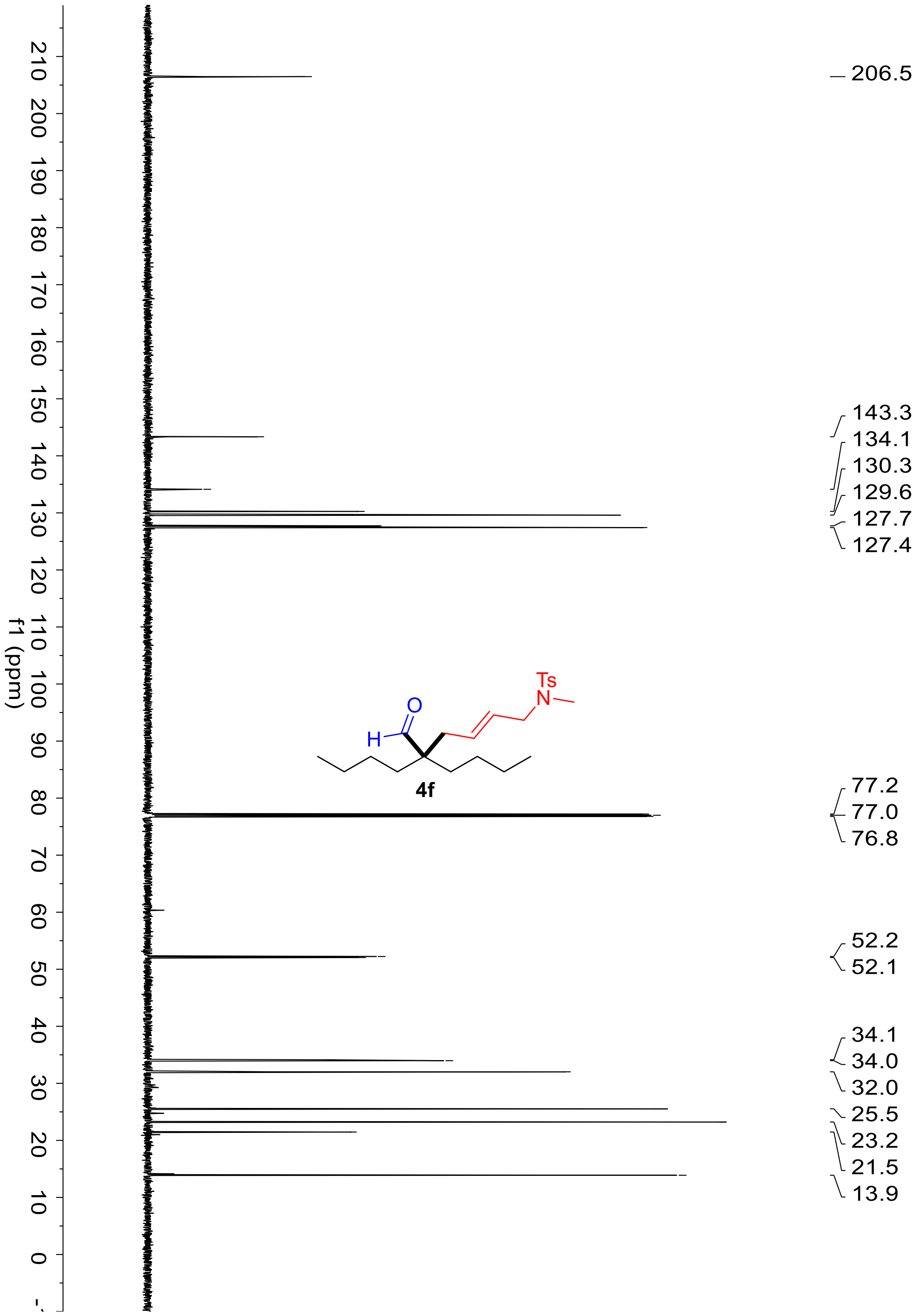
4d

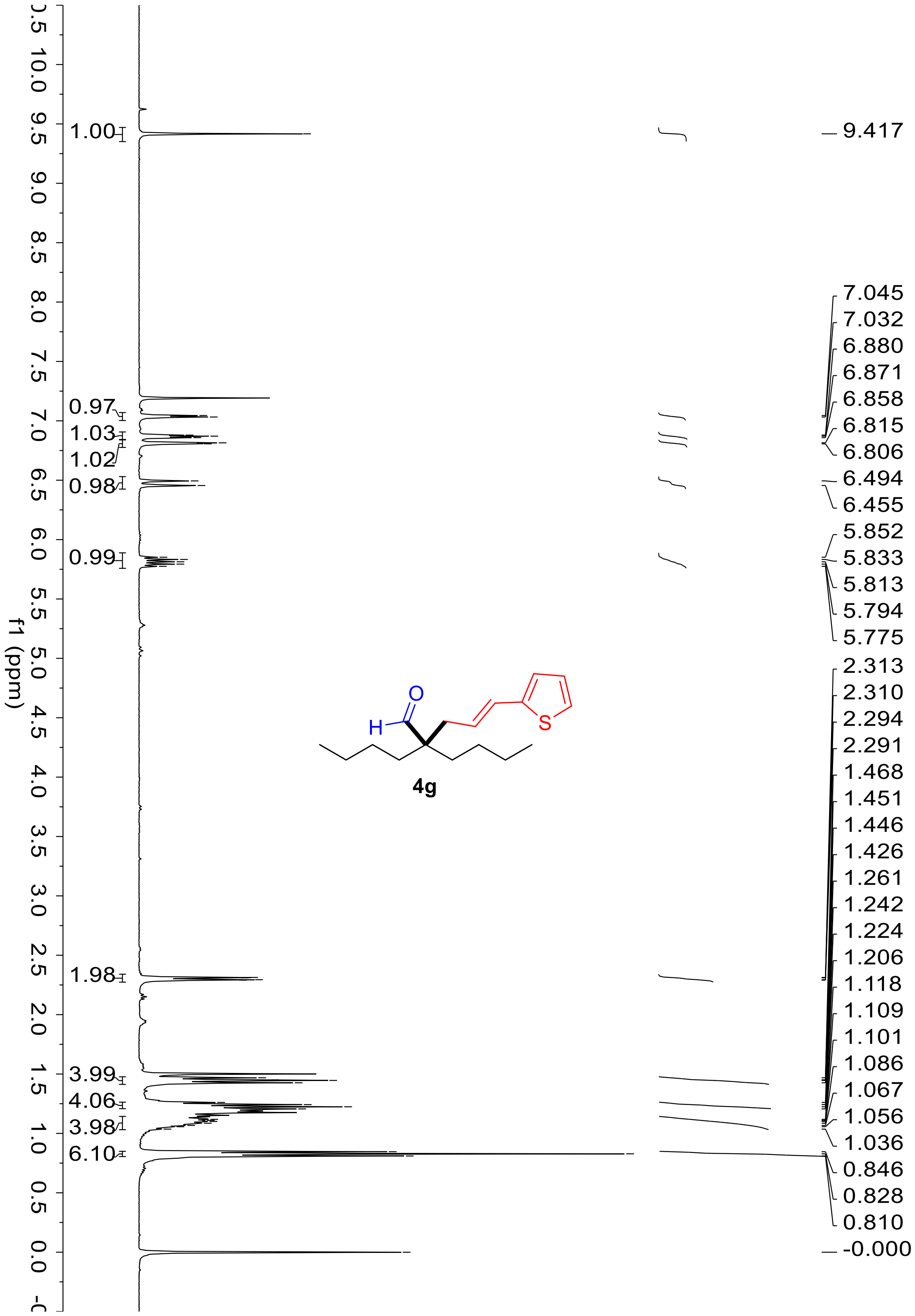


4e
f1 (ppm)
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
0.97
4.22
2.31
4.02
1.01
1.04
1.03
2.04
2.12
2.04
9.685
7.281
7.269
7.256
7.235
7.222
7.211
7.120
7.108
5.926
5.914
5.898
5.886
5.869
5.857
5.219
5.202
5.154
5.126
3.006
2.983
2.842
2.819
2.273
2.261
0.000
O
H

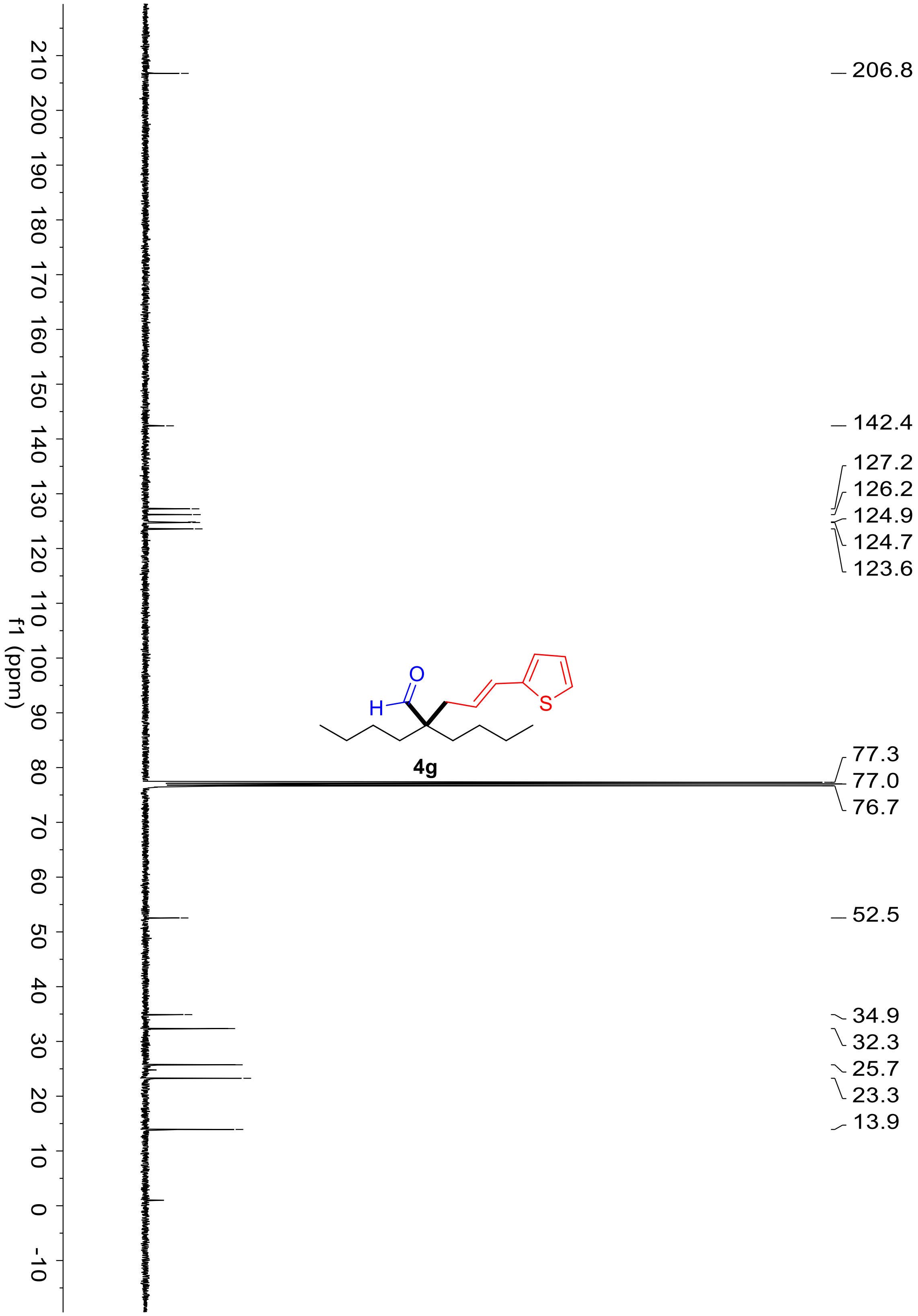

206.5
136.3
133.2
130.4
128.3
126.7
119.3
77.2
77.0
76.8
53.5
40.2
35.4
O
H
4e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

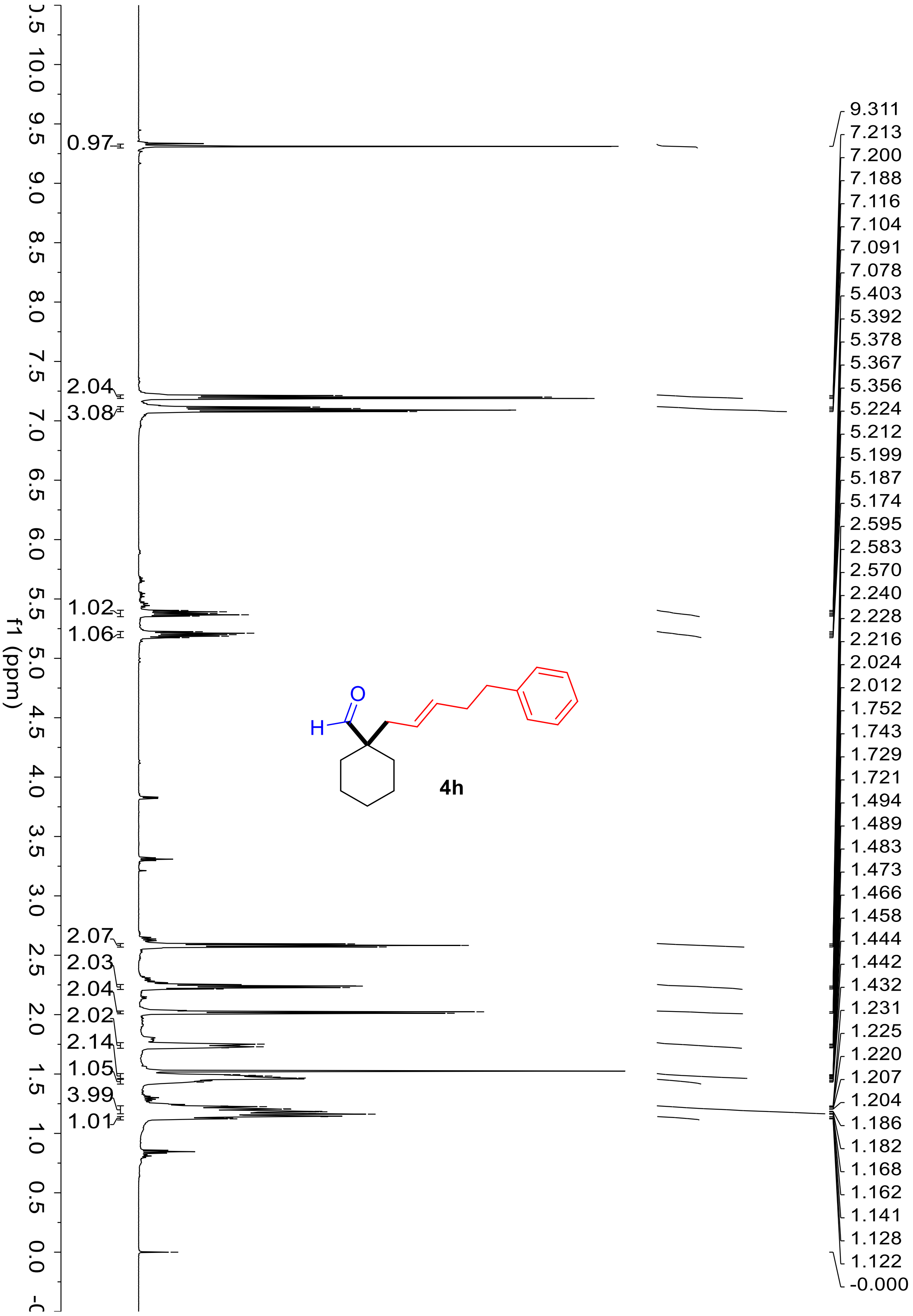

4f
Ts
N
O
H
f1 (ppm)
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1.00
2.03
2.02
2.06
2.01
3.03
3.06
2.05
3.99
4.03
4.02
6.06
9.322
7.592
7.579
7.258
7.244
5.350
5.344
5.340
5.335
5.331
3.484
3.477
2.536
2.363
2.145
2.140
2.135
1.366
1.352
1.338
1.209
1.197
1.185
1.173
1.086
1.075
1.064
1.052
1.046
1.039
1.031
1.025
1.018
1.012
1.005
0.995
0.983
0.818
0.805
0.793
-0.000


206.5
143.3
134.1
130.3
129.6
127.7
127.4
77.2
77.0
76.8
52.2
52.1
34.1
34.0
32.0
25.5
23.2
21.5
13.9
Ts
N
O
H
4f
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


9.5
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
0.97
1.03
1.02
0.98
0.99
1.98
3.99
4.06
3.98
6.10
9.417
7.045
7.032
6.880
6.871
6.858
6.815
6.806
6.494
6.455
5.852
5.833
5.813
5.794
5.775
2.313
2.310
2.294
2.291
1.468
1.451
1.446
1.426
1.261
1.242
1.224
1.206
1.118
1.109
1.101
1.086
1.067
1.056
1.036
0.846
0.828
0.810
-0.000
H
O
S

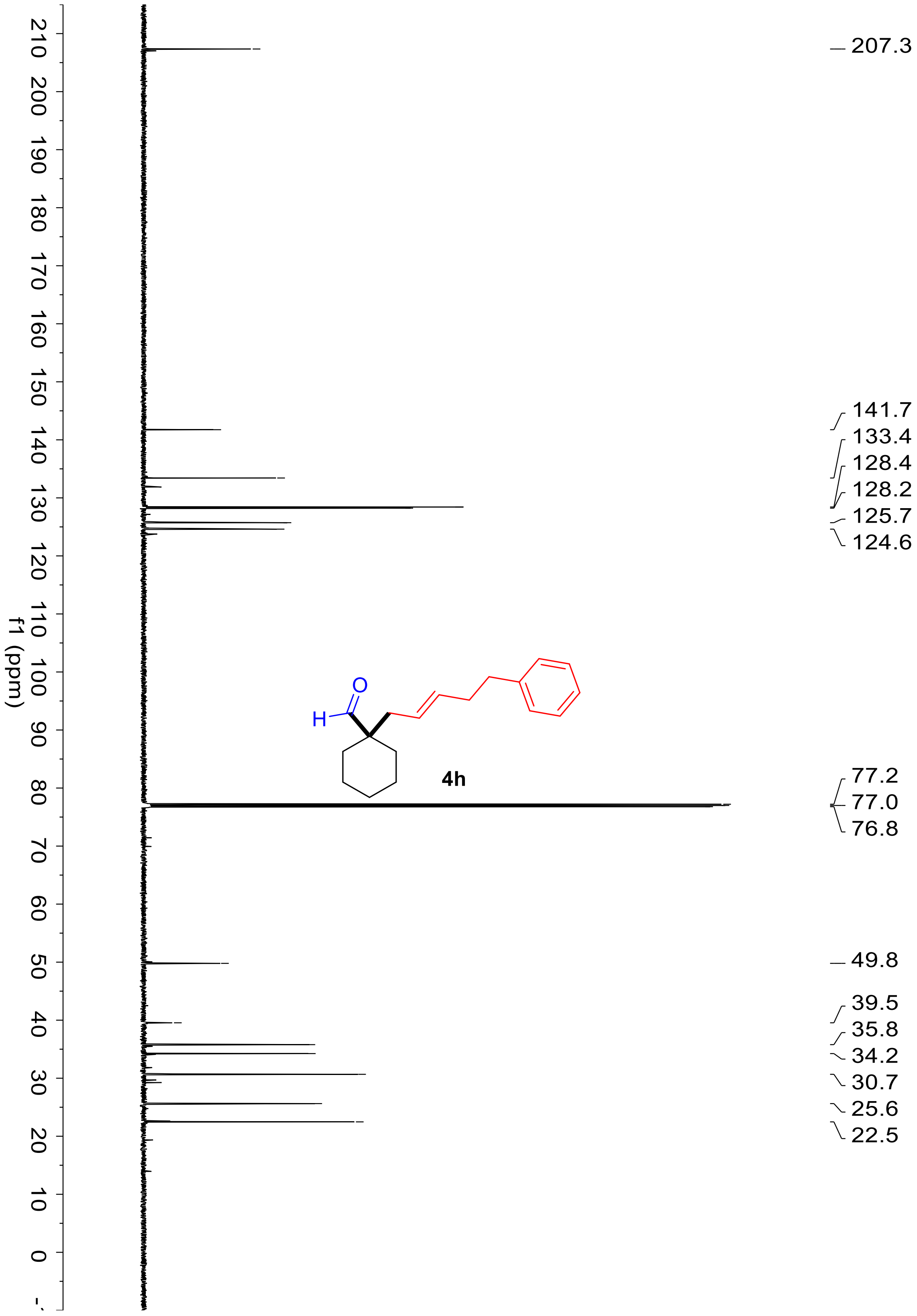
4g

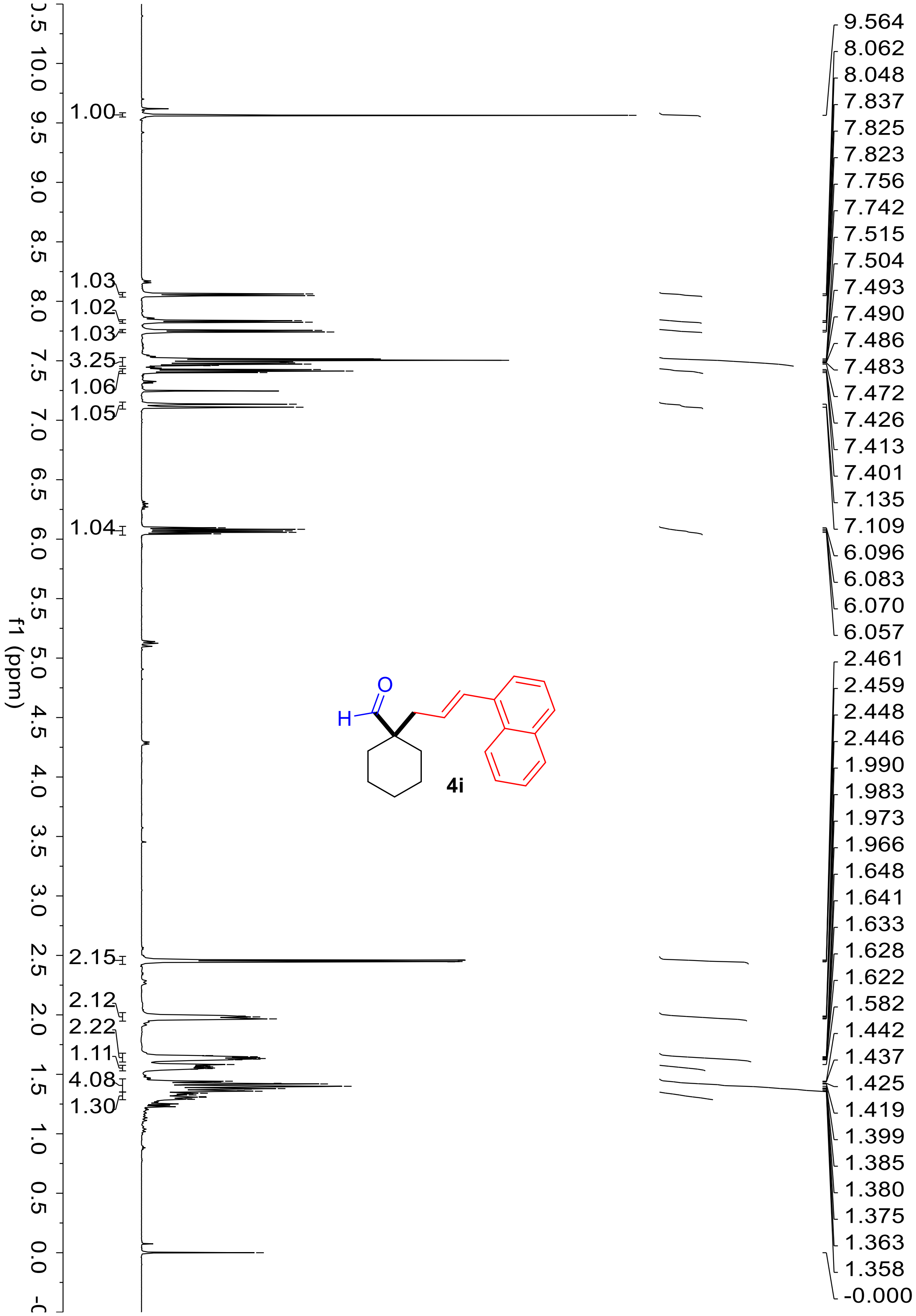

206.8
142.4
127.2
126.2
124.9
124.7
123.6
77.3
77.0
76.7
52.5
34.9
32.3
25.7
23.3
13.9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
O
H
S
4g



4h

f1 (ppm)
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
0.97
2.04
3.08
1.02
1.06
2.07
2.03
2.04
2.02
2.14
1.05
3.99
1.01
9.311
7.213
7.200
7.188
7.116
7.104
7.091
7.078
5.403
5.392
5.378
5.367
5.356
5.224
5.212
5.199
5.187
5.174
2.595
2.583
2.570
2.240
2.228
2.216
2.024
2.012
1.752
1.743
1.729
1.721
1.494
1.489
1.483
1.473
1.466
1.458
1.444
1.442
1.432
1.231
1.225
1.220
1.207
1.204
1.186
1.182
1.168
1.162
1.141
1.128
1.122
-0.000
O
H


207.3
141.7
133.4
128.4
128.2
125.7
124.6
77.2
77.0
76.8
49.8
39.5
35.8
34.2
30.7
25.6
22.5
O
H
4h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



).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
1.03
1.02
1.03
3.25
1.06
1.05
1.04
2.15
2.12
2.22
1.11
4.08
1.30
O
H
4i
9.564
8.062
8.048
7.837
7.825
7.823
7.756
7.742
7.515
7.504
7.493
7.490
7.486
7.483
7.472
7.426
7.413
7.401
7.135
7.109
6.096
6.083
6.070
6.057
2.461
2.459
2.448
2.446
1.990
1.983
1.973
1.966
1.648
1.641
1.633
1.628
1.622
1.582
1.442
1.437
1.425
1.419
1.399
1.385
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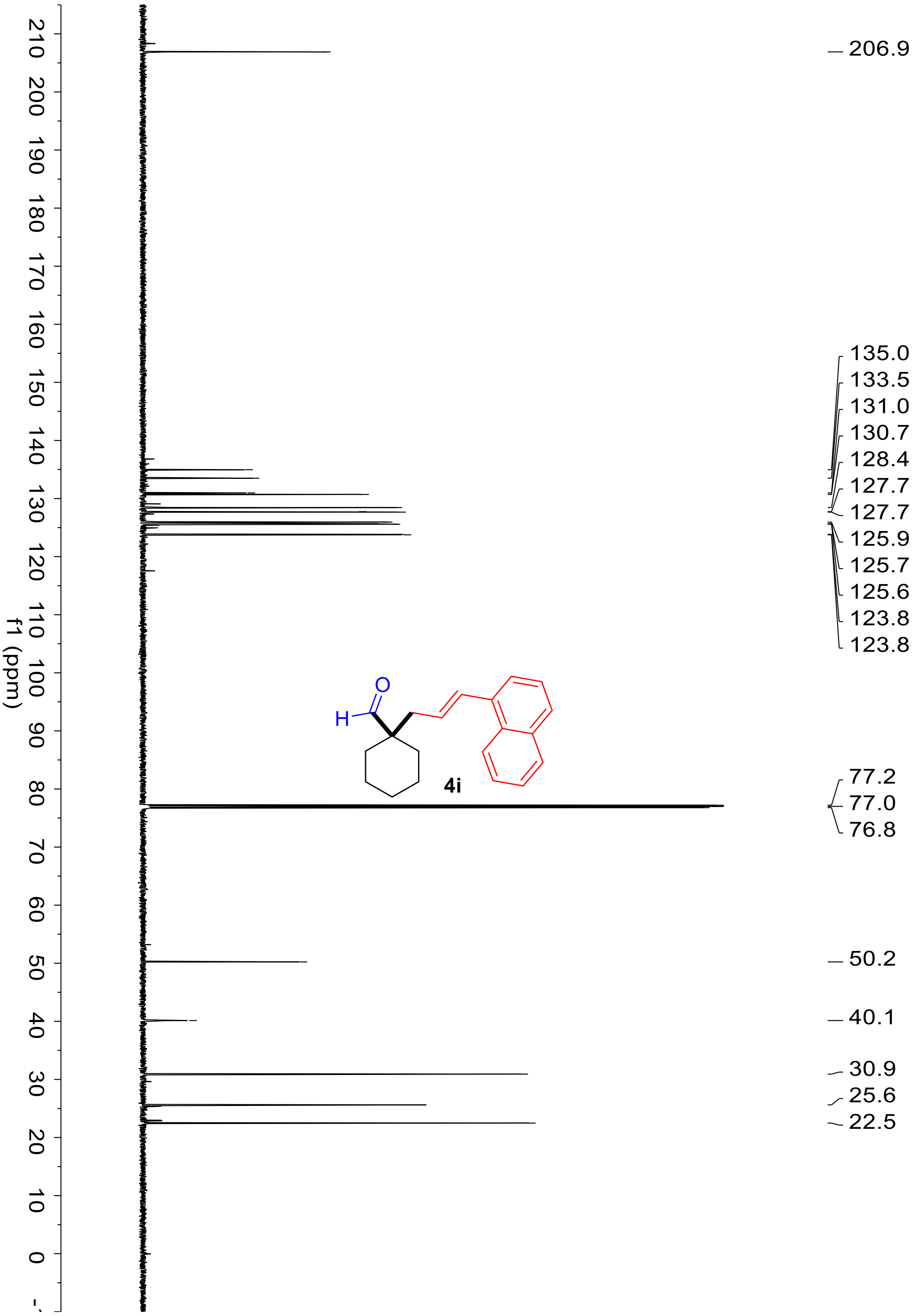
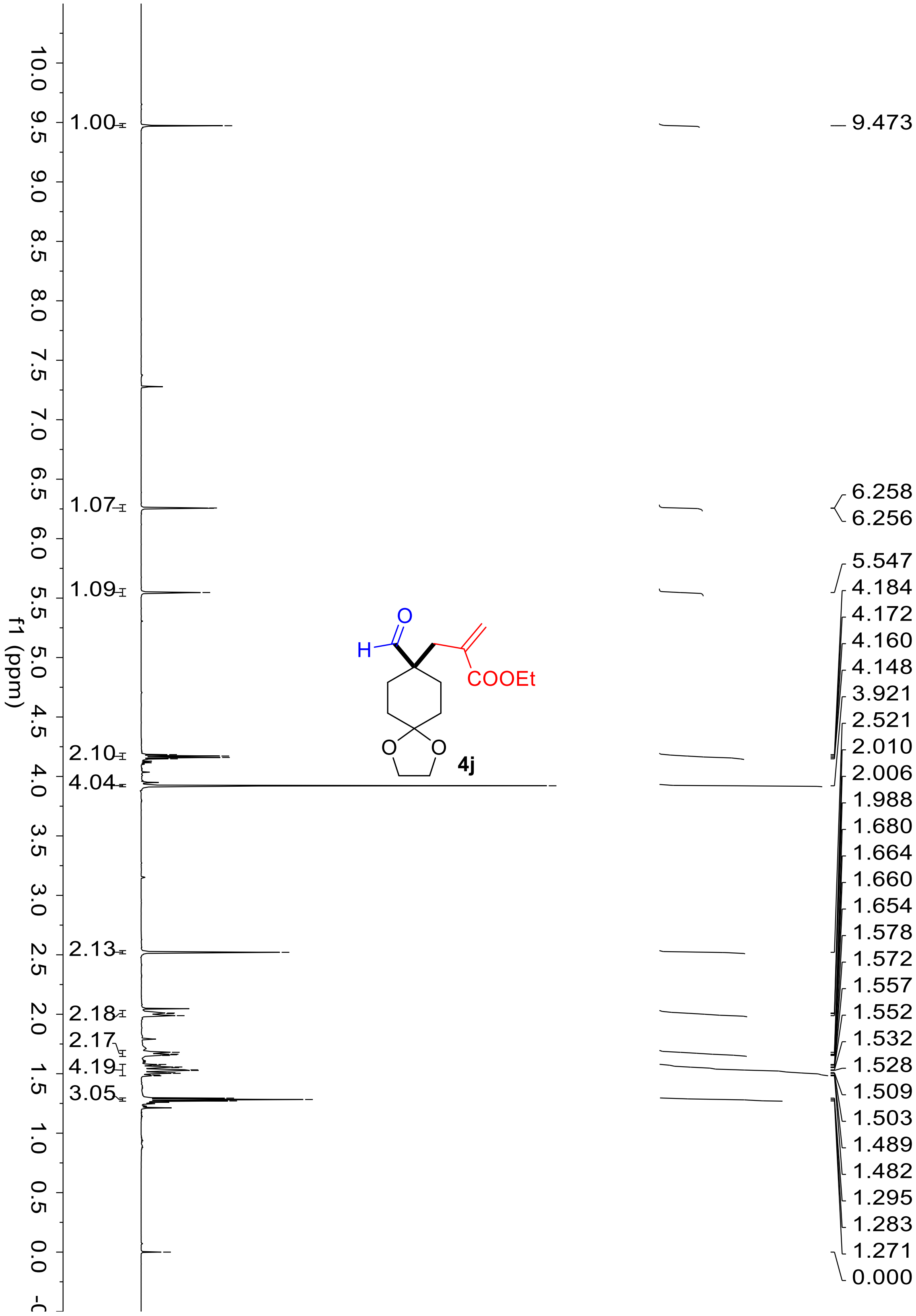
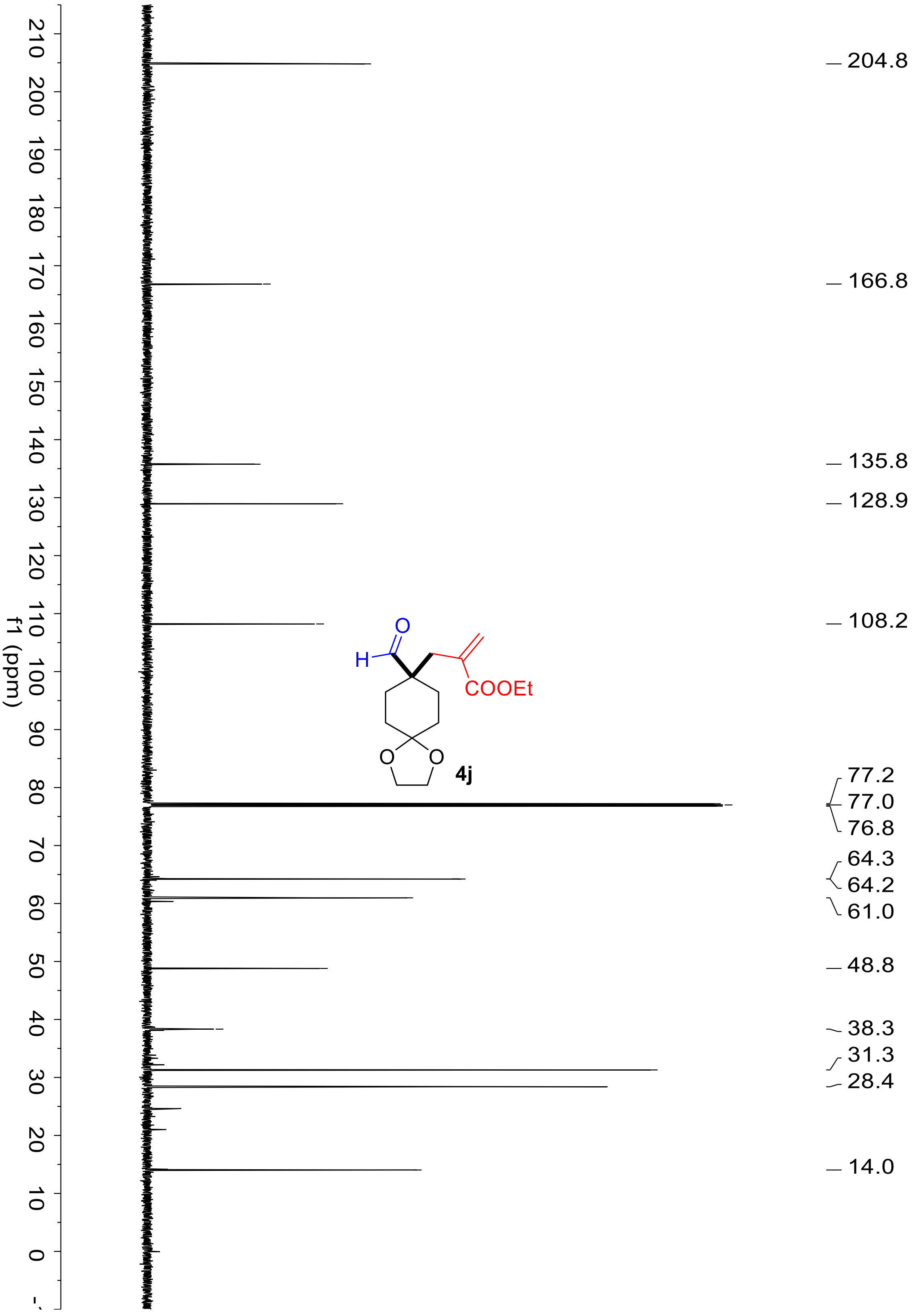
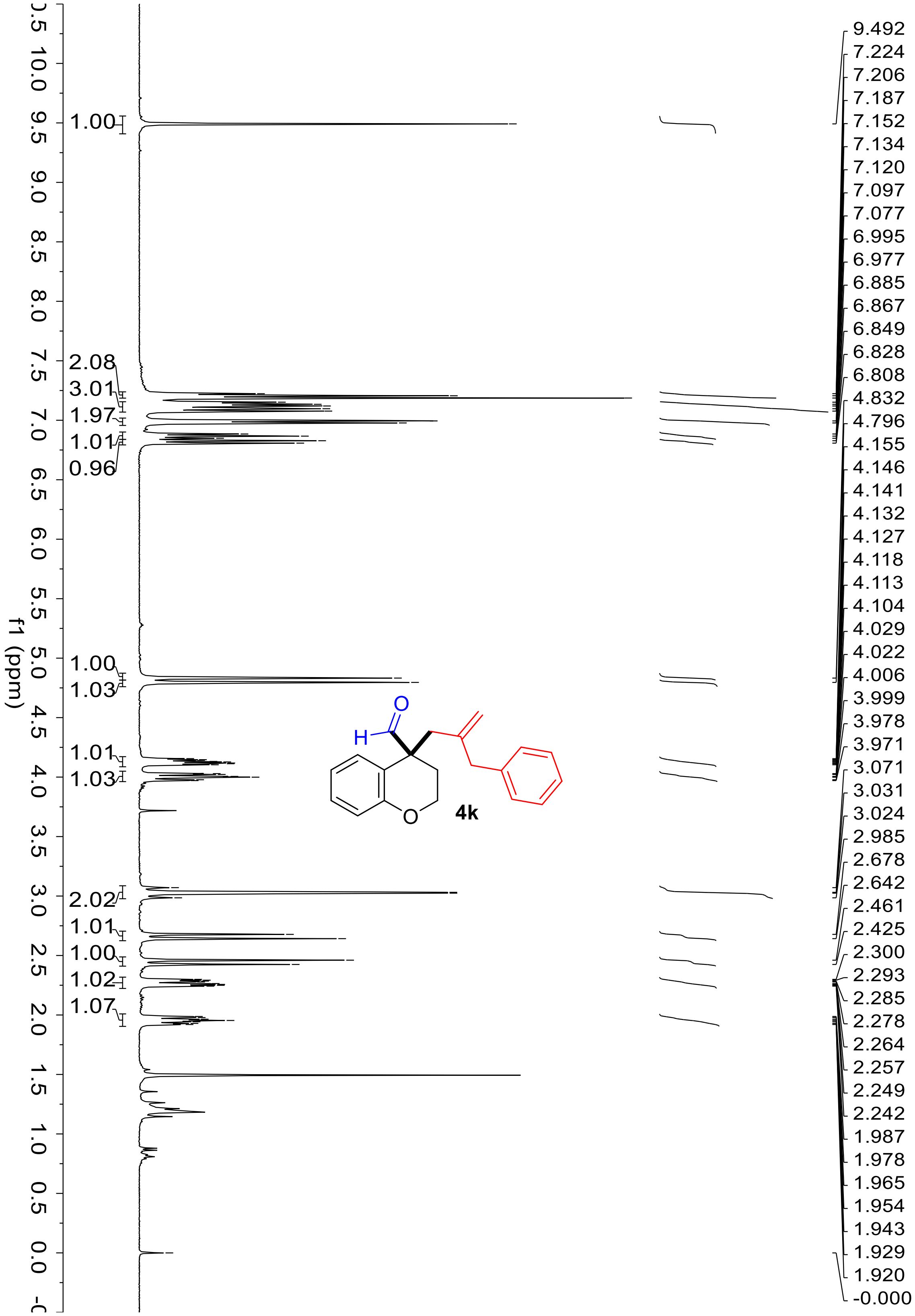
1.375
1.363
1.358
-0.000


206.9
135.0
133.5
131.0
130.7
128.4
127.7
127.7
125.9
125.7
125.6
123.8
123.8
77.2
77.0
76.8
50.2
40.1
30.9
25.6
22.5
H
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

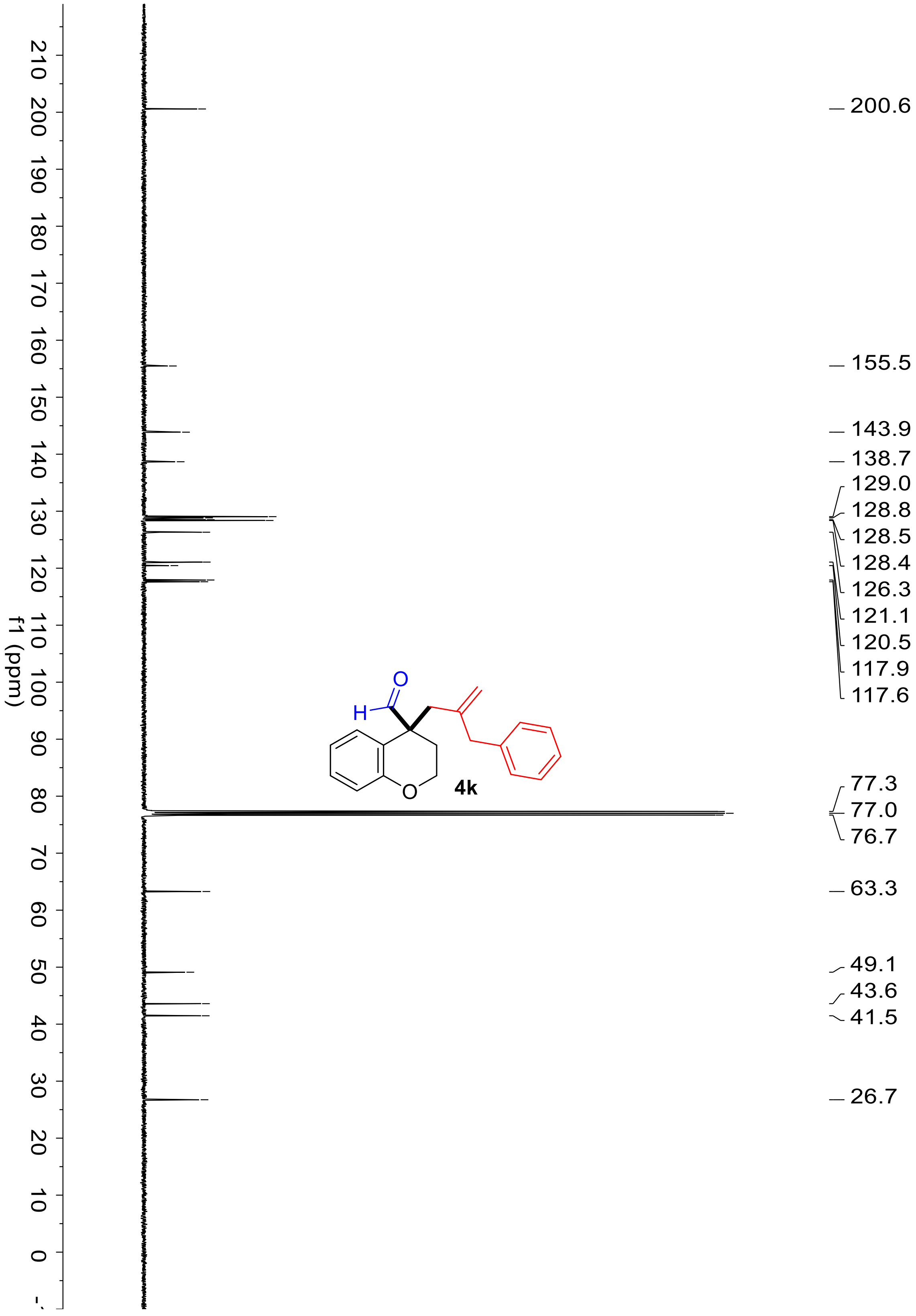
4i

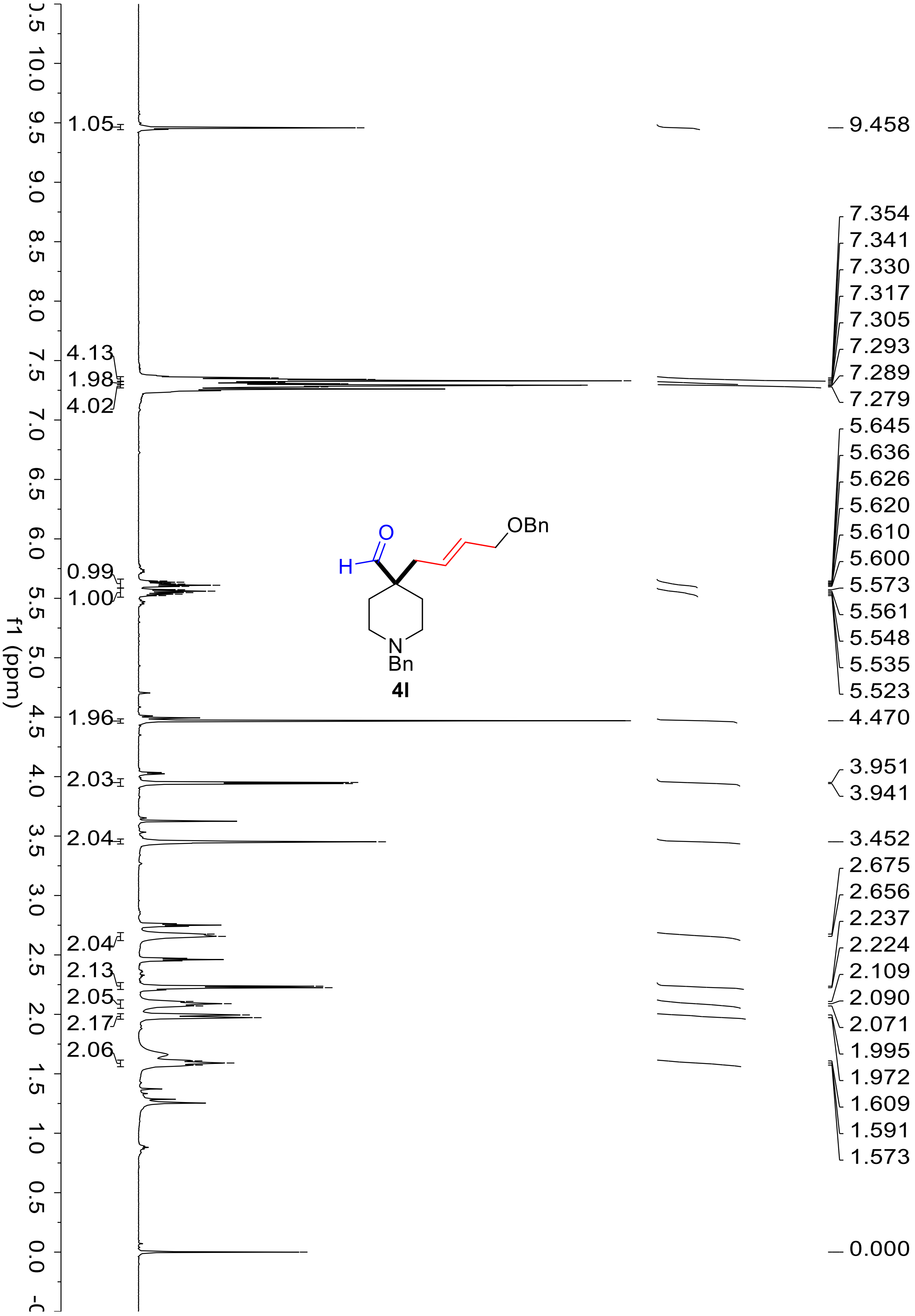

4j
H
O
COOEt
O
O
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
1.00
1.07
1.09
2.10
4.04
2.13
2.18
2.17
4.19
3.05
9.473
6.258
6.256
5.547
4.184
4.172
4.160
4.148
3.921
2.521
2.010
2.006
1.988
1.680
1.664
1.660
1.654
1.578
1.572
1.557
1.552
1.532
1.528
1.509
1.503
1.489
1.482
1.295
1.283
1.271
0.000


4j
H
O
COOEt
O
O
204.8
166.8
135.8
128.9
108.2
77.2
77.0
76.8
64.3
64.2
61.0
48.8
38.3
31.3
28.4
14.0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

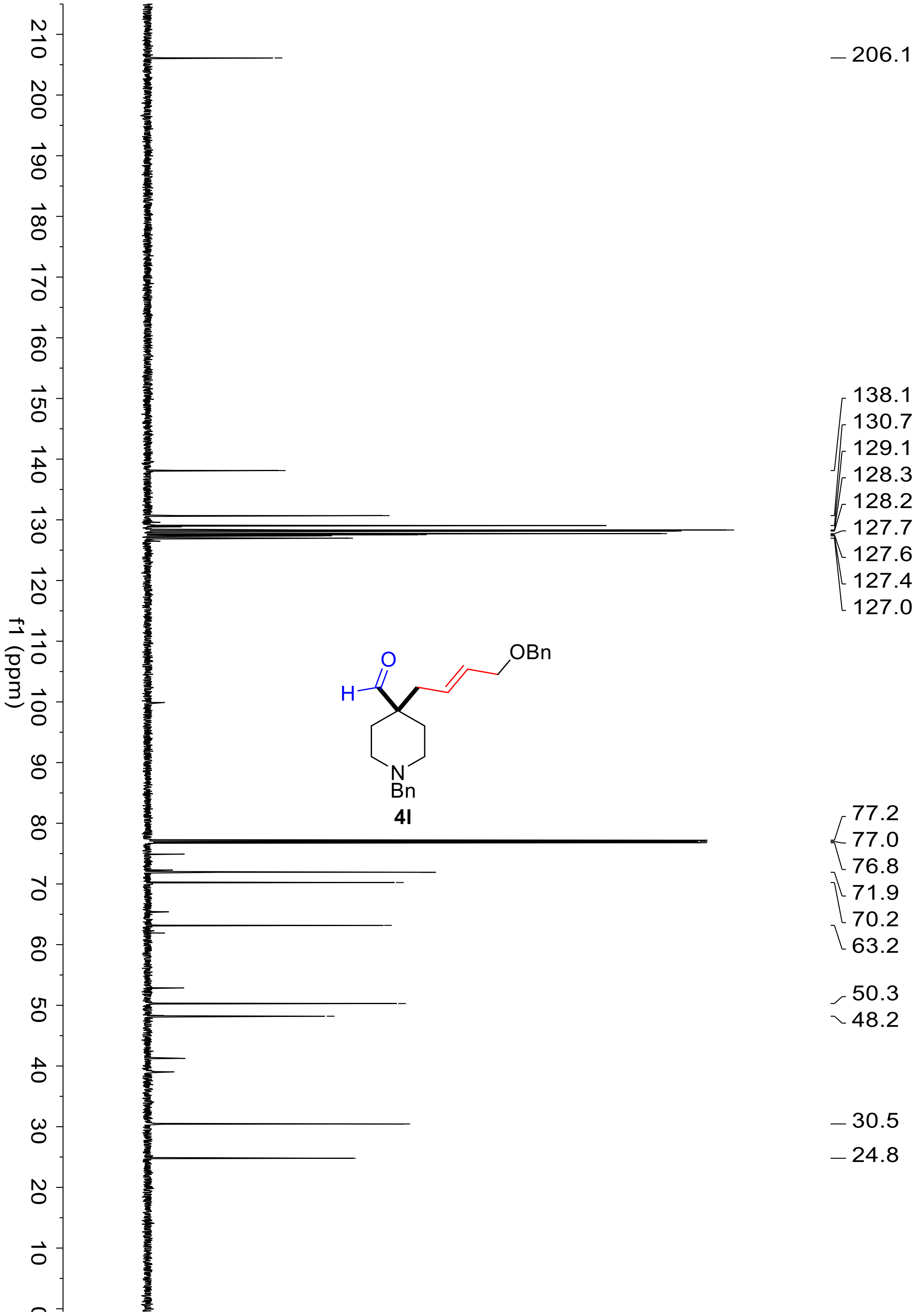

9.492
7.224
7.206
7.187
7.152
7.134
7.120
7.097
7.077
6.995
6.977
6.885
6.867
6.849
6.828
6.808
4.832
4.796
4.155
4.146
4.141
4.132
4.127
4.118
4.113
4.104
4.029
4.022
4.006
3.999
3.978
3.971
3.071
3.031
3.024
2.985
2.678
2.642
2.461
2.425
2.300
2.293
2.285
2.278
2.264
2.257
2.249
2.242
1.987
1.978
1.965
1.954
1.943
1.929
1.920
-0.000
1.00
2.08
3.01
1.97
1.01
0.96
1.00
1.03
1.01
1.03
2.02
1.01
1.00
1.02
1.07
O
H
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

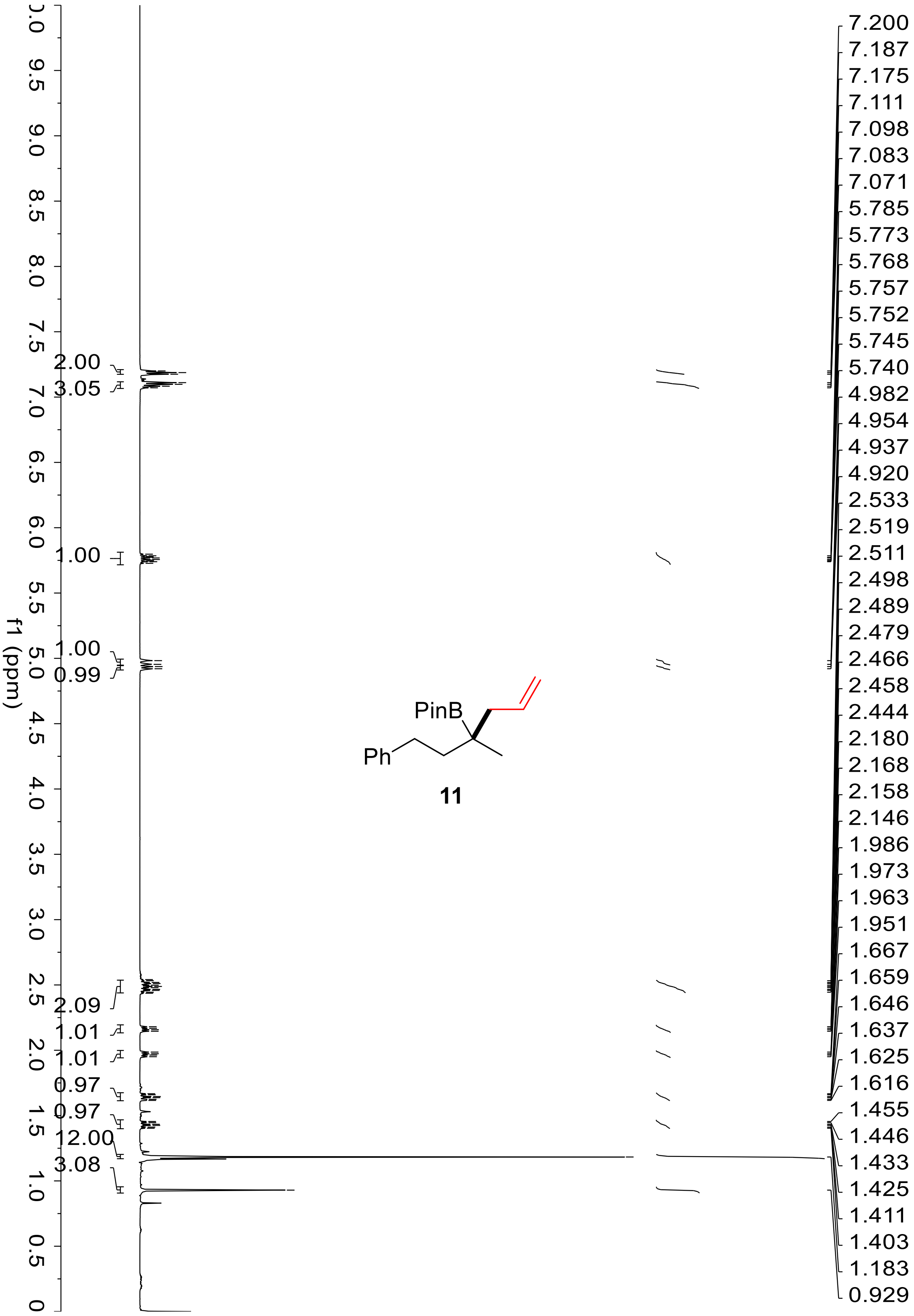
4k


200.6
155.5
143.9
138.7
129.0
128.8
128.5
128.4
126.3
121.1
120.5
117.9
117.6
77.3
77.0
76.7
63.3
49.1
43.6
41.5
26.7
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
H
O
4k

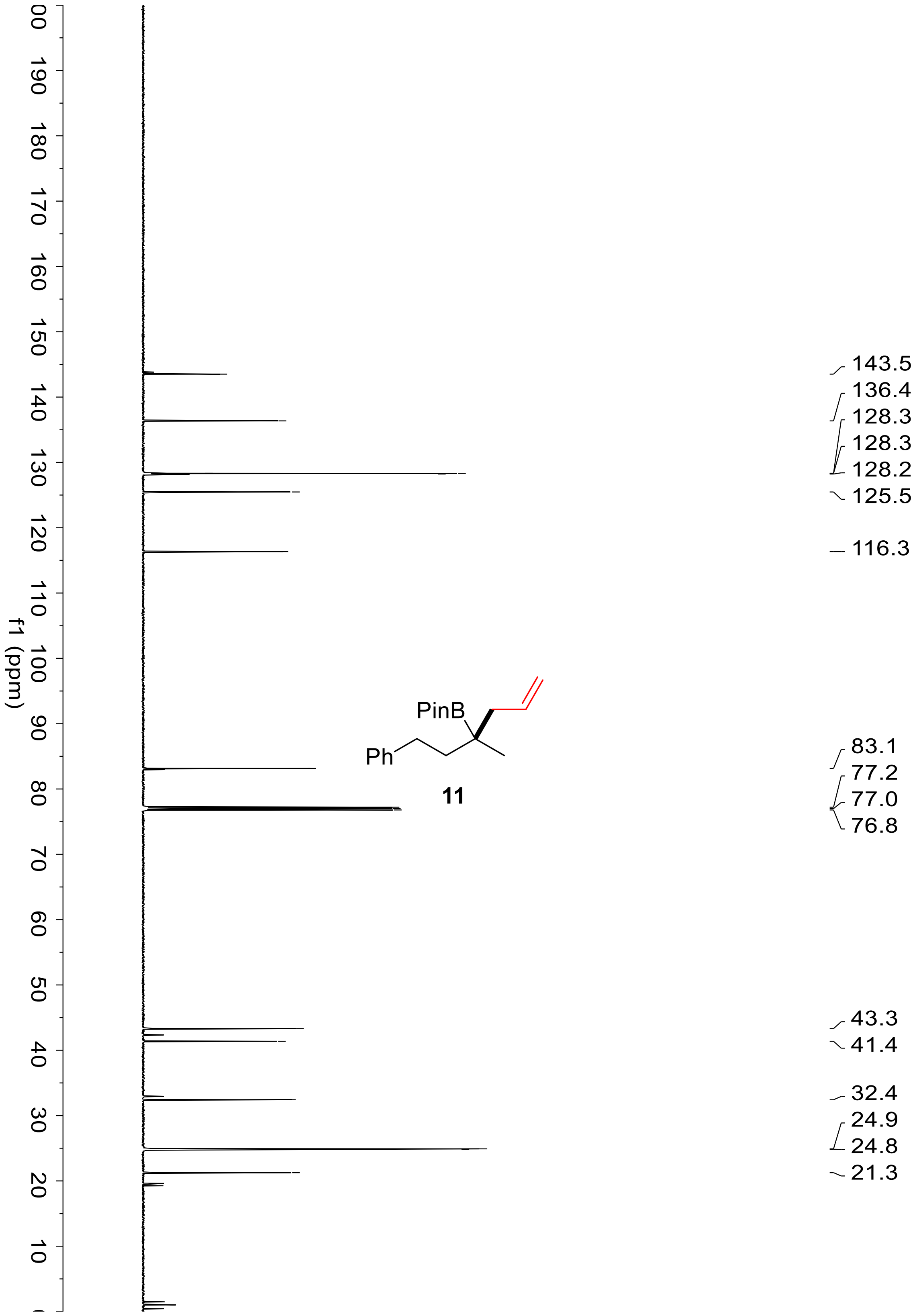


9.458
7.354
7.341
7.330
7.317
7.305
7.293
7.289
7.279
5.645
5.636
5.626
5.620
5.610
5.600
5.573
5.561
5.548
5.535
5.523
4.470
3.951
3.941
3.452
2.675
2.656
2.237
2.224
2.109
2.090
2.071
1.995
1.972
1.609
1.591
1.573
0.000
1.05
4.13
1.98
4.02
0.99
1.00
1.96
2.03
2.04
2.04
2.13
2.05
2.17
2.06
f1 (ppm)
OBn
O
H
N
Bn
4l

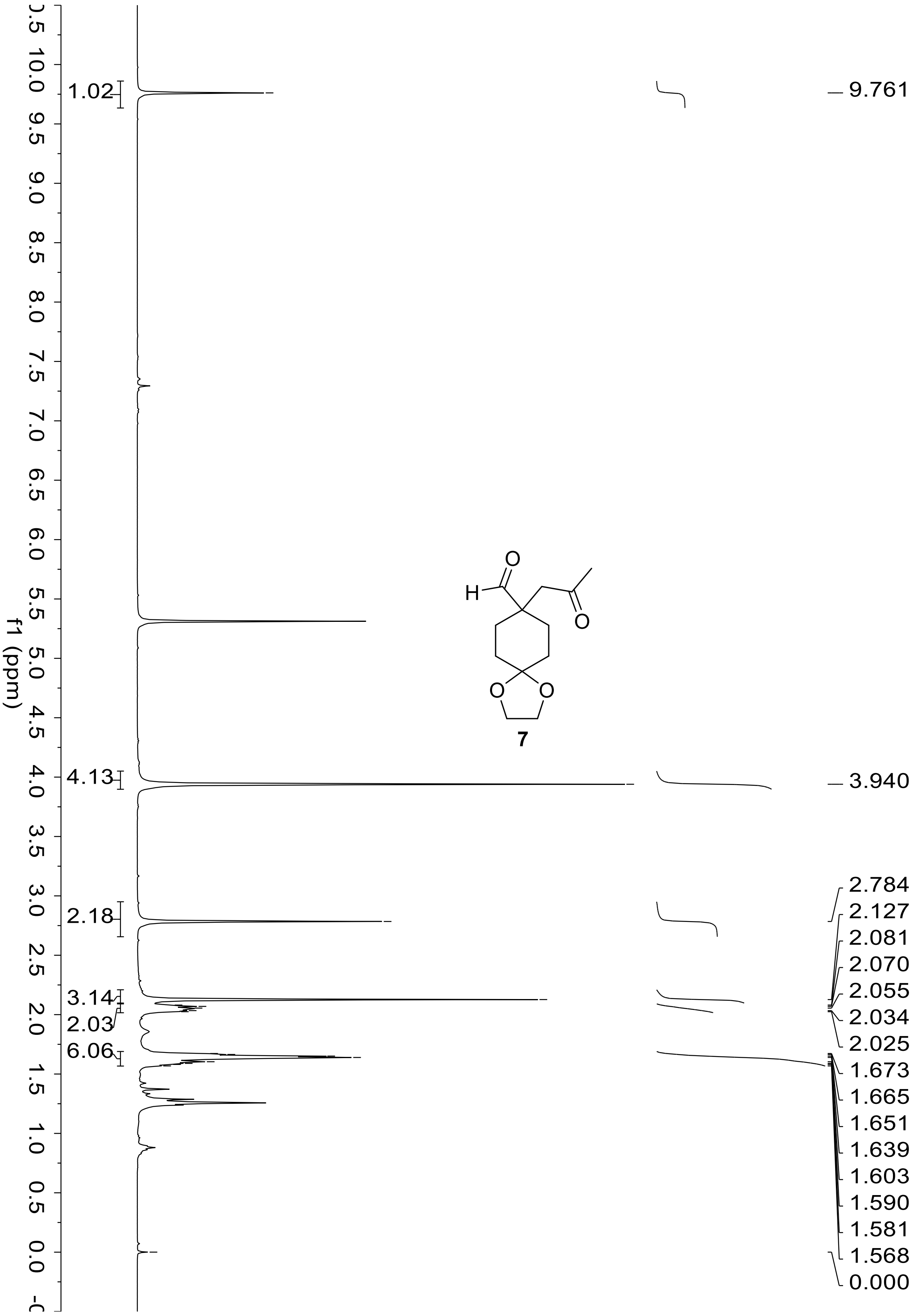

206.1
138.1
130.7
129.1
128.3
128.2
127.7
127.6
127.4
127.0
77.2
77.0
76.8
71.9
70.2
63.2
50.3
48.2
30.5
24.8
O
H
OBn
N
Bn
4l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.200
7.187
7.175
7.111
7.098
7.083
7.071
5.785
5.773
5.768
5.757
5.752
5.745
5.740
4.982
4.954
4.937
4.920
2.533
2.519
2.511
2.498
2.489
2.479
2.466
2.458
2.444
2.180
2.168
2.158
2.146
1.986
1.973
1.963
1.951
1.667
1.659
1.646
1.637
1.625
1.616
1.455
1.446
1.433
1.425
1.411
1.403
1.183
0.929
2.00
3.05
1.00
1.00
0.99
2.09
1.01
1.01
0.97
0.97
12.00
3.08
).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
f1 (ppm)
PinB
Ph

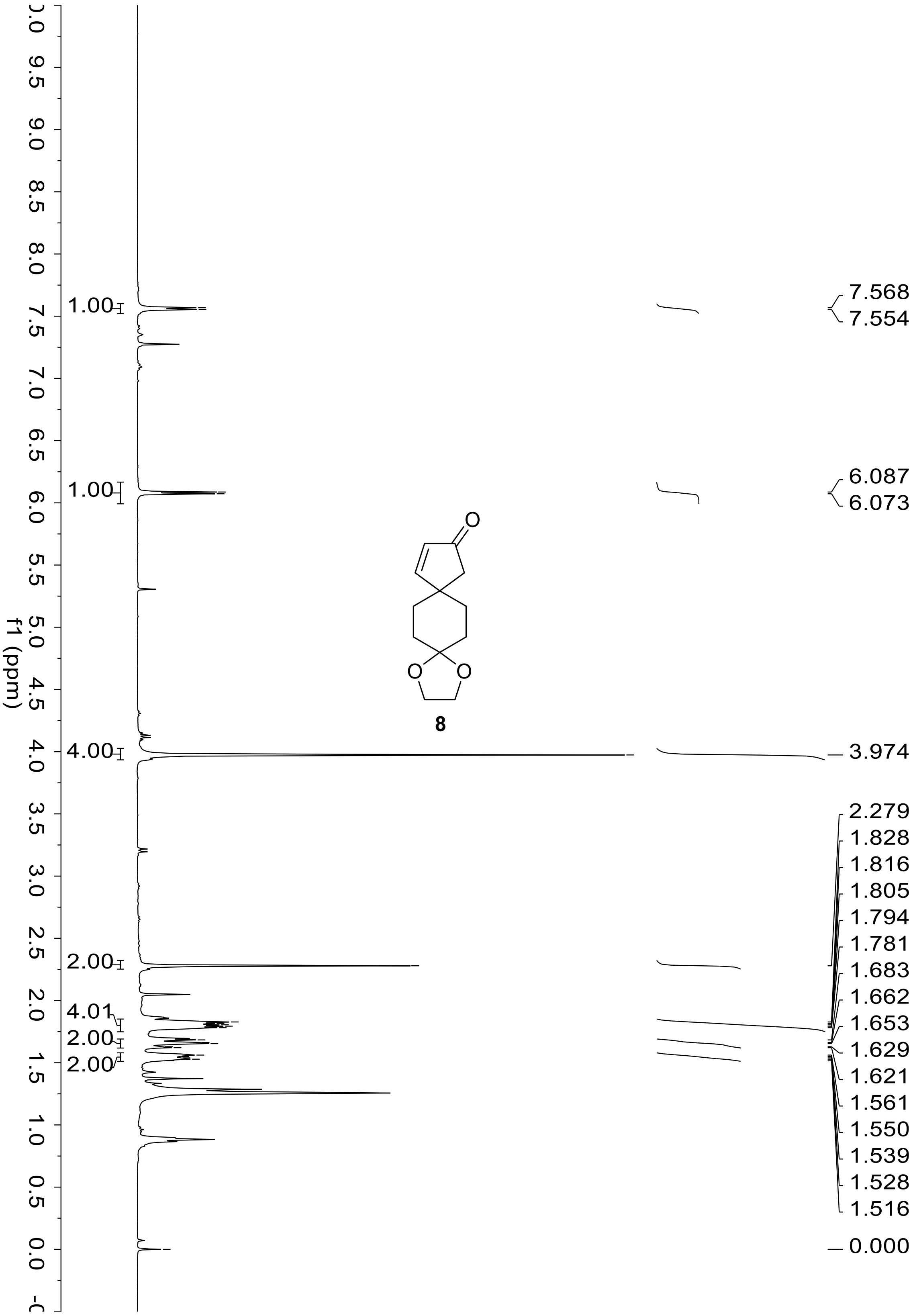
11


143.5
136.4
128.3
128.3
128.2
125.5
116.3
83.1
77.2
77.0
76.8
43.3
41.4
32.4
24.9
24.8
21.3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
PinB
Ph

11



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
1.02
4.13
2.18
3.14
2.03
6.06
9.761
3.940
2.784
2.127
2.081
2.070
2.055
2.034
2.025
1.673
1.665
1.651
1.639
1.603
1.590
1.581
1.568
0.000
O
H
O
O
O
7


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
1.00
1.00
4.00
2.00
4.01
2.00
2.00
7.568
7.554
6.087
6.073
3.974
2.279
1.828
1.816
1.805
1.794
1.781
1.683
1.662
1.653
1.629
1.621
1.561
1.550
1.539
1.528
1.516
0.000
O
O
O
8