Nickel catalyzed tandem conversion of paraformaldehyde:methanol to hydrogen and formate/chemo- and stereoselective hydrogenation of alkynes under neutral conditions

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Contents

1. General Information

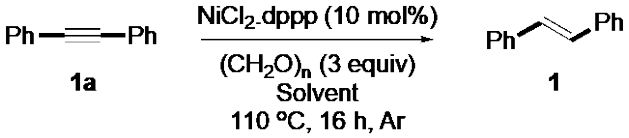
All catalytic experiments were carried out using standard Schlenk techniques. All solvents were reagent grade or better. Methanol was refluxed over magnesium and distilled under an argon atmosphere and stored over molecular sieves. Metal complexes and other chemicals used in catalysis reactions were used without additional purification. Thin-layer chromatography (TLC) was performed using silica gel precoated aluminium plates, which were visualized with UV light at 254 nm or under iodine. Column chromatography was performed with SiO_2 (SilicycleSiliaflash F60 (230-400 mesh). ^{1}H NMR (200 or 400 or 500 MHz), $^{13}C\{1H\}$ NMR (50 or 101 or 126 MHz) spectra were recorded on the NMR spectrometer. Deuterated chloroform was used as the solvent, and chemical shift values (δ) are reported in parts per million relative to the residual signals of this solvent [δ 7.27 for ^{1}H (chloroform-d), δ 77.0 for $^{13}C\{1H\}$ (chloroform-d). Abbreviations used in the NMR follow-up experiments: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. GC analysis was carried out using an HP-5 column (30 m, 0.25 mm, 0.25μ). All the calculations in this study have been performed with density functional theory (DFT), with the aid of the Turbomole 7.1 suite of programs,[1] using the PBE functional.[2] The TZVP[3] basis set has been employed. The resolution of identity (RI),[4] along with the multipole accelerated resolution of identity (marij)[5] approximations, have been employed for an accurate and efficient treatment of the electronic Coulomb term in the DFT calculations. Solvent corrections were incorporated with optimization calculations using the COSMO model,[6] with methanol (ε = 32.5) as the solvent. The values reported are ΔG values, with zero-point energy corrections, internal energy, and entropic contributions included through frequency calculations on the optimized minima with the temperature taken to be 298.15 K. Harmonic frequency calculations were performed for all stationary points to confirm them as local minima or transition state structures.

2. Experimental Section

General procedure for the preparation of *E*-selective alkenes from internal alkynes

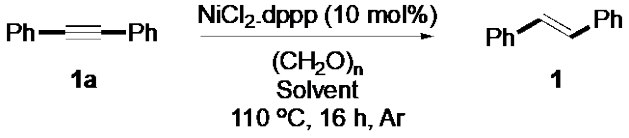
In an oven-dried screw cap reaction tube (15 mL) containing alkyne (0.5 mmol) and paraformaldehyde (1.5 mmol), [1,3-Bis(diphenylphosphino)propane]dichloronickel(II)-$NiCl_2$.dppp (10 mol%) and methanol (1 mL) added in a gentle stream of argon. Then the reaction mixture was stirred with a magnetic stirring bar at 110 °C in an oil-bath for 16 h. After completion of the reaction, the crude mixture was cooled to room temperature, then filtered through a celite filter and washed with ethyl acetate (3×5 mL), followed by the solvent was removed under vacuum, and finally, the residue was purified by silica gel column chromatography (230–400 mesh size) using petroleum-ether or pentane and ethyl acetate as an eluent to give the alkenes.

Supplementary Table S1: Effect of Solvent



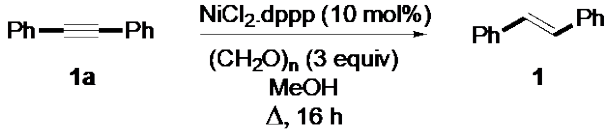
Entry	Solvent	Yield of 1 (%)	*E/Z*
1	MeOH	78	99:1
2	EtOH	72	99:1
3	i- PrOH	32	99:1
4	t- BuOH	19	90:10
5	t- amyl alcohol	10	82:18
6	H_2O	n.r	–

Supplementary Table S2: Effect of Paraformaldehyde



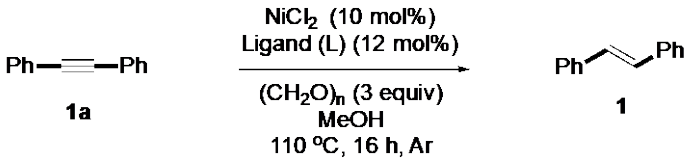
Entry	Equiv of $(HCHO)_n$	Yield of 1 (%)	*E/Z*
1	0	n.r	–
2	1	56	94:6
3	2	63	97:3
4	3	74	98:2
5	4	76	98:2
6	5	78	99:1

Supplementary Table S3: Effect of Temperature



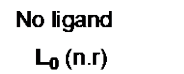
Entry	Temperature (°C)	Yield of 1 (%)	*E/Z*
1	rt	n.r	–
2	50	n.r	–
3	80	48	96:4
4	110	78	99:1
5	130	74	99:1

Supplementary Table S4: Effect of Ligand

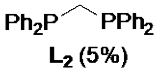


(i) Variation of Ligands

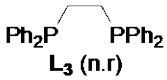
No ligand
L_0 (n.r)



L_1 (n.r)

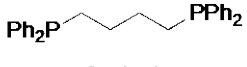


L_2 (5%)

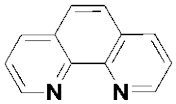


L_3 (n.r)

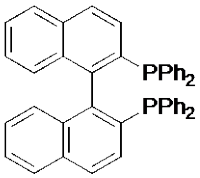
L_4 (73 %) (*E/Z* : 99:1)



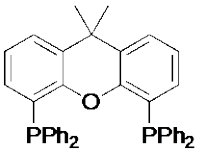
L_5 (n.r)



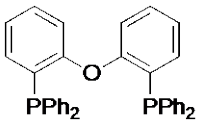
L_6 (n.r)



L_7 (3%)



L_8 (n.r)



L_9 (n.r)

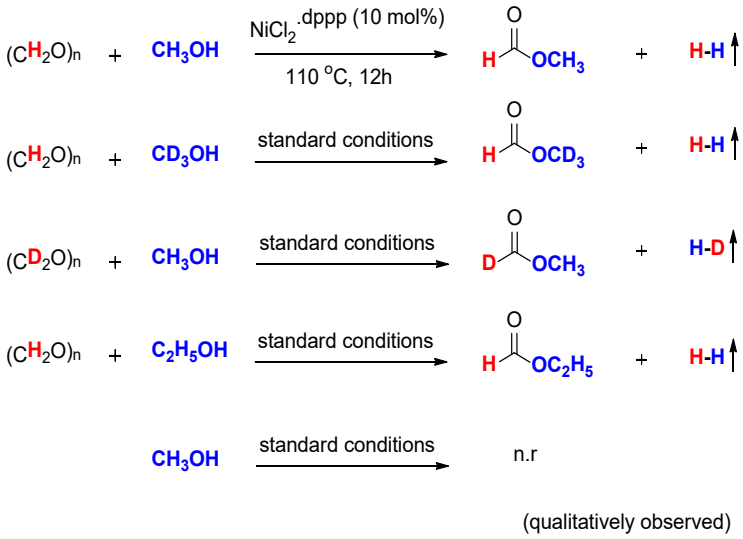
(ii) Ratio of $NiCl_2$: L

Entry	Ratio	Yield of 1 (%)	*E/Z*
1	0:1	n.r	–
2	1:0	n.r	–
3	1:1	65	96:4
4	1:1.2	73	99:1

3. Mechanistic Investigation

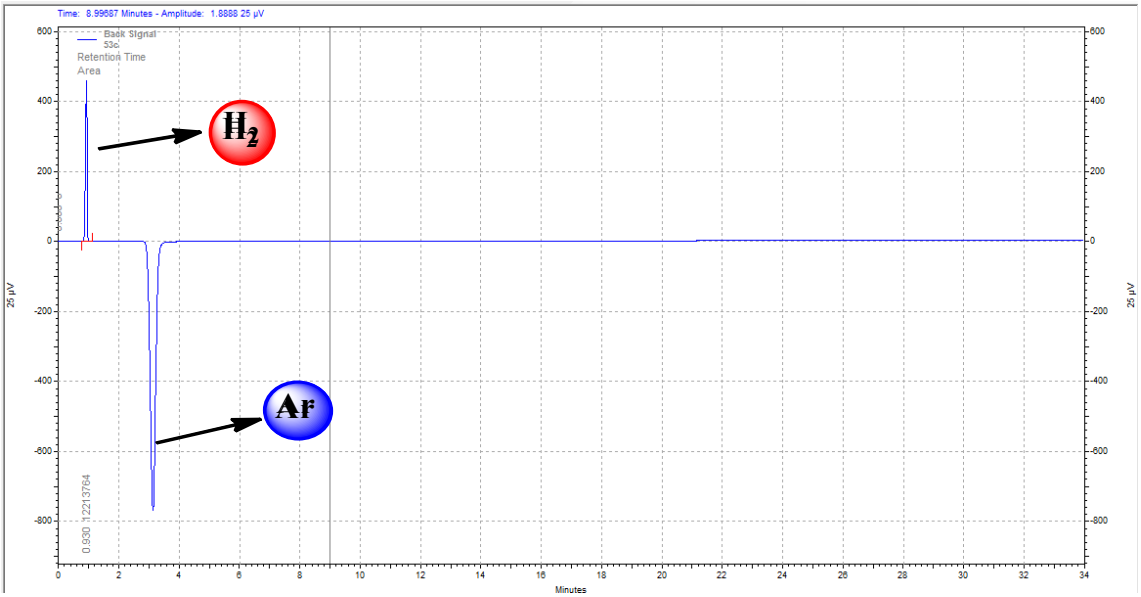
3.1 H_2 detection

To an oven-dried 10 mL screw-capped vial, paraformaldehyde (1.5 mmol), [1,3-Bis(diphenylphosphino)propane]dichloronickel(II)-$NiCl_2$.dppp (10 mol%) and methanol (1 mL) were added under a gentle stream of argon. Then the reaction mixture was stirred for 16 h at 110 °C (bath temperature). After completion of the reaction, the crude mixture was cooled to room temperature, followed by the sample was submitted to GC for detection of H_2 gas and GC-MS.



Supplementary Scheme S1: Formation of hydrogen gas and methyl formate.

GC data for the detection of molecular Hydrogen



Area % Report

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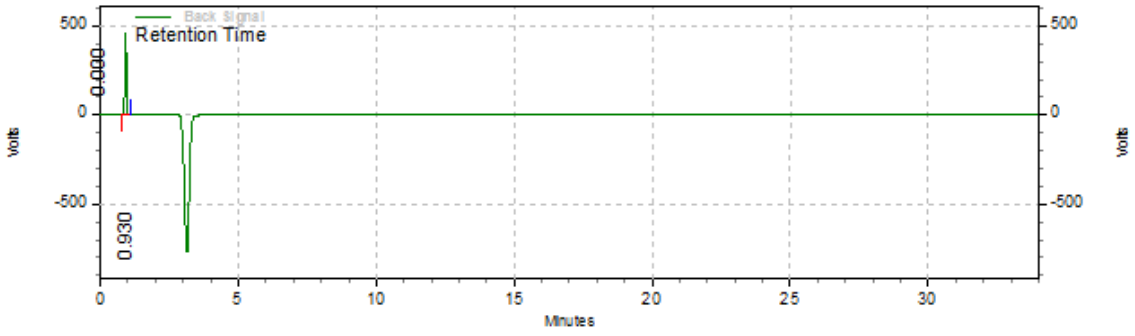
Acquired: 8/8/2016 12:01:28 PM
Printed: 8/8/2016 2:36:02 PM



Back Signal
Results

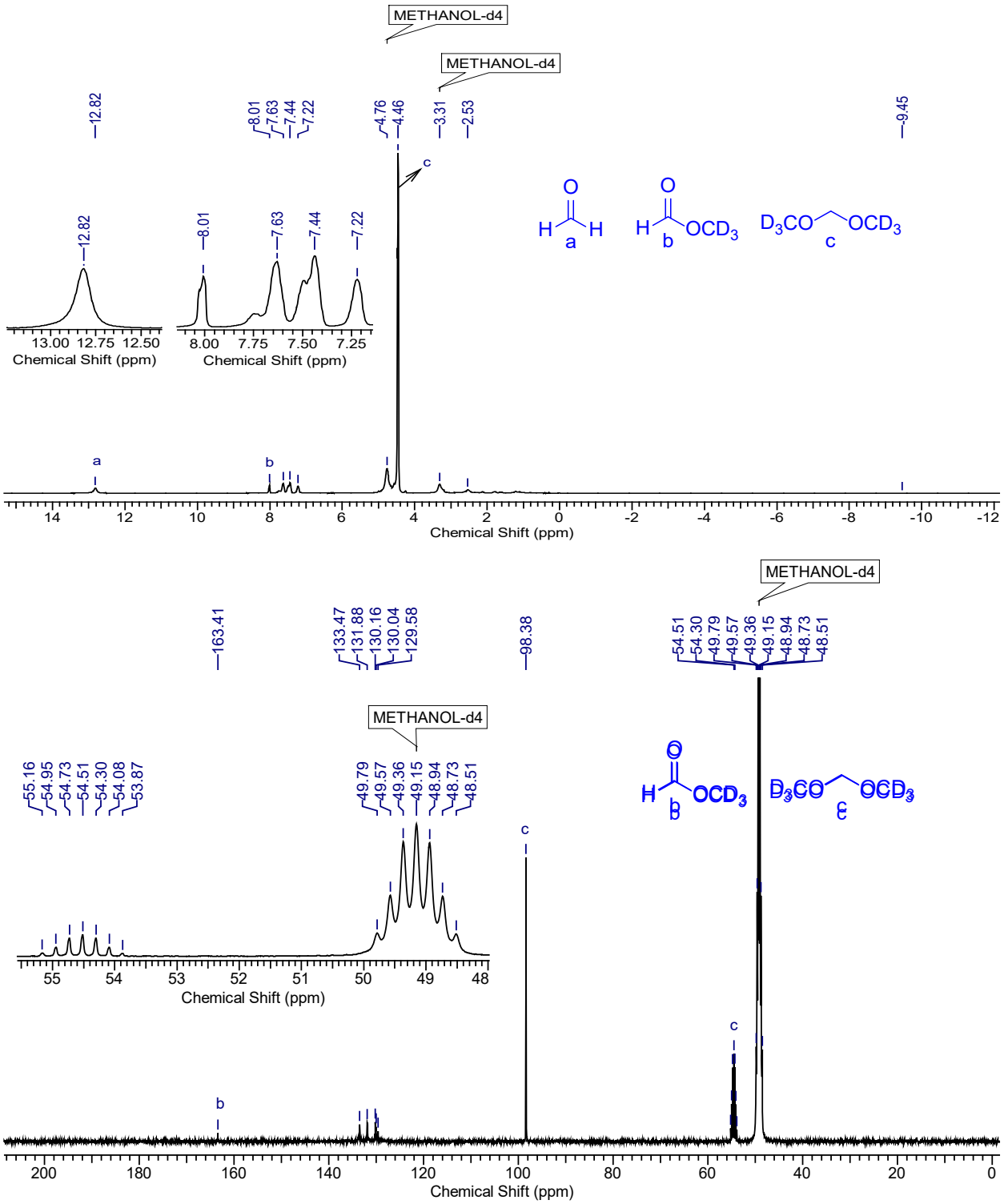
Retention Time	Area	Area %	Height	Height %
0.000	0	0.00	0	0.00
0.930	12213764	100.00	3527989	100.00
Totals	12213764	100.00	3527989	100.00

Supplementary Figure S1 & S2: Detection of hydrogen gas

3.2 Detection of reaction intermediate and byproducts

To an oven-dried screw-capped low-pressure *J-young* NMR tube, paraformaldehyde (1 mmol), [1,3-Bis(diphenylphosphino)propane]dichloronickel(II)-$NiCl_2$.dppp (10 mol%) and methanol-D4 (0.6 mL) were added under a gentle stream of argon. Then the NMR tube was carefully closed by the screw cap. Then, the reaction mixture was stirred for 16 h at 110 °C (bath temperature). After completion of the reaction, the crude mixture was cooled to room temperature, and the sample was submitted for NMR measurement. The reaction intermediates, such as methyl formate, and Ni-hydride, were detected by NMR and conformed by chromatographic analysis (shown below). Similarly, the combination of methanol/ethanol and deuterated paraformaldehyde was performed, and the corresponding products were identified through GC and GC-MS.

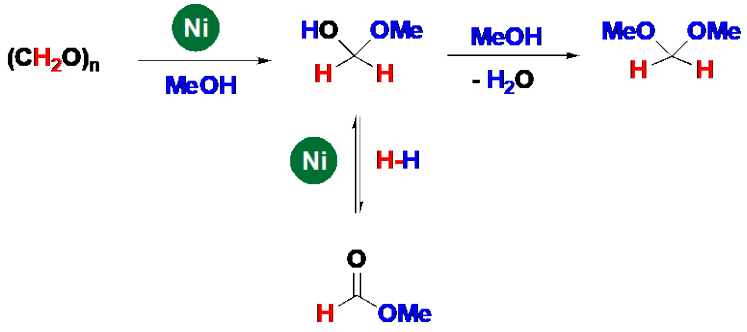
3.2.1. ^{1}H and ^{13}C NMR of reaction mixture without diphenyl acetylene

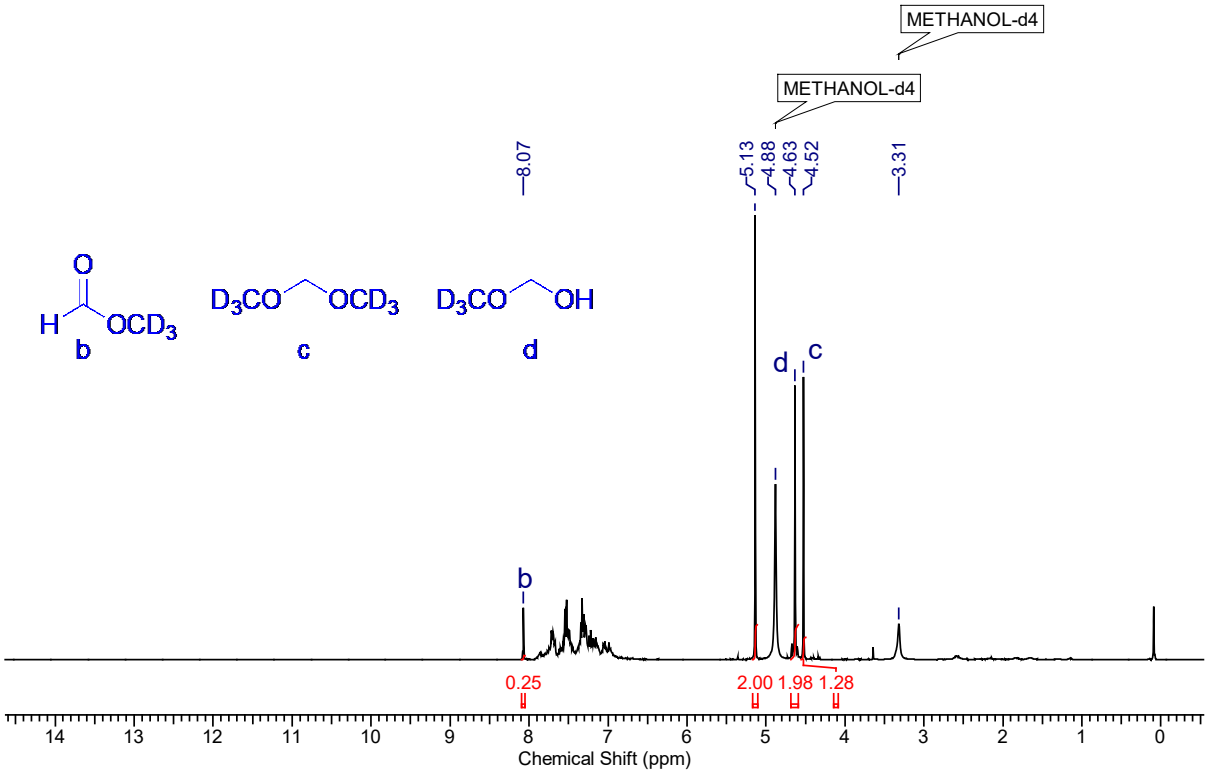


Supplementary Figure S3 & S4: ^{1}H and ^{13}C NMR detection of reaction intermediates from the reaction of paraformaldehyde, and MeOH-D4 in the presence of $NiCl_2$.dppp catalyst.

3.2.2 ^{1}H NMR of reaction mixture with diphenyl acetylene

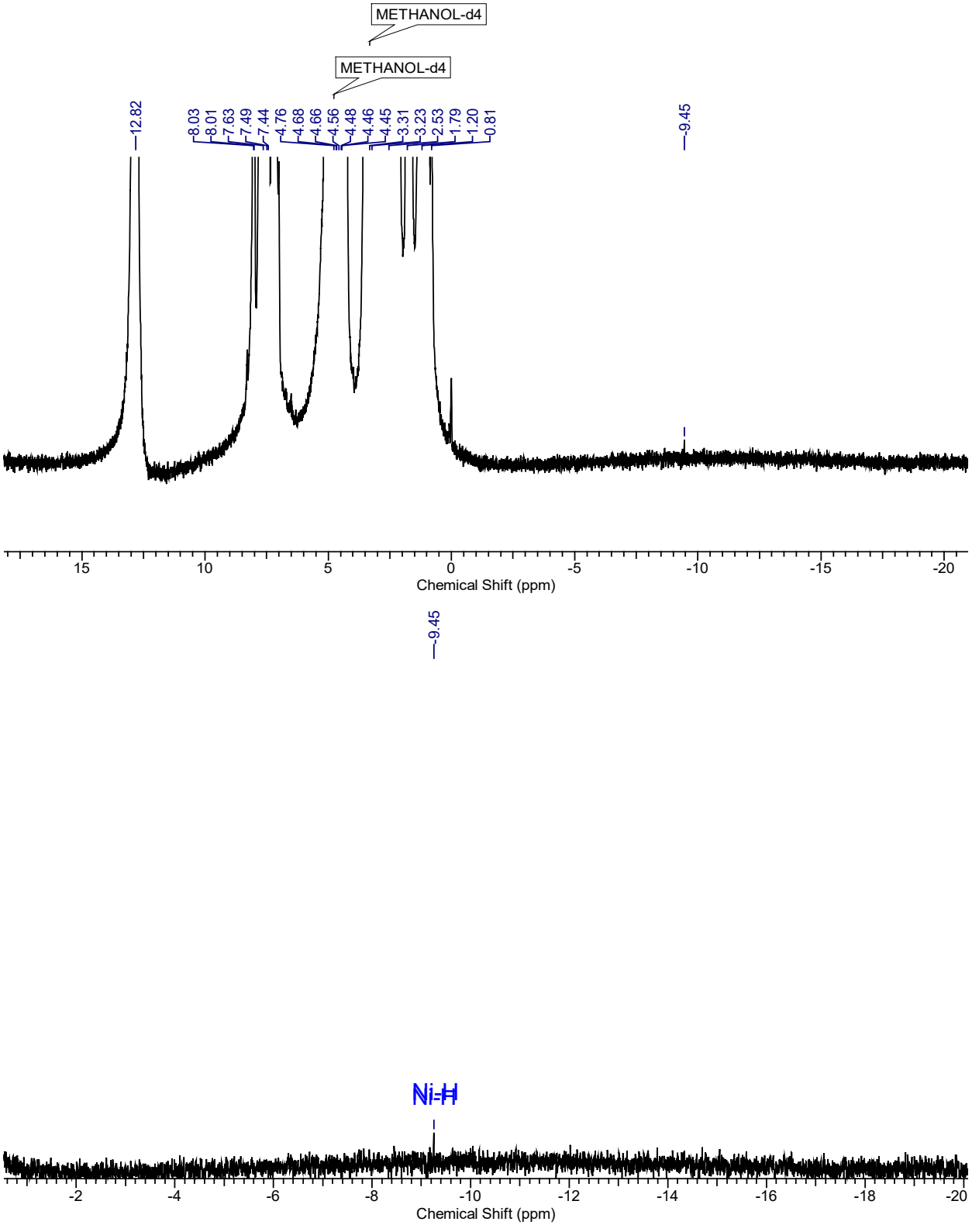
To an oven-dried screw-capped vial, diphenyl acetylene (0.25 mmol), paraformaldehyde (0.75 mmol), [1,3-Bis(diphenylphosphino)propane]dichloronickel(II)-$NiCl_2$.dppp (10 mol%) and methanol-D4 (0.5 mL) were added under a gentle stream of argon. Then the reaction mixture was stirred for 16 h at 110 °C (bath temperature). Upon finishing the reaction, 0.25 mmol of the internal standard (dibromomethane) was introduced to the reaction mixture. Subsequently, a representative sample was drawn from the reaction mixture, diluted with methanol-D4, and then submitted for ^{1}H NMR analysis. As a result, the yield of methyl formate: methoxymethanol (hemiacetal): dimethoxymethane (acetal) was determined to be 8.7%: 33%: 21.3% concerning 0.75 mmol of paraformaldehyde. Their ratio, expressed as a percentage, is approximately (13.81: 52.38: 33.81). Consequently, we can understand that out of 0.75 mmol of paraformaldehyde, 66% undergoes conversion into hemiacetal and methyl formate, utilized in the semihydrogenation reaction, while the remaining 34% contributes to acetal formation.





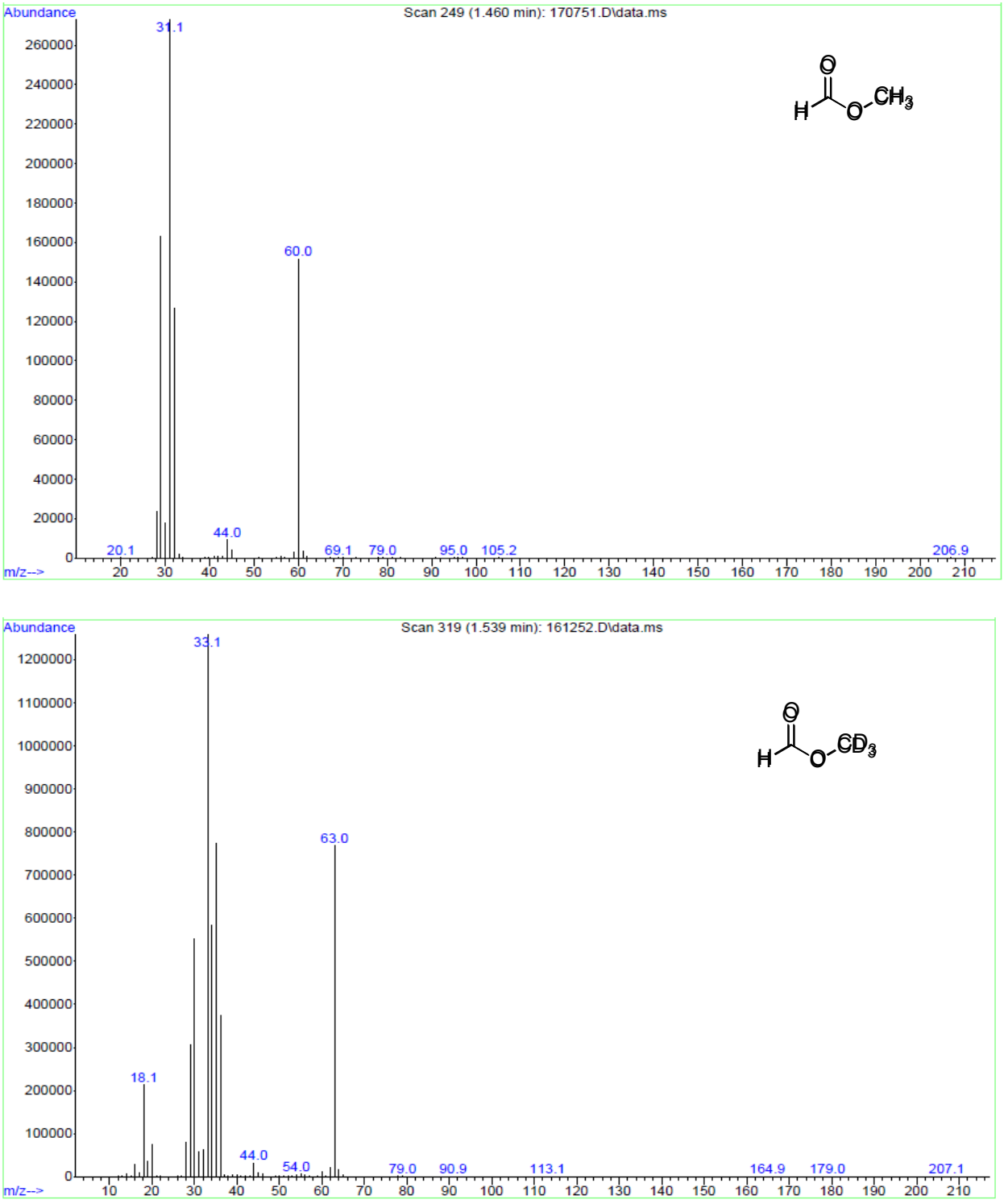
Supplementary Figure S5: ^{1}H NMR detection of reaction intermediates from the reaction of diphenyl acetylene, paraformaldehyde, and MeOH-D4 in the presence of $NiCl_2$.dppp catalyst.

3.2.3. Detection of Ni-H intermediate

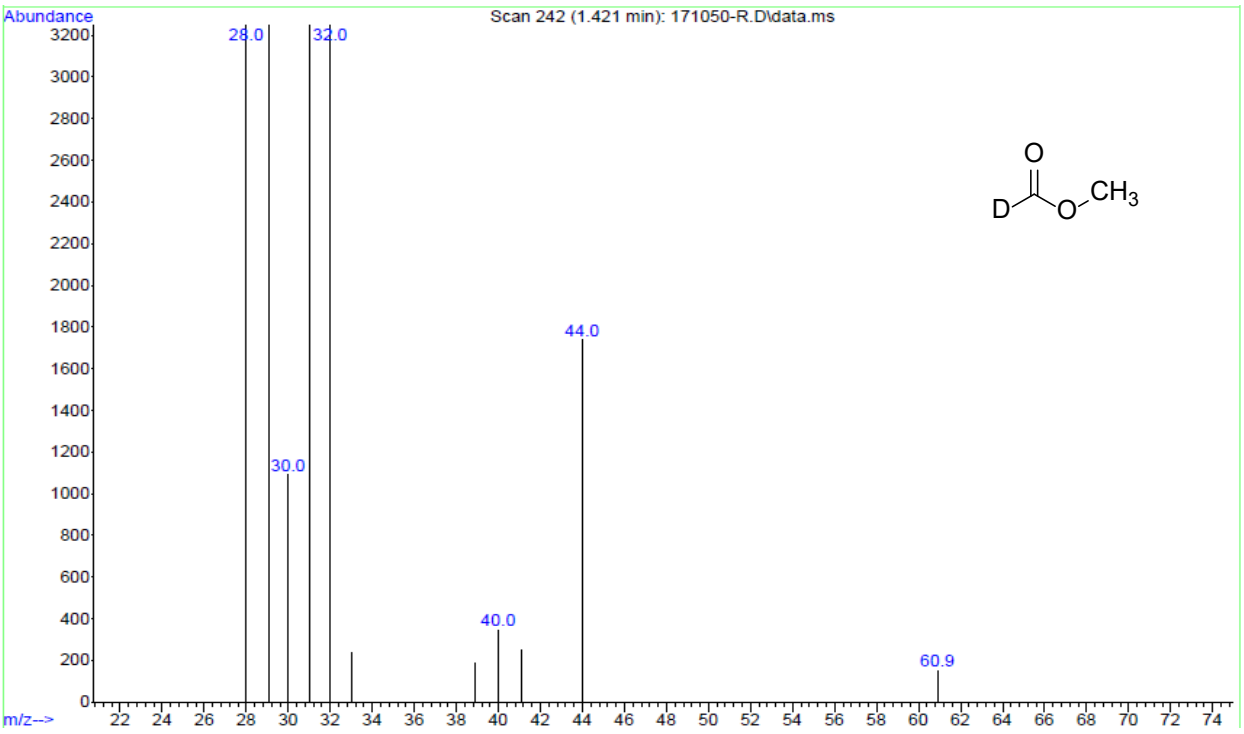


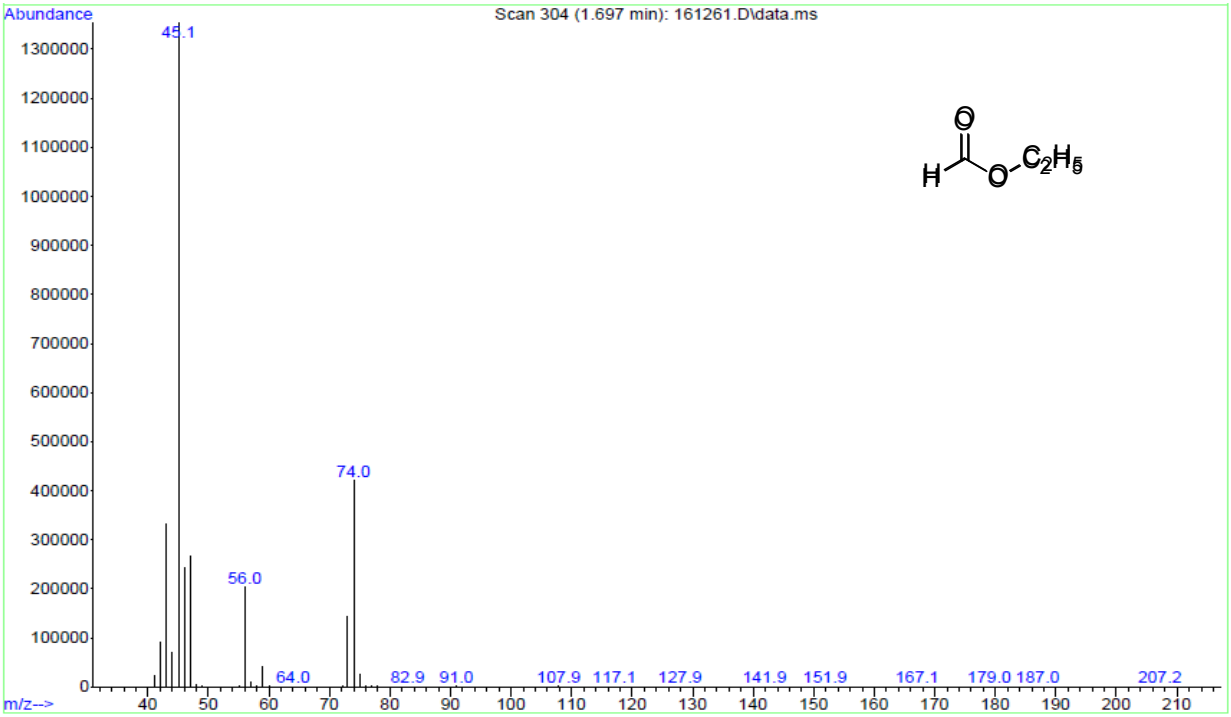
Supplementary Figure S6 & S7: Detection of Ni-H

3.2.4. GC-MS data for various formate byproduct



Supplementary Figure S8 & S9: Detection of reaction intermediates by GCMS

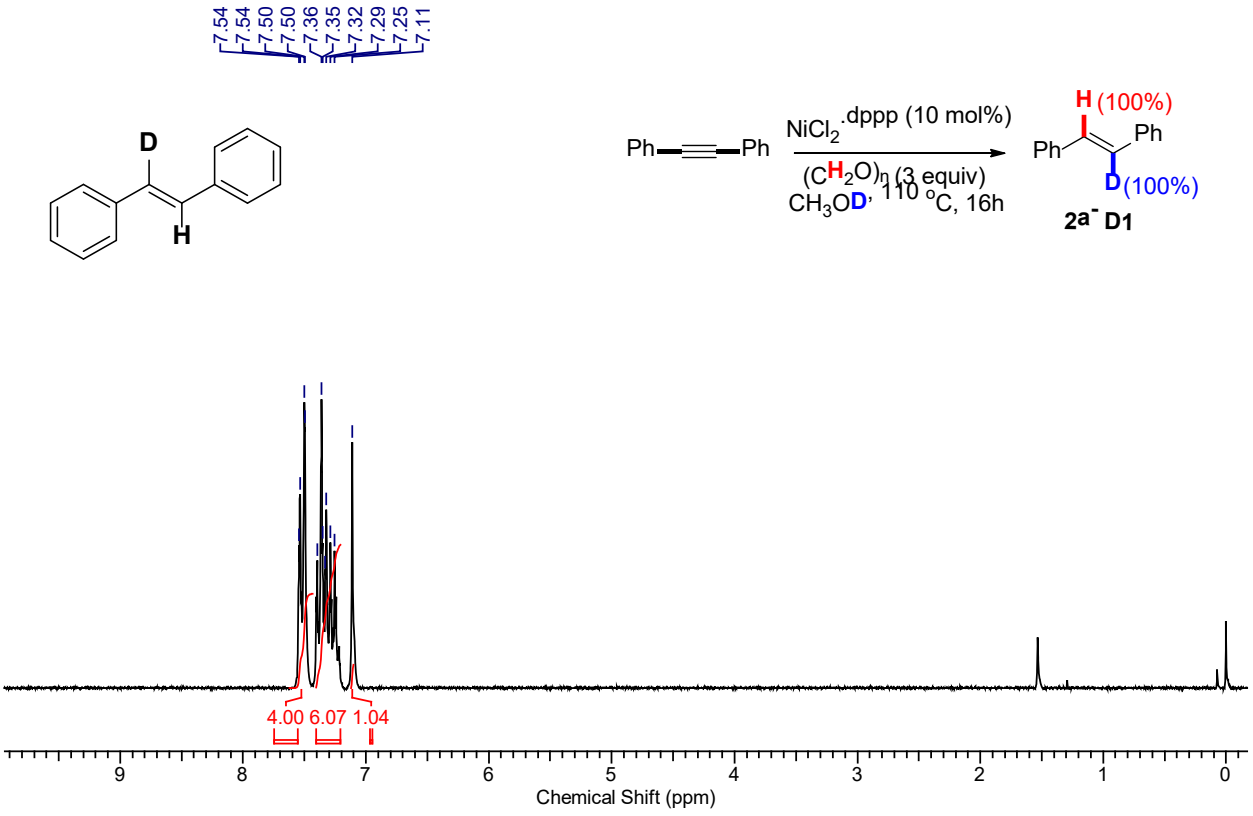




Supplementary Figure S10 & S11: Detection of various formate byproducts by GCMS

3.3 Deuterium labeling experiment

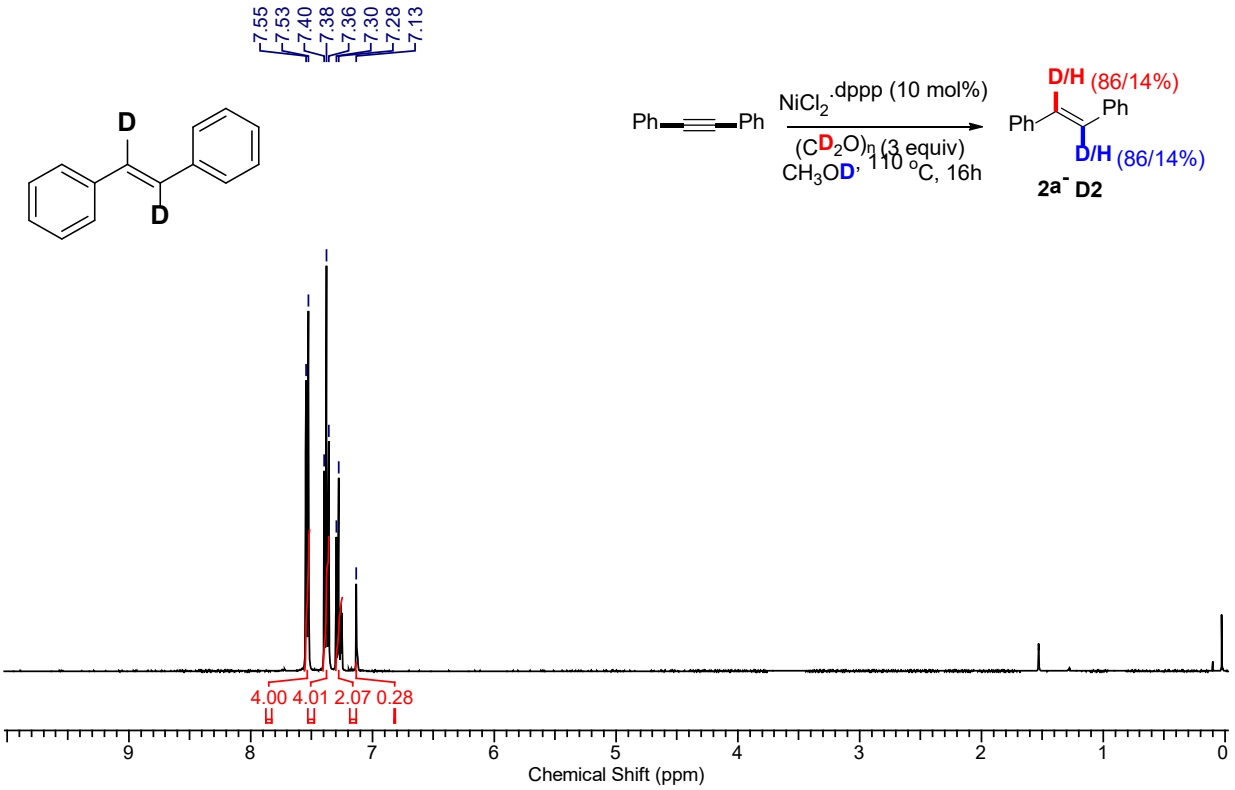
(i) To an oven-dried 10 mL screw-capped vial, alkyne (0.5 mmol), paraformaldehyde (1.5 mmol), [1,3-Bis(diphenylphosphino)propane]dichloronickel(II)-$NiCl_2$.dppp (10 mol%) and CH_3OD (1 mL) were added under a gentle stream of argon. Then the reaction mixture was stirred for 16 h at 110 °C (bath temperature). After completion of the reaction, the crude mixture was cooled to room temperature, followed by filtered through a celite pad with several washings (3 x 3 mL ethyl acetate), and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (eluent: pet ether) to afford the desired product.



Supplementary Figure S12: Deuterium labeling experiment

(ii) To an oven-dried 10 mL screw-capped vial, alkyne (0.5 mmol), paraformaldehyde-D_2 (1.5 mmol), [1,3-Bis(diphenylphosphino)propane]dichloronickel(II)-$NiCl_2$.dppp (10 mol%) and CH_3OD (1 mL) were added under a gentle stream of argon. Then the reaction mixture was stirred for 16 h at 110 °C (bath temperature). After completion of the reaction, the crude mixture was cooled to room temperature, followed by filtration through a celite pad with several washings (3 x

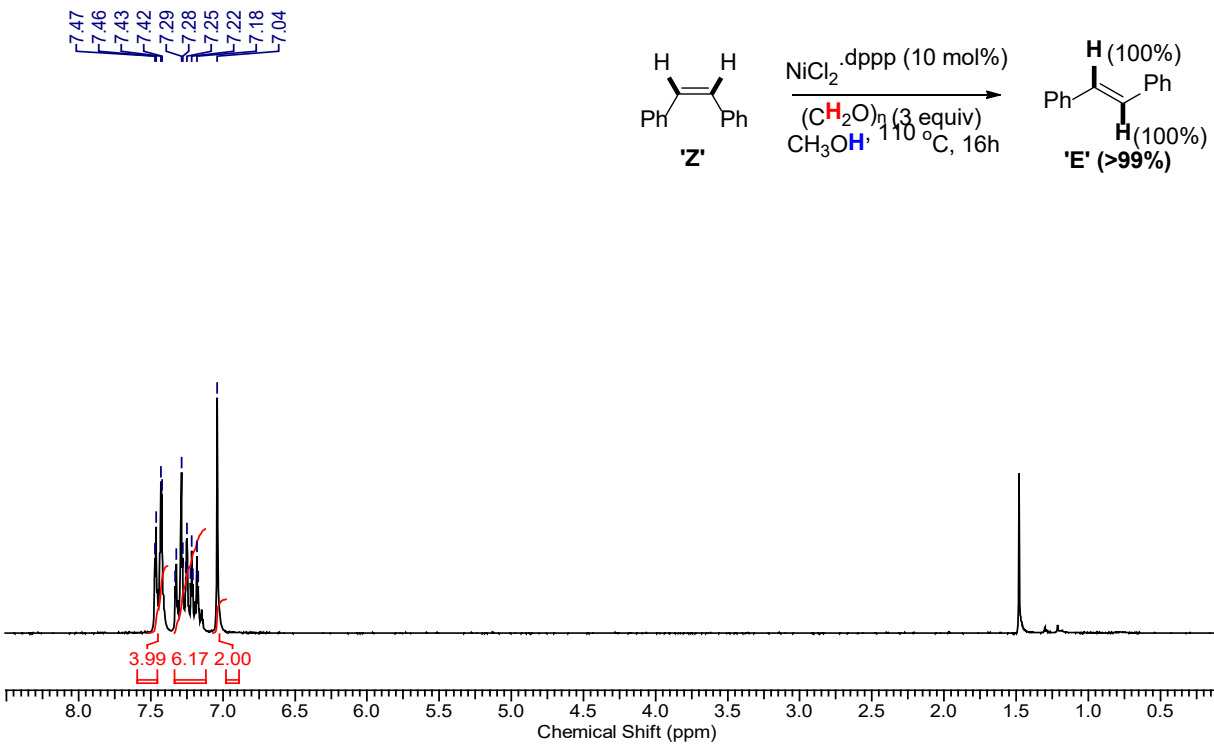
3 mL ethyl acetate) and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (eluent: pet ether) to afford the desired product.

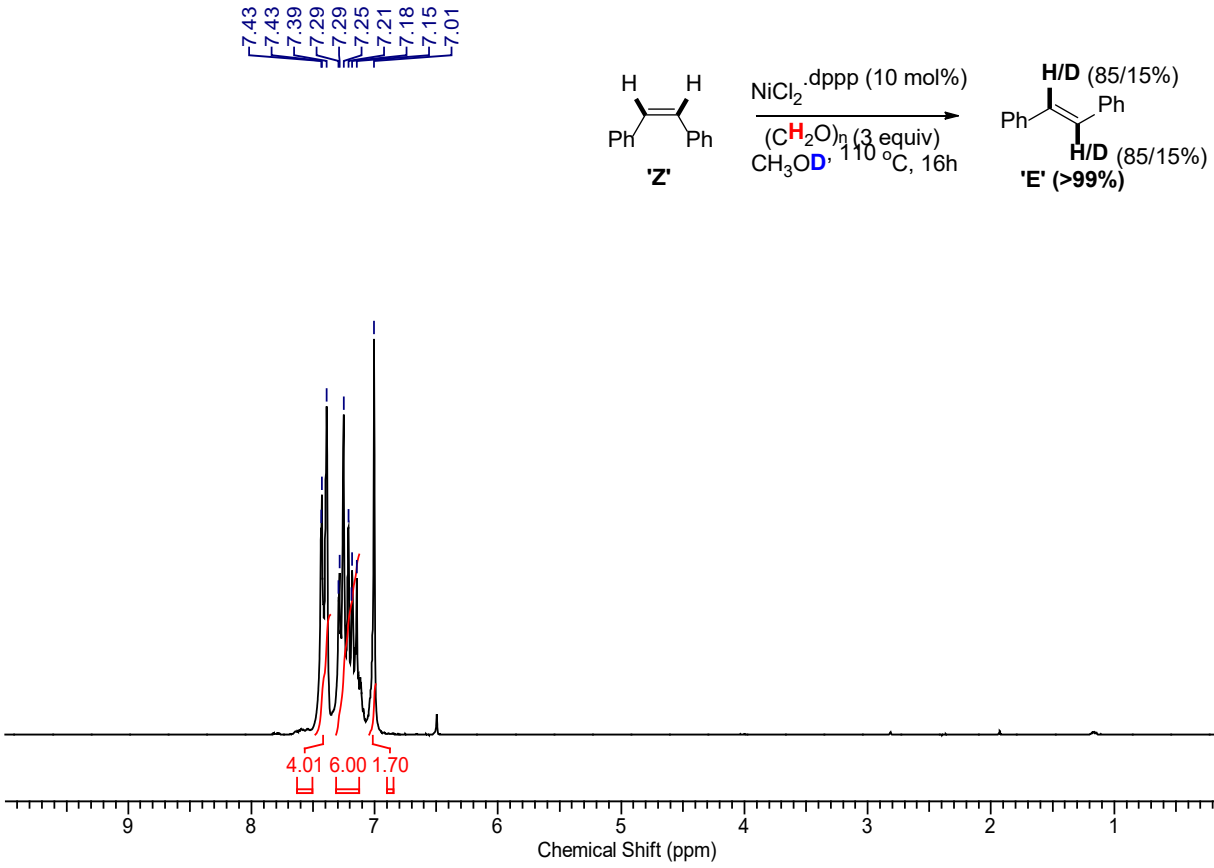


Supplementary Figure 13: Deuterium labeling experiment

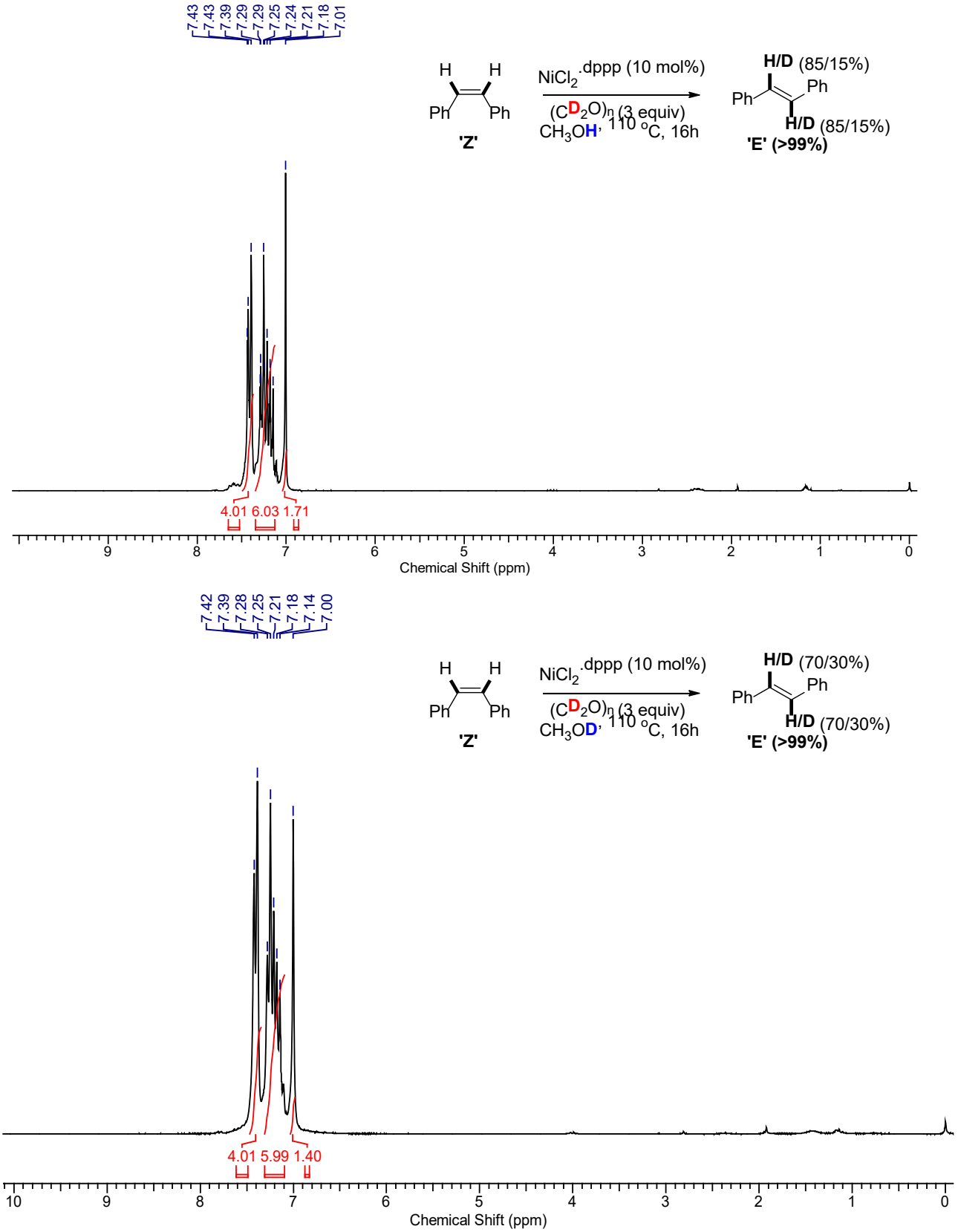
3.4 Isomerization experiment

To an oven-dried 10 mL screw-capped vial, cis-stilbene (0.5 mmol), paraformaldehyde (1.5 mmol), [1,3-Bis(diphenylphosphino)propane]dichloronickel(II)-$NiCl_2$.dppp (10 mol%) and CH_3OH (1 mL) were added under a gentle stream of argon. Then the reaction mixture was stirred for 16 h at 110 °C (bath temperature). After completion of the reaction, the crude mixture was cooled to room temperature, followed by filtration through a celite pad with several washings (3 x 3 mL ethyl acetate) and concentrated *in vacuo*. The yield of alkene was determined by GC and NMR spectroscopy. Similarly, the isomerization reaction was performed with different combinations of deuterated methanol and deuterated paraformaldehyde using cis-stilbene, and the crude mixture was analyzed by GC and NMR measurements.





Supplementary Figures S14 & S15: *Cis* to *trans* isomerization reaction



Supplementary Figures S16 & S17: *Cis* to *trans* isomerization reaction

3.5 Selective removal of alkyne and alkene impurities

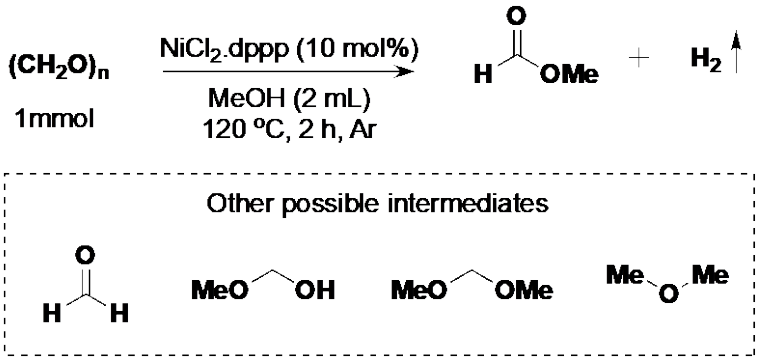
To an oven-dried 30 mL screw-capped vial, alkyne (0.05 mmol) or cis-stilbene (0.05 mmol) or both, trans-stilbene (5 mmol), paraformaldehyde (15 mmol). [1,3-Bis(diphenylphosphino)-propane]dichloronickel(II)-$NiCl_2$.dppp (10 mol%) and CH_3OH (8 mL) were added under a gentle stream of argon. The mixture was stirred for 12 h at 110 °C (bath temperature), followed by cooling to room temperature, and filtered through a celite pad with several washings with ethyl acetate and concentrated *in vacuo*. Then the crude mixture was analyzed by GC and NMR.

3.6 Homogenous test

a) Mercury test: To an oven-dried 10 mL screw-capped vial, alkyne (0.5 mmol), paraformaldehyde (2.5 mmol), $NiCl_2$ (10 mol%), Bis (1,3)-diphenyl phosphino propane (dppp) (20 mol%), 2 drops of mercury and methanol (1 mL) were added under a gentle stream of argon. The mixture was stirred for 12 hrs at 110 °C (bath temperature), followed by cooling to room temperature. Finally, the crude mixture was filtered through a celite pad with several washings (3 x 3 mL ethyl acetate) and concentrated *in vacuo*. The yield of alkene was determined by GC (75% of **1**).

b) Hot-filtration test: To an oven-dried 10 mL screw-capped vial, alkyne (0.5 mmol), paraformaldehyde (2.5 mmol), $NiCl_2$ (10 mol%), Bis (1,3)-diphenyl phosphino propane (dppp) (20 mol%), and methanol (1 mL) were added under a gentle stream of argon. The mixture was stirred for 3 hrs at 110 °C (bath temperature), followed by cooling to room temperature. After that, the reaction mixture was filtered using a syringe filter under argon atmosphere (at this stage, the crude reaction mixture was analyzed by GC (52% of **1**). Then, the reaction mixture was transferred into another 15 mL oven-dried sealed tube under an argon atmosphere, and the reaction tube was sealed and heated at 110 ^{o}C (bath temperature) with stirring for 16 h. After cooling to room temperature, the crude reaction mixture was quantitatively analyzed by GC (76% of **1**), and it was observed that the yield of 1a increased.

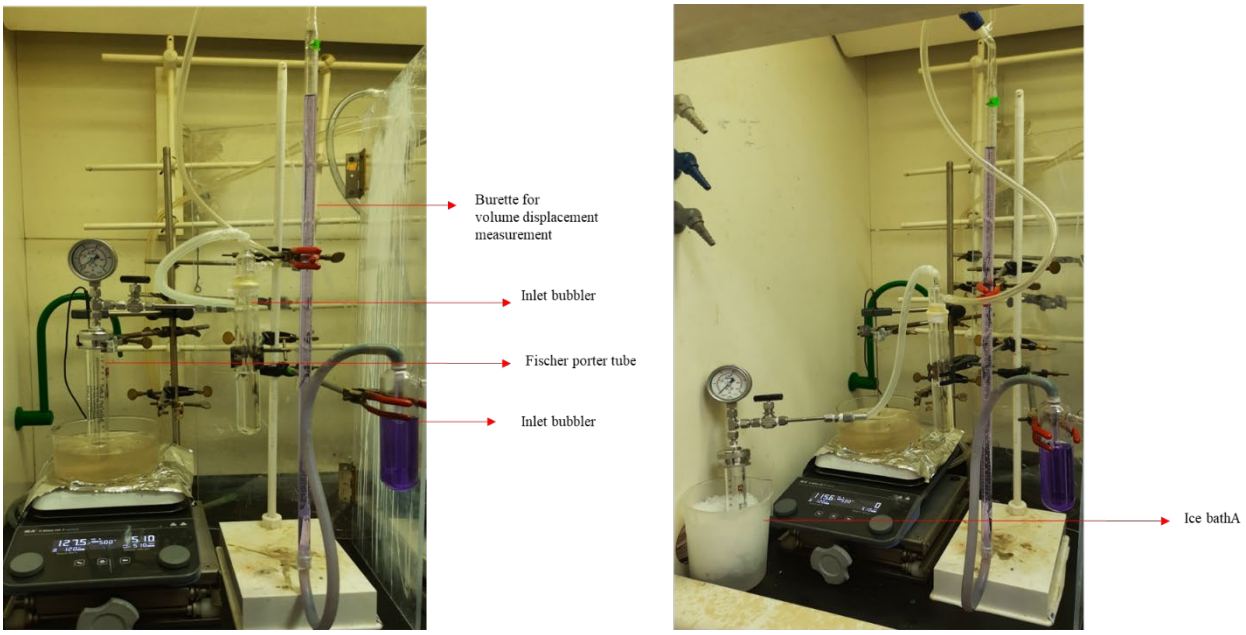
3.7 H_2 Quantification



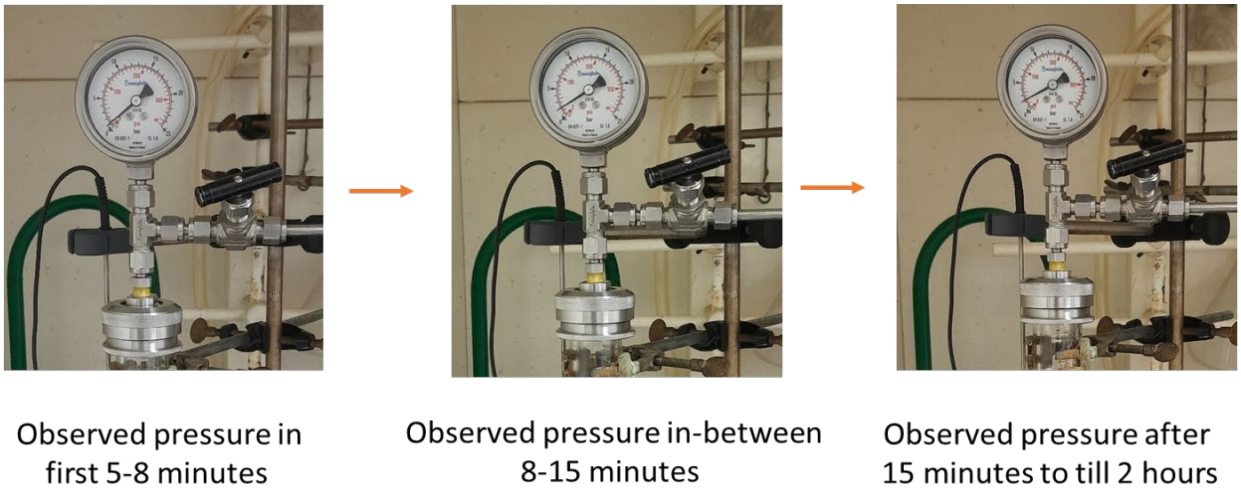
Supplementary Scheme S2: Formation of methyl formate and H_2 gas and other possible intermediates from the reaction mixture**.**

Procedure for the H_2 Quantification: Fischer porter tube (100 mL) was used with Pressure gauge (Swagelok) connected over it. An oven-dried Fischer Porter tube was taken, charged with 5 mol% catalyst ($NiCl_2$.dppp), 1 mmol of paraformaldehyde, and 2 mL anhydrous methanol, and connected with a pressure gauge. The Fischer Porter tube was dipped in a preheated oil bath at a temperature of 120 C and continued for 2 hours with constant monitoring of changes in pressure in the pressure gauge. In the initial 5-8 minutes, the pressure reached ~ 1 bar, and it reached ~2 bar within the next 5-10 minutes. Later, the pressure remains constant for a longer time, even after 16 hours. To analyze the H_2 gas, the Fischer tube was taken out from the oil bath after 2 hours and kept in the ice bath for 5-10 minutes. Then, pressure was released, and volume displacement was calculated.

It was found to be 10-13.5 mL displacement in a burette after several attempts. The same reaction conditions were followed without using the catalyst ($NiCl_2$.dppp), the volume of released gas was analyzed by displacement in the burette, and it was found to be around 2-3 mL after several attempts.



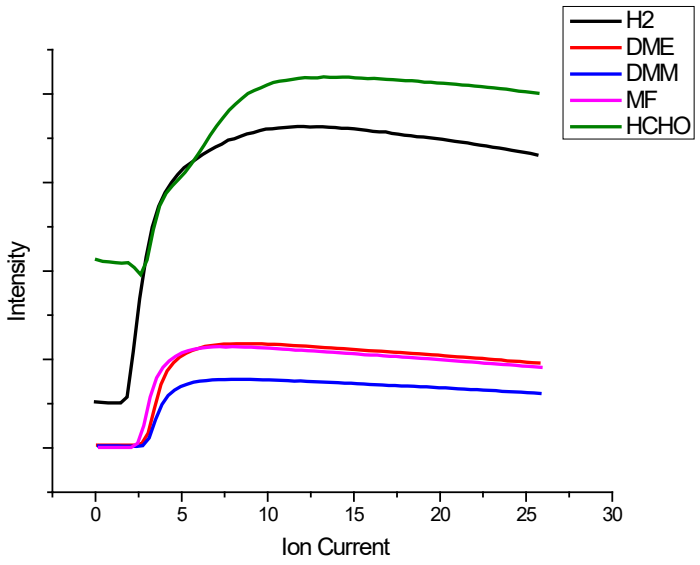
Supplementary Figure S18: H_2 Quantification setup



Supplementary Figure S19: Pressure difference observed in pressure gauge

Reaction in Parr reactor: To observe the precise pressure after 2 hours at ^{0}C and pressure change during the course of the reaction, Reaction was tried in the Parr reactor also with the same reaction condition. It is observed that, pressure reached up to 2.5-3 bar after 2 hours, and after detaching from the heating band and brought to 10-15 ^{0}C, pressure remained 0.2 bar.

Conclusion: After considering all the experiments (with catalyst and without catalyst), the volume of H_2 gas detected is around 8-10 mL. Hence the efficiency of the catalyst will be around 35% (expected H_2 gas volume for 1 mmol paraformaldehyde is 22.4 mL, (8/22.4)*100 = 35.71%).



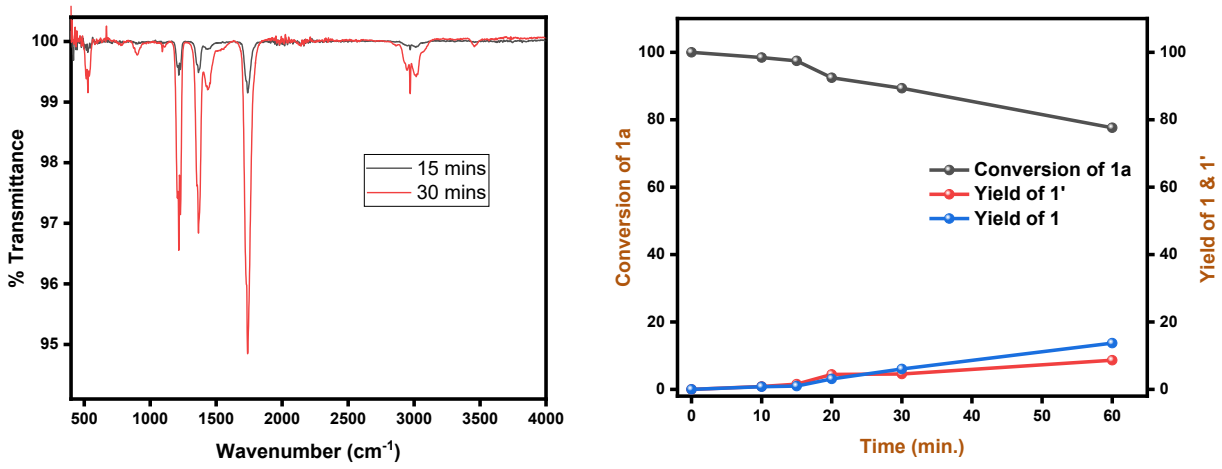
Supplementary Figure S20: Analysis of gaseous samples: Evolved gas analyzer

Reaction condition: Reaction was carried out in 10 mL reaction tube, paraformaldehyde (1 mmol), $NiCl_2$(dppp) (5mol%), and MeOH (2 mL) heated at 120 °C for 2hrs.

4. Rate Order Determination

4.1 Kinetics study

We performed infrared (IR) spectroscopy to follow the reaction at its initial stages. Our observations revealed a continuous rise in alkene formation over time, and notably, no distinct induction time was observed, especially for this particular reaction. We observed a steady increase in alkene formation over time, and no clear induction time was detected. The IR spectroscopy data for the crude reaction mixture at 15 and 30 minutes are shown below,



Supplementary Figure S21: Kinetic study

4.2 Determination of order of the reaction

4.2a Rate order determination for 1a.

The rate order of the semihydrogenation reaction with various reaction components was determined by the initial rate method. The data of the concentration of the product vs time (min) plot was fitted linear with Origin Pro 8. The slope of the linear fitting represents the reaction rate. The order of the reaction was then determined by plotting the log (rate) vs log (conc) for a particular component. Initially, to determine the order of the semihydrogenation reaction on **1a**, the initial rates at different low and high initial concentrations of **1a** were recorded. The final data was obtained by averaging the results of three independent runs for each experiment.

For low concentrations of **1a**, To an oven-dried 10 mL screw-capped vial, paraformaldehyde (30 mg, 1 mmol), $NiCl_2$.dppp (13.5 mg, 10 mol%), a specific amount of **1a** (0.25 mmol scale) (as shown in table S5a), mesitylene (34 µL, 0.25 mmol) as internal standard and methanol (2 mL) was added under a gentle stream of argon. The reaction was carried out individually for each time interval. The mixture was stirred at 120 °C (bath temperature). At regular intervals, the reaction vessel was removed and cooled to ambient temperature, and an aliquot of sample was withdrawn to the GC vial. Finally, the sample was diluted with EtOAc and subjected to GC analysis. The

concentration of product **2a** obtained in each sample was determined with respect to the internal standard mesitylene.

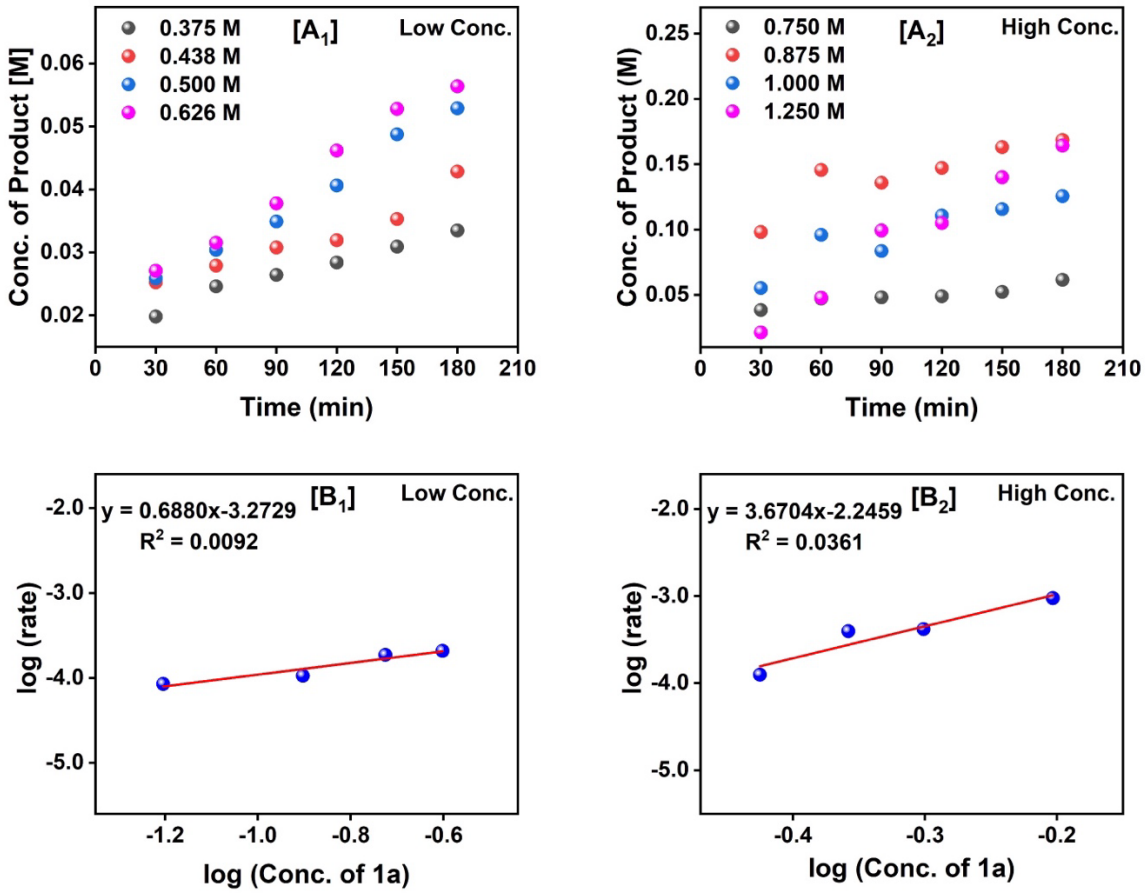
For high concentrations of 1a, To an oven-dried 10 mL screw-capped vial, paraformaldehyde (90 mg, 3 mmol), $NiCl_2$.dppp (54.2 mg, 10 mol%), a specific amount of **1a** (1 mmol scale) (as shown in table S5b), mesitylene (68 µL, 0.5 mmol) as internal standard and methanol (2 mL) was added under a gentle stream of argon. The reaction was carried out individually for each time interval. The mixture was stirred at 120 °C (bath temperature). At regular intervals, the reaction vessel was removed and cooled to ambient temperature, and an aliquot of sample was withdrawn to the GC vial. Finally, the sample was diluted with EtOAc and subjected to GC analysis. The concentration of product **1** obtained in each sample was determined with respect to the internal standard mesitylene.

Supplementary Table S5a. Rate of nickel-catalyzed semihydrogenation reaction at different low concentrations of **1a**.

Experiment	Amount of 1a (gm)	Initial concentration of 1a [M]	Initial Rate $[Mmin^{-1}] \times 10^{-3}$
1	**0.022**	**0.0625**	**0.085**
2	**0.044**	**0.125**	**0.106**
3	**0.067**	**0.188**	**0.186**
4	**0.089**	**0.25**	**0.208**

Supplementary Table S5b. Rate of nickel-catalyzed semihydrogenation reaction at different high concentrations of **1a**.

Experiment	Amount of 1a (gm)	Initial concentration of 1a [M]	Initial Rate $[Mmin^{-1}] \times 10^{-3}$
1	**0.134**	**0.375**	**0.124**
2	**0.156**	**0.438**	**0.396**
3	**0.178**	**0.500**	**0.417**
4	**0.223**	**0.626**	**0.949**



Supplementary Figure S22: The graph of (A_1) Product concentration *vs*. time with different low concentrations of **1a**. (B_1) log (rate) vs. log (conc. of **1a** at low conc.). (A_2) Product concentration *vs*. time with different high concentrations of **1a**. (B_2) log (rate) vs. log (conc. of **1a** at high conc.).

4.2b Rate order determination for $(CH_2O)_n$.

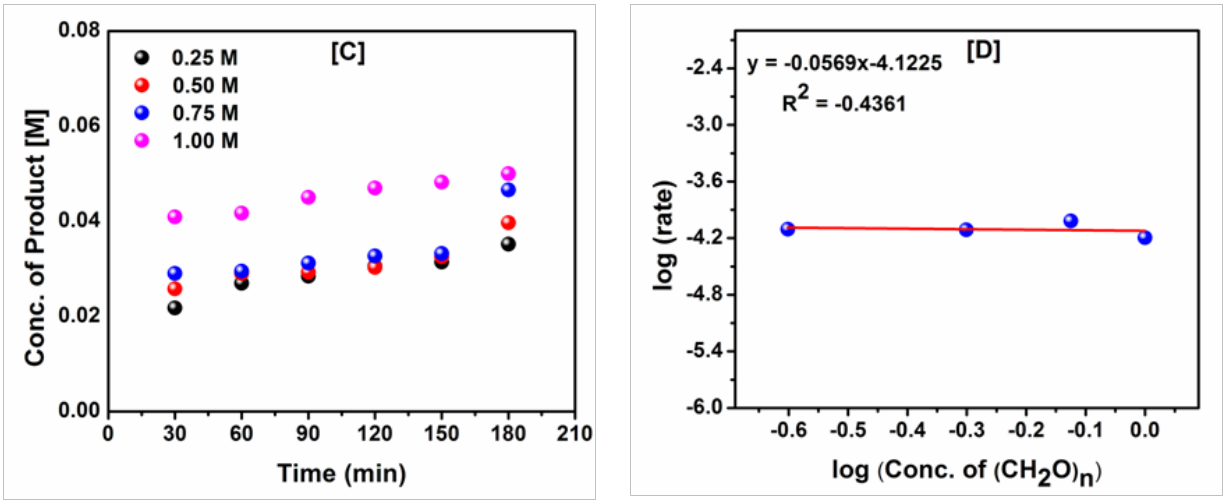
To determine the order of the semihydrogenation reaction on $(CH_2O)_n$, the initial rates at different initial concentrations of $(CH_2O)_n$ were recorded. The final data was obtained by averaging the results of three independent runs for each experiment.

To an oven-dried 10 mL screw-capped vial, diphenyl acetylene (44.5 mg, 0.25 mmol), $NiCl_2$.dppp (13.5 mg, 10 mol%), a specific amount of paraformaldehyde (as shown in table S6), mesitylene (34 µL, 0.25 mmol) as internal standard and methanol (2 mL) were added under a gentle stream of argon. The reaction was carried out individually for each time interval. The mixture was stirred at 120 °C (bath-temperature). At regular intervals, the reaction vessel was removed and cooled to

ambient temperature, and an aliquot of sample was withdrawn to the GC vial. Finally, the sample was diluted with EtOAc and subjected to GC analysis. The concentration of product **1** obtained in each sample was determined with respect to the internal standard mesitylene.

Supplementary Table S6. Rate of nickel-catalyzed semihydrogenation reaction at different initial concentration of **$(CH_2O)_n$.**

Experiment	Amount of $(CH_2O)_n$ (gm)	Initial concentration of $(CH_2O)_n$ [M]	Initial Rate [$Mmin^{-1}$] x 10^{-3}
1	**0.015**	**0.25**	**0.0786**
2	**0.030**	**0.50**	**0.0771**
3	**0.045**	**0.75**	**0.0957**
4	**0.060**	**1.00**	**0.0638**



Supplementary Figure S23: The graph of (C) Time-dependent formation of **1** at different initial concentration of $(CH_2O)_n$. (D) Plot of log (rate) *vs* log (conc. of $(CH_2O)_n$.

4.2c Rate order determination for cat. Ni.

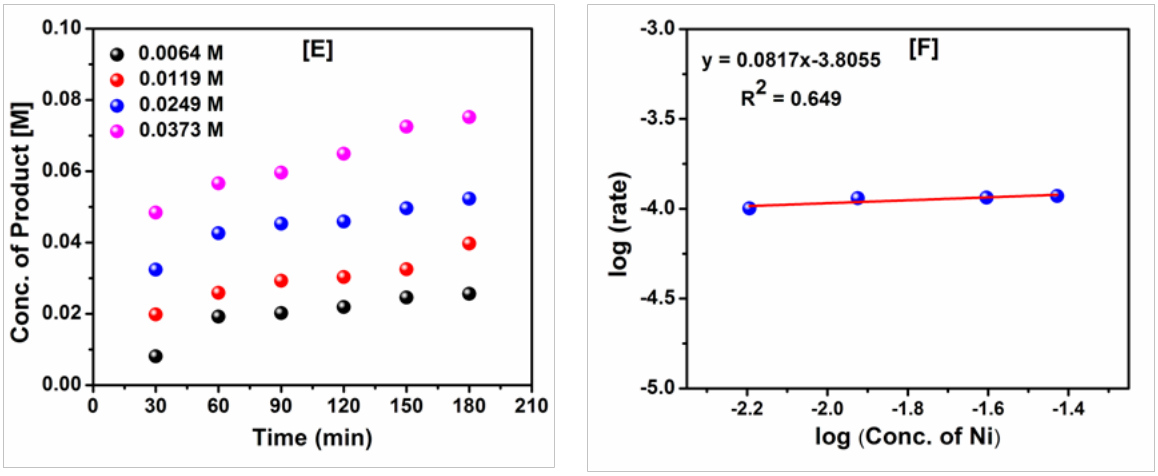
To determine the order of the semihydrogenation reaction in cat.[Ni], the initial rates at different initial concentrations of cat. Ni was recorded. The final data was obtained by averaging the results of three independent runs for each experiment.

To an oven-dried 10 mL screw-capped vial, diphenyl acetylene (44.5 mg, 0.25 mmol), paraformaldehyde (30 mg, 1 mmol), a specific amount of $NiCl_2$.dppp (as shown in table S7),

mesitylene (34 μL, 0.25 mmol) as internal standard, and methanol (2 mL) were added under a gentle stream of argon. The reaction was carried out individually for each time interval. The mixture was stirred at 120 °C (bath temperature). At regular intervals, the reaction vessel was removed and cooled to ambient temperature, and an aliquot of sample was withdrawn to the GC vial. Finally, the sample was diluted with EtOAc and subjected to GC analysis. The concentration of product **1** obtained in each sample was determined with respect to the internal standard mesitylene.

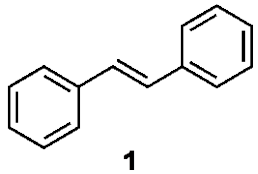
Supplementary Table S7. Rate of nickel-catalyzed semihydrogenation reaction at different initial concentration of **Cat. Ni.**

Experiment	Amount of cat. Ni (gm)	Initial concentration of cat. Ni [M]	Initial Rate [Mmin^{-1}] x 10^{-3}
1	**0.007**	**0.0064**	**0.1003**
2	**0.013**	**0.0119**	**0.1145**
3	**0.027**	**0.0249**	**0.1153**
4	**0.040**	**0.0373**	**0.1178**



Supplementary Figure S24. The graph of (E) Time-dependent formation of **1** at different initial concentration of cat.Ni. (F) Plot of log (rate) *vs* log (conc. of cat. Ni).

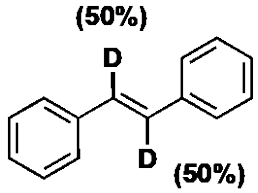
5. Characterization Data



1

***(E)*-1,2-diphenylethene (1)**

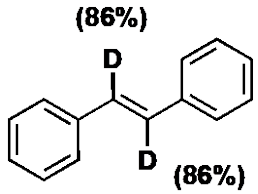
White solid; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56-7.54 (m, 4H), 7.41-7.38 (m, 4H), 7.32-7.28 (m, 2H), 7.15 (s, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 137.28, 128.65, 127.59, 126.48 ppm.



1-D1

(*E*)-1,2 –diphenylethene-D_1 (1-D_1)

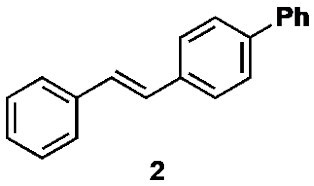
White solid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 7.54-7.50 (m, 4H), 7.36-7.25 (m, 6H), 7.11 (s, 1H); ^{13}C NMR (50 MHz, Chloroform-*d*) δ 137.32, 128.68, 127.61, 126.50 ppm.



1-D2

(*E*)-1,2-diphenylethene-D_2 (1-D_2)

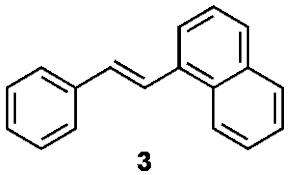
White solid; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55-7.53 (m, 4H), 7.40 -7.36 (m, 4H), 7.30-7.28 (m, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 137.21, 128.66, 127.58, 126.47 ppm.



2

(*E*)-4-styryl-1,1'-biphenyl (2)

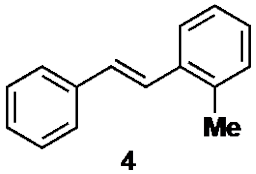
White solid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 7.58-7.18 (m, 14H), 7.08 (s, 2H); ^{13}C NMR (50 MHz, Chloroform-*d*) δ 140.67, 140.33, 137.32, 136.38, 128.79, 128.70, 128.19, 127.65, 127.34, 126.92, 126.52 ppm.



3

(*E*)-1-styrylnaphthalene (3)

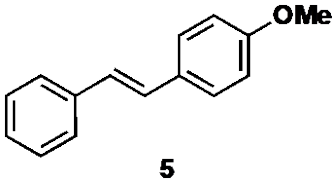
White solid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 8.15 (d, *J* = 8.0 Hz, 1H), 7.83-7.67 (m, 4H), 7.55-7.41 (m, 4H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.28-7.22 (m, 1H), 7.18-7.01 (m, 2H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 137.61, 135.02, 133.72, 131.77, 131.40, 129.04, 128.74, 128.61, 128.03, 127.77, 126.68, 126.08, 125.82, 125.69, 123.77, 123.62 ppm.



4

(*E*)-1-methyl-2-styrylbenzene (4)

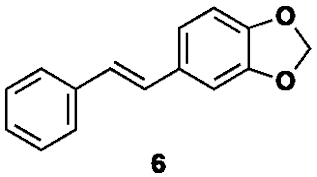
Pale yellow liquid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 7.64-7.52 (m, 3H), 7.43-7.28 (m, 4H), 7.24-7.19 (m, 3H), 7.01 (d, *J* = 16.1 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (50 MHz, Chloroform-*d*) d 137.68, 136.39, 135.80, 130.39, 130.01, 128.67, 127.57, 126.55, 126.19, 125.36, 19.90 ppm.



5

(*E*)-1-methoxy-4-styrylbenzene (5)

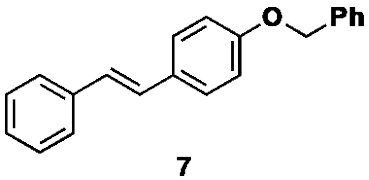
White solid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 7.52-7.23 (m, 7H), 7.12-7.00 (dd, *J = 7.4, 4.8* Hz, 2H), 6.92-6.88 (m, 2H), 3.83 (s, 3H); ^{13}C NMR (50 MHz, Chloroform-*d*) δ 159.31, 137.65, 130.15, 128.63, 128.21, 127.70, 127.20, 126.62, 126.24, 114.14, 55.32 ppm.



6

(*E*)-5-Styrylbenzo[d] [1,3]dioxole (6)

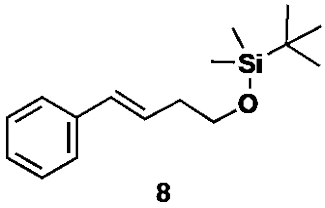
Pale yellow solid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 7.50-7.46 (m, 2H), 7.34-7.25 (m, 3H), 7.07 (d, *J* = 1.6 Hz, 1H), 7.00-6.93 (m, 3H), 6.80 (d, *J* = 8.0 Hz, 1H), 5.97 (s, 2H); ^{13}C NMR (50 MHz, Chloroform-*d*) δ 148.14, 147.31, 137.40, 131.88, 128.65, 128.34, 127.35, 127.02, 126.29, 121.45, 108.41, 105.55, 101.11 ppm.



7

(*E*)-1-(benzyloxy)-4-styrylbenzene (7)

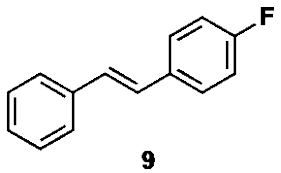
White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51–7.34 (m, 11H), 7.24 (d, *J* = 7.3 Hz, 2H), 7.08 (d, *J* = 16.3 Hz, 1H), 7.01-6.98 (m, 3H), 5.11 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.46, 137.59, 136.86, 128.60, 128.14, 128.00, 127.71, 127.47, 126.71, 126.24, 115.05, 70.03 ppm.



8

(*E*)-tert-butyldimethyl((4-phenylbut-3-en-1-yl)oxy)silane (8)

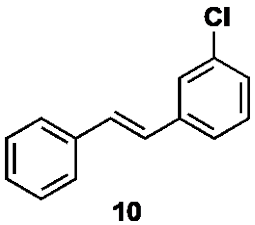
Colourless liquid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 7.37-7.29 (m, 5H), 6.45 (d, *J* = 15.8 Hz 1H), 6.30-6.19 (m, 1H), 3.74 (t, *J* = 6.7 Hz, 2H), 2.44 (q, *J* = 6.9 Hz, 2H), 0.92 (s, 9H), 5.76 (s, 6H); ^{13}C NMR (50 MHz, Chloroform-*d*) δ 137.71, 131.62, 128.46, 126.94, 125.97, 125.01, 62.98, 36.92, 36.65, 25.95, 5.24 ppm.



9

(*E*)-1-fluoro-4-styrylbenzene (9)

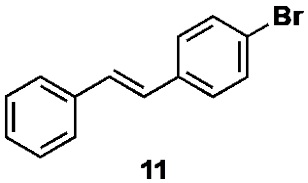
White solid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 7.52-7.44 (m, 4H), 7.39-7.35 (m, 1H), 7.33-7.29 (m, 2H), 7.09-7.00 (m, 4H); ^{13}C NMR (50 MHz, Chloroform-*d*) δ 164.78, 159.87, 137.16, 133.48, 128.69, 128.05, 127.89, 127.65, 127.47, 126.42, 115.81, 115.39 ppm.



10

(*E*)-1-chloro-4-styrylbenzene (10)

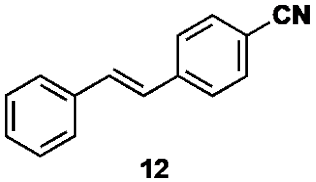
White solid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 7.53-7.49 (m, 3H), 7.40-7.20 (m, 6H), 7.12 (d, *J* = 16.2 Hz, 1H), 7.01 (d, *J* = 16.4 Hz, 1H); ^{13}C NMR (50 MHz, Chloroform-*d*) δ, 139.23, 136.80, 134.63, 130.12, 129.85, 128.74, 128.02, 127.47, 127.20, 126.64, 126.29, 124.73 ppm.



11

(*E*)-1-bromo-4-styrylbenzene (11)

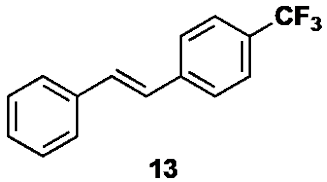
White solid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 7.52-7.46 (m, 3H), 7.41-7.26 (m, 6H), 7.10-7.06 (m, 2H); ^{13}C NMR (50 MHz, Chloroform-*d*) δ 136.28, 131.77, 129.43, 128.73, 127.96, 127.89, 127.63, 127.40, 126.55 ppm.



12

(*E*)-4-styrylbenzonitrile (12)

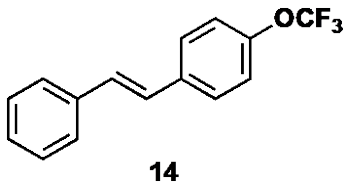
White solid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 7.59-7.44 (m, 6H), 7.35-7.24 (m, 3H), 7.15 (d, *J = 14.7* Hz, 1H), 7.00 (d, *J = 16.2* Hz, 1H); ^{13}C NMR (50 MHz, Chloroform-*d*) δ 141.80, 136.25, 132.44, 128.82, 128.61, 126.87, 126.83, 126.69, 118.99, 110.54 ppm.



13

(*E*)-1-styryl-4-(trifluoromethyl) benzene (13)

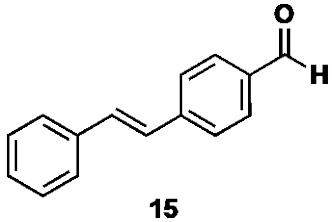
White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62-7.54 (m, 6H), 7.42-7.32 (m, 3H), 7.22 (d, *J* = 16.4 Hz, 1H), 7.13 (d, *J* = 16.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 140.80, 136.62, 131.20, 128.79, 128.28, 127.11, 126.77, 126.56, 125.64, 125.60 ppm.



14

(*E*)-1-styryl-4-(trifluoromethoxy) benzene (14)

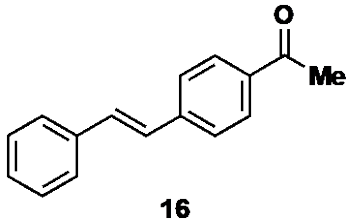
White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55-7.52 (m, 4H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.31-7.29 (m, 2H), 7.23-7.21 (m, 2H), 7.08 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.45, 136.89, 136.10, 129.70, 128.74, 127.93, 127.65, 127.08, 126.57, 121.18 ppm.



15

(*E*)-4-styrylbenzaldehyde (15)

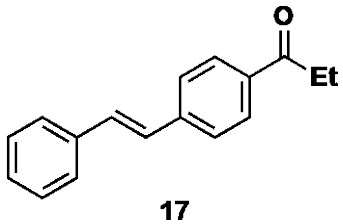
Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.01 (s, 1H), 7.89 (d, *J* = 8.3 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 7.1 Hz, 2H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.36-7.33 (m, 1H), 7.28 (d, *J* = 16.1 Hz, 1H), 7.16 (d, *J* = 16.3 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 191.662, 143.41, 136.51, 135.29, 132.18, 130.23, 128.82, 128.49, 127.31, 126.89 ppm. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{15}H_{12}O$ 209.0961; Found 209.0954



16

(*E*)-1-(4-styrylphenyl) ethanone (16)

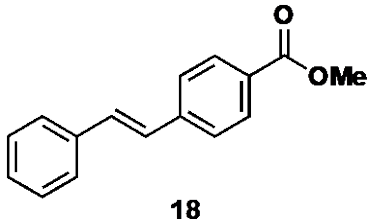
White solid; ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 8.39 Hz 2H), 7.51 (d, *J* = 8.3 Hz, 2H), 7.46 (d, *J* = 7.6 *Hz,* 2H), 7.31 (t, *J* = 7.2 Hz, 2H), 7.24-7.23 (m, 1H), 7.15 (d, *J* = *16.4* Hz, 1H), 7.05 (d, *J* = 16.4 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 197.46, 141.99, 136.67, 135.93, 131.45, 128.77, 128.29, 127.42, 126.79, 126.47, 26.56 ppm.



17

(*E*)-1-(4-styrylphenyl) propan-1-one (17)

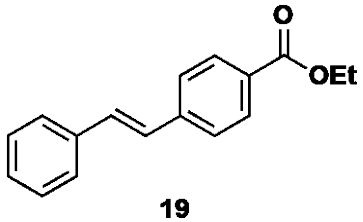
White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 8.4 Hz, 2H), 7.54-7.46 (m, 4H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.29-7.21 (m, 1H), 7.18 (d, *J* = 16.3 Hz, 1H), 7.09 (d, *J* = 16.3 Hz, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.33, 141.63, 136.69, 131.05, 129.91, 1129.19, 128.70, 128.14, 127.52, 126.71, 126.21, 60.85, 14.30 ppm.



18

(*E*)-methyl 4-styrylbenzoate (18)

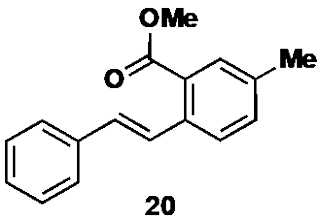
White solid; ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 8.3 Hz, 2H), 7.49-7.45 (m, 4H), 7.31-7.28 (t, *J* = 7.6 Hz, 2H), 7.23-7.20 (m, 1H), 7.13 (d, *J* = 16.4 Hz, 1H), 7.04 (d, *J* = 16.4 Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.87, 141.81, 136.73, 131.21, 130.01, 128.89, 128.76, 128.22, 127.54, 126.76, 126.29, 52.05 ppm.



19

(*E*)-Ethyl 4-styrylbenzoate (19)

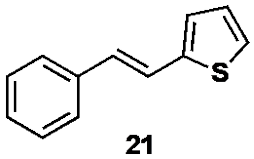
White solid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 8.02 (d, *J* = 8.3 Hz, 2H), 7.57-7.50 (m, 4H), 7.40-7.28 (m, 3H), 7.20 (d, *J* = 14.0 Hz, 1H), 7.10 (d, *J* = 16.2 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 1H), 1.39 (s, *J* = 6.91 Hz, 2H); ^{13}C NMR (50 MHz, Chloroform-*d*) δ 166.35, 141.66, 136.73, 131.08, 129.94, 129.23, 128.72, 128.16, 127.57, 126.74, 126.23, 60.86, 14.31 ppm.



20

methyl (*E*)-5-methyl-2-styrylbenzoate (20)

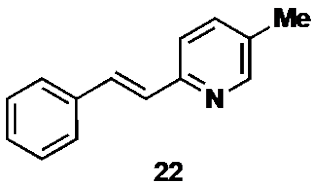
Yellow liquid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 16.2 Hz, 1H), 7.75 (s, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 7.5 Hz, 2H), 7.36 (q, *J* = 8.7 Hz, 3H), 7.28 (d, *J* = 8.6 Hz, 2H), 6.99 (d, *J* = 16.2 Hz, 1H), 3.94 (s, 3H), 2.40 (s, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.03, 137.06, 132.96, 131.05, 130.57, 128.61, 128.39, 127.64, 127.27, 126.84, 126.74, 52.06, 21.00 ppm.



21

(*E*)-2-styrylthiophene (21)

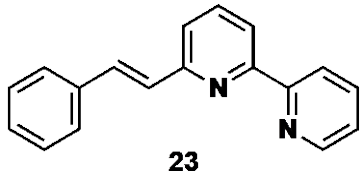
Pale yellow solid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 7.51-7.46 (m, 2H), 7.39-7.29 (m, 3H), 7.26-7.19 (m, *2*H), 7.08 (d, *J* = 2.9 Hz, 1H), 7.04-7.00 (m, 1H), 6.94 (d, *J* = 16.2 Hz, 1H); ^{13}C NMR (50 MHz, Chloroform-*d*) δ 142.87, 136.95, 128.68, 128.32, 127.57, 126.28, 126.07, 124.32, 121.76 ppm.



22

(*E*)-5-methyl-2-styrylpyridine (22)

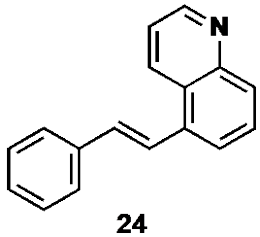
Pale yellow solid; ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.36 (s, 1H), 7.53-7.19 (m, 8H), 7.08 (d, *J* = 16.1 Hz, 1H), 2.27 (s, 3H); ^{13}C NMR (126 MHz, Chloroform-*d*) δ 153.02, 150.10, 137.03, 136.83, 131.65, 128.67, 127.93, 126.96, 121.51, 18.29 ppm.



23

(*E*)-6-styryl-2,2'-bipyridine (23)

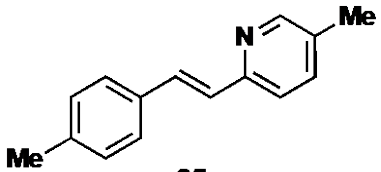
White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.71-8.67 (m, 1H), 8.55 (dd, *J* = 28.3, 8.0 Hz, 1H), 8.33 (dd, *J* = 40.5, 8.7 Hz, 1H), 7.90-7.55 (m, 5H), 7.45-7.23 (m, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.92, 149.10, 142.84, 137.41, 136.87, 132.78, 132.07, 128.71, 128.37, 127.13, 123.72, 122.07, 121.29, 120.32, 119.46 ppm. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{14}N_2$ 259.1230; Found 259.1226



24

(*E*)-5-styrylquinoline (24)

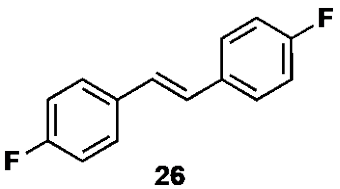
Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.97 (d, *J* = 5.5 Hz, 1H), 8.58 (d, *J* = 8.6 Hz, 1H), 8.09 (d, *J* = 8.3 Hz, 1H), 7.84-7.71 (m, 3H), 7.61 (d, *J* = 7.5 Hz, 2H), 7.49-7.42 (m, 2H), 7.38 (d, *J* = 21.4 Hz, 1H), 7.34-7.26 (m, 1H), 7.19 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 150.24, 137.14, 135.36, 132.86, 132.22, 129.28, 129.16, 128.80, 128.12, 126.73, 124.17, 123.88, 120.92 ppm. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{13}N$ 232.1121; Found 232.1118



25

(*E*)-5-methyl-2-(4-methylstyryl) pyridine (25)

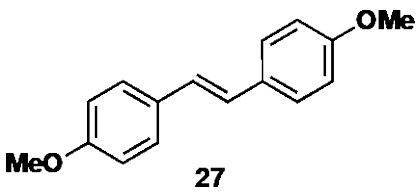
Brown solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.44 (s, 1H), 7.68 (d, *J* = 16.2 Hz, 1H), 7.70-7.66 (m, 1H), 7.52-7.47 (m, 3H), 7.23-7.21 (m, 1H), 7.22 (d, *J* = 16.1 Hz, 1H), 2.40 (s, 3H), 2.38 (s, 3H);^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.71, 146.71, 139.25, 133.17, 132.37, 129.54, 127.41, 121.74, 21.39, 18.25 ppm.



26

(*E*)-1,2-bis(4-fluorophenyl) ethane (26)

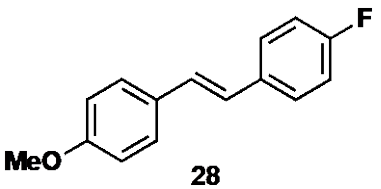
White solid; ^{1}H NMR (200 MHz, Chloroform-*d*) δ 7.51-7.44 (m, 4H), 7.11-7.02 (m, 4H), 6.99 (s, 2H); ^{13}C NMR (50 MHz, Chloroform-*d*) d 164.80, 159.88, 133.38, 127.98, 127.82, 127.27, 115.85, 115.42 ppm.



27

(*E*)-1,2-bis(4-methoxyphenyl) ethene (27)

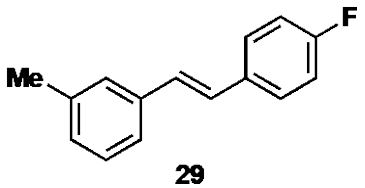
White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 (d, *J* = 8.7 Hz, 4H), 6.97-6.85 (m, 6H), 3.84 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.99, 130.48, 127.40, 126.17, 114.09, 55.31 ppm.



28

(*E*)-1-fluoro-4-(4-methoxystyryl) benzene (28)

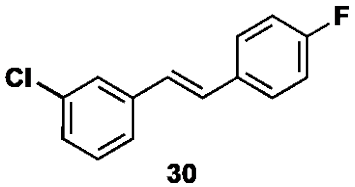
Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 (dd, *J* = 8.6, 6.1 Hz, 4H), 7.05 (t, *J* = 8.7 Hz, 2H), 6.97 (d, *J* = 14.1 Hz, 2H), 6.92 (d, *J* = 16.8 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.31, 133.80, 129.96, 128.00, 127.62, 125.39, 115.63, 115.42, 114.14, 55.29 ppm. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{15}H_{13}FO$ 229.1024; Found 229.1012



29

(*E*)-1-(4-fluorostyryl)-3-methylbenzene (29)

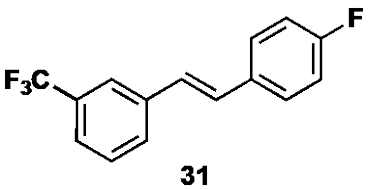
White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.33-7.25 (m, 3H), 7.25 (d, *J* = 7.5 Hz, 1H), 7.11-7.04 (m, 4H), 7.00 (d, *J* = 16.4 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.51, 161.05, 138.24, 137.09, 133.61, 128.58, 128.48, 127.96, 127.25, 127.12, 123.62, 115.69, 115.47, 21.42 ppm.



30

(*E*)-1-chloro-3-(4-fluorostyryl) benzene (30)

Colourless liquid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 (dd, *J* = 8.6, 5.3 Hz, 3H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.31-7.24 (m, 3H), 7.10-7.06 (m, 3H), 6.95 (d, *J* = 16.3 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.76, 161.30, 139.04, 134.64, 132.99, 129.87, 128.85, 128.19, 127.51, 126.95, 126.19, 124.66, 115.81, 115.59 ppm.

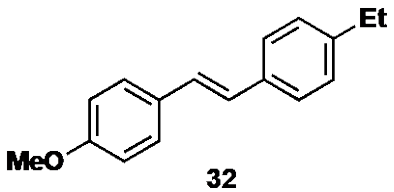


31

(*E*)-1-fluoro-4-(4-(trifluoromethyl) styryl) benzene (31)

White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.63-7.58 (m, 4H), 7.53-7.50 (m, 2H), 7.16 (d, *J* = 16.3 Hz, 1H), 7.09 (t, *J* = 8.7 Hz, 2H), 7.04 (d, *J* = 16.4 Hz, 1H); ^{13}C NMR (101 MHz,

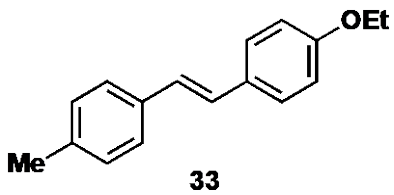
Chloroform-*d*) δ 163.90, 161.43, 140.61, 132.82, 129.91,129.42, 129.10, 128.35, 128.27, 126.87, 126.48, 125.65, 122.84, 115.87, 115.65 ppm.



32

(*E*)-1-ethyl-4-(4-methoxystyryl) benzene (32)

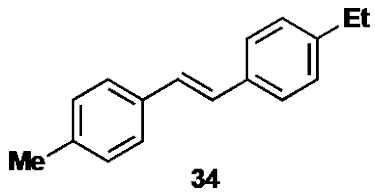
White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 (dd, *J* = 11.2, 8.4 Hz, 4H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.05 (d, *J* = 16.3 Hz, 1H), 6.98 (d, *J* = 16.3 Hz, 1H), 6.92 (d, *J* = 8.7 Hz, 2H), 3.85 (s, 3H), 2.67 (q, *J* = 7.6 Hz, 2H), 1.27 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.11, 143.45, 135.09, 130.33, 128.13, 127.56, 127.26, 126.55, 126.21, 114.08, 55.29, 28.60, 15.53 ppm. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{18}O$ 239.1431; Found 239.1427



33

(*E*)-1-ethoxy-4-(4-methylstyryl) benzene (33)

White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 (d, *J* = 8.7 Hz, 2H), 7.40 (d, *J* = 8.1 Hz, 2H), 7.17 (d, *J* = 7.9 Hz, 2H), 7.03 (d, *J* = 16.3 Hz, 1H), 6.96 (d, *J* = 16.3 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 2H), 4.07 (q, *J* = 7.0 Hz, 2H), 2.37 (s, 3H), 1.44 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.50, 137.00, 134.87, 130.15, 129.33, 127.54, 127.26, 126.41, 126.12, 114.63, 63.46, 21.21, 14.83 ppm. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{18}O$ 239.1431; Found 239.1427

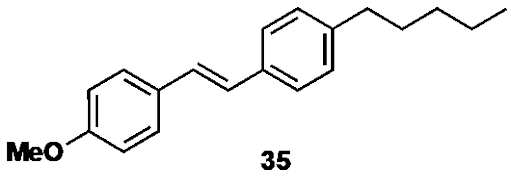


34

(*E*)-1-ethyl-4-(4-methylstyryl) benzene (34)

White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 (dd, *J* = 9.8, 8.2 Hz, 4H), 7.21 (dd, *J* = 10.6, 8.1 Hz, 4H), 7.09 (s, 2H), 2.69 (q, *J* = 7.6 Hz, 2H), 2.39 (s, 3H), 1.29 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.66, 137.23, 134.96, 134.71, 129.34, 128.15, 127.61,

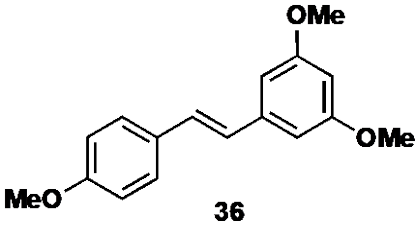
126.36, 28.61, 21.22, 15.54 ppm. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{18}$ 223.1482; Found 223.1469.



35

(*E*)-1-methoxy-4-(4-pentylstyryl) benzene (35)

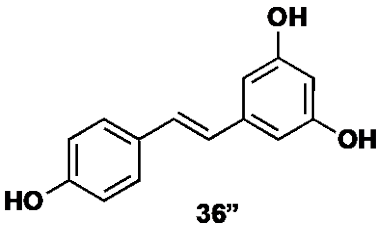
White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 (dd, *J* = 15.1, 8.4 Hz, 4H), 7.17 (d, *J* = 8.1 Hz, 2H), 7.04 (d, *J* = 16.3 Hz, 1H), 6.97 (d, *J* = 16.4 Hz, 1H), 6.95-6.89 (m, 2H), 3.84 (s, 3H), 2.63-2.59 (m, 2H), 1.67-1.63 (m, 2H), 1.36-1.33 (m, 4H), 0.92-0.89 (m, 3H);^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.13, 142.23, 135.07, 130.38, 128.73, 127.59, 127.26, 126.62, 126.17, 114.11, 55.35, 35.70, 31.53, 31.16, 22.58, 14.07 ppm. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{24}O$ 281.1900; Found 281.1890.



36

(*E*)-1,3-dimethoxy-5-(4-methoxystyryl) benzene (36)

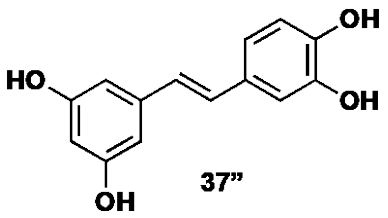
Pale yellow liquid. ^{1}H NMR (200 MHz, Chloroform-d) δ = 7.55-7.41 (m, 2H), 7.02 (s, 1H), 6.98-6.91 (m, 2H), 6.91-6.87 (m, 1H), 6.67 (d, *J* = 2.1 Hz, 2H), 6.39 (t, *J* = 2.2 Hz, 1H), 3.84 (s, 9H).^{13}C NMR (50 MHz, Chloroform-d) δ 161.97, 159.40, 139.70, 129.94, 128.74, 127.78, 126.58, 114.14, 104.35, 99.64, 55.35 ppm.



36”

(*E*)-5-(4-hydroxystyryl) benzene-1,3-diol (36’’)

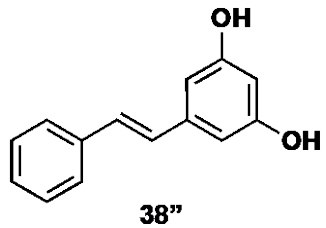
White solid. ^{1}H NMR (200 MHz, DMSO-d_6) δ 8.59 (s, 1H), 8.25 (s, 2H), 6.32 (d, J = 8.6 Hz, 2H), 5.84-5.67 (m, 4H), 5.33 (s, 2H), 5.06-5.05 (m, 1H); ^{13}C NMR (50 MHz, DMSO-d_6) δ 158.64, 157.33, 139.47, 128.27, 128.04, 125.81, 115.74, 104.53, 101.97 ppm.



37”

(*E*)-4-(3,5-dihydroxystyryl)benzene-1,2-diol (37”)

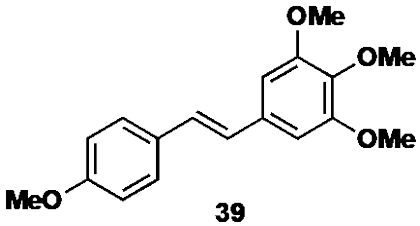
White solid, ^{1}H NMR (400 MHz, Methanol-d_4) d ppm 6.98 (s, 1H) 6.91-6.73 (m, 2H), 6.44 (s, 2H) 6.16 (s, 1H) ppm.



38”

(*E*)-5-styrylbenzene-1,3-diol (38”)

White solid, ^{1}H NMR (400 MHz, Methanol-d_4) d 7.50 (d, J=7.38 Hz, 2H), 7.33 (t, J=7.63 Hz, 2H), 7.19-7.26 (m, 1H), 6.95-7.08 (m, 2H), 6.49 (d, J = 2.13 Hz, 2H), 6.20 (t, J = 2.13 Hz, 1H); ^{13}C NMR (Methanol-d_4 ,101MHz) δ 159.91, 140.90, 138.95, 130.08, 129.83, 129.60, 128.67, 127.61, 106.23, 103.36, 49.79, 49.58, 49.37, 49.15, 48.94, 48.72, 48.51 ppm.



39

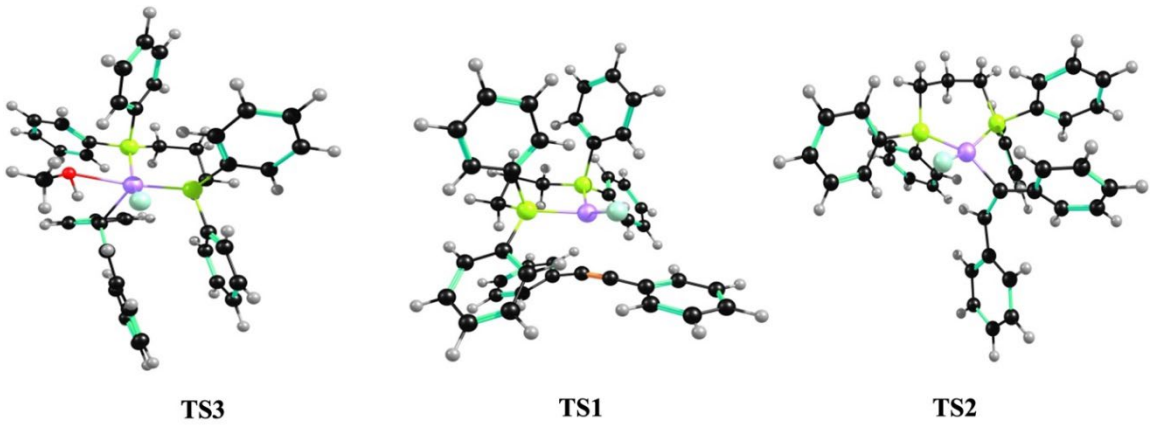
(*E*)-1,2,3-trimethoxy-5-(4-methoxystyryl) benzene (39)

White solid. ^{1}H NMR (200 MHz, Chloroform-d) δ 7.46 (d, J = 8.8 Hz, 2H), 6.96-6.89 (m, 3H), 6.73 (s, 2H), 3.92 (s, 6H), 3.88 (s, 3H), 3.84 (s, 3H); ^{13}C NMR (50 MHz, Chloroform-d) δ 159.30, 153.39, 137.71, 133.43, 130.02, 127.74, 127.61, 126.55, 114.15, 103.37, 60.92, 56.11, 55.29 ppm.

6. DFT Studies and Reaction Mechanism

Full quantum chemical calculations were performed using density functional theory (DFT) at the dispersion and solvent-corrected PBE/TZVP level of theory to understand the mechanism (Figs. S27-S28) of the alkyne hydrogenation reaction in the presence of the Ni(II).dppe catalyst **I**. The values (in kcal/mol) were calculated at the PBE/TZVP level of theory with DFT, with methanol (ε = 32.5) modeled as the solvent The reaction is initiated at the square planar complex **A** (precatalyst Ni(II)). In the presence of a methanol solvent, one of the chloride ligands is replaced by the methoxy group of MeOH (complex **II**). In the next step, complex **II** reacts with paraformaldehyde. The methoxy ligand of complex **II** is substituted by hydride *via* intermediate **III** to form a new Ni(II) catalyst **I**, which acts as the catalyst in the entire diphenylacetylene to (*E*)-stilbene transfer hydrogenation cycle.

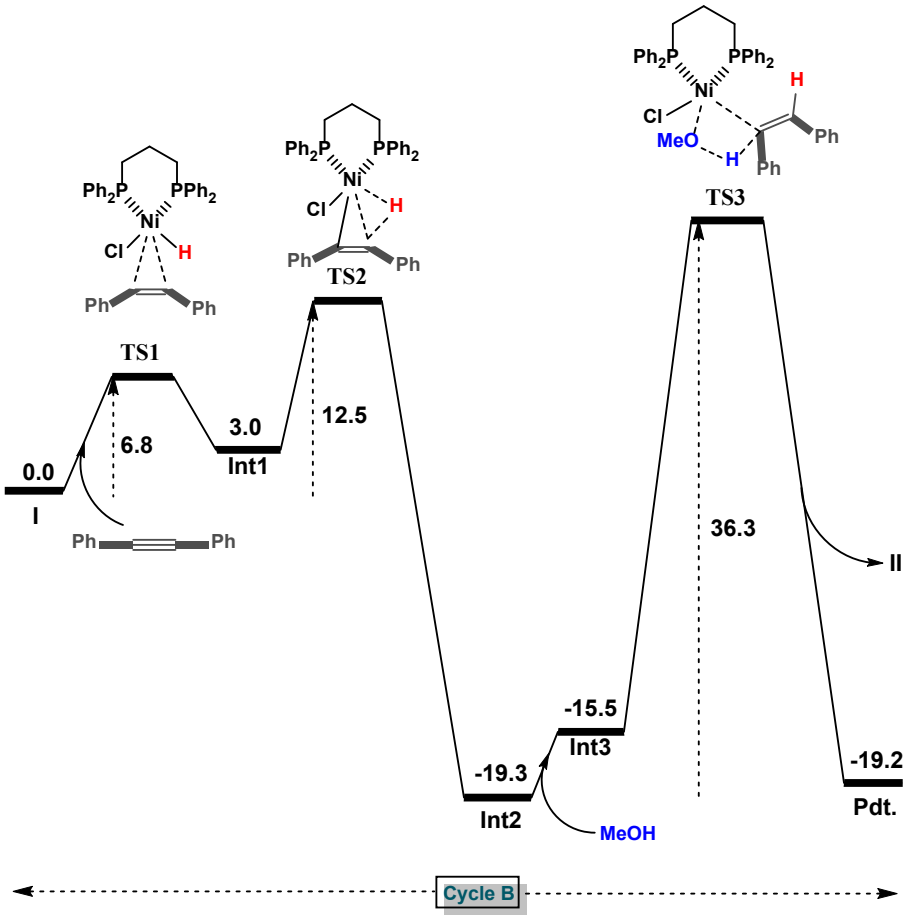
In the first step of the catalytic cycle, diphenylacetylene **1a** approaches the square planar catalyst **I** and makes a square pyramidal π-complex, **Int-1** (Fig S28, Cycle B). The reaction free energy for this π-complex formation step is 3.0 kcal/mol, and this step goes through the transition state **TS1** with an activation free energy of 6.8 kcal/mol. In the next step, the reaction proceeds through **TS2** with an intramolecular rearrangement occurring, with the hydride being transferred from the Ni(II) center to one of the alkyne carbons. Consequently, the π-complex is broken, and the covalent Ni(II)-C bond (**Int-2**) is formed. The reaction free energy and the activation energy barriers are -22.3 kcal/mol and 12.5 kcal/mol, respectively. The next step, corresponding to the interaction of methanol with the Ni(II) center, leads to the formation of **Int-3**. The free energy increases by 3.8 kcal/mol. The distance between the Ni(II) center and the methanol oxygen is 3.75 Å, suggesting a weak interaction. This step proceeds *via* a four-membered transition state (**TS3**), where the proton is transferred to the alkyne carbon, along with the simultaneous breaking of the Ni(II)-C bond and the formation of the Ni(II)-O bond. Thus, (*Z*)-stilbene is formed, and catalyst **II** is regenerated. The free energy and activation energy barrier for the product formation step is 0.1 kcal/mol and 36.3 kcal/mol, respectively. These values indicate that the reaction would be favorable under the conditions.



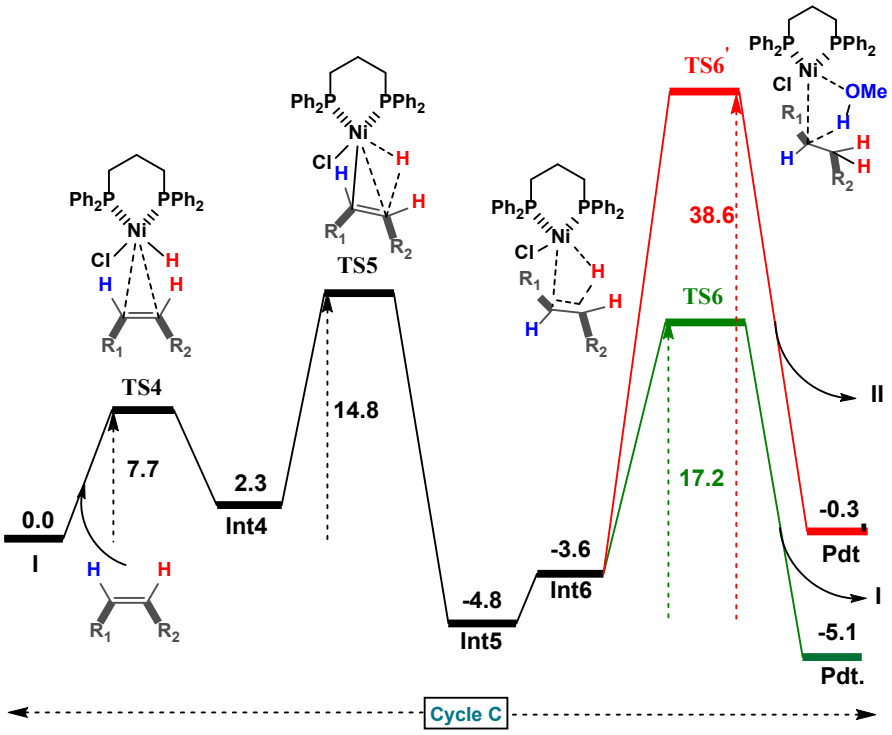
Supplementary Figure S25. Transition state geometries for the nickel catalyst.

The formation of (*E*)-stilbene may also be explained *via* the alkene isomerization cycle shown in Fig. S28 (Cycle C). In the first step of this cycle, the catalyst species **I** interact with (*Z*)-stilbene, leading to **Int-4**. This step is endergonic, with a binding free energy value of 2.3 kcal/mol, which compares well with the binding energy of diphenylacetylene to the catalyst **I** (3.0 kcal/mol) (in Cycle B, discussed above). The activation-free energy barrier for this step is 7.7 kcal/mol. In the next step, the hydride is transferred from Ni(II) of **Int-4** to the closest carbon of (*Z*)-stilbene, leading to **Int-5**. This hydrogenation by hydride transfer occurs through **TS5**, with a low activation barrier of 14.8 kcal/mol, and leads to sp^3 hybridization of the carbon atom of (*Z*)-stilbene. Rotation along the C−C bond of this complex leads to the conversion of **Int-5** to **Int-6** (Fig. S28, Cycle C). This step is thermodynamically a little endergonic by 1.2 kcal/mol. Now, in the next step, there are two possibilities: either β-H transfer to the Ni center from **Int-6** *via* **TS6** with a free energy barrier of 17.2 kcal/mol leading to (*E*)-stilbene **(Pdt)** and the regeneration of the catalyst **I** (shown in green in Fig. S27), or the complete hydrogenation *via* interaction of methanol with **Int-6** and the subsequent four-membered **TS6'**, where methanol transfers its proton to the carbon center and

the Ni(II)-C bond is broken at the same time, leading to the formation of the alkane (**Pdt'**) and the regeneration of the catalyst **II** (shown in red in Fig.S27). The free energy and activation energy barriers for these steps are 17.2 kcal/mol and 38.6 kcal/mol, respectively. Therefore, the complete hydrogenation pathway is thermodynamically and kinetically unfavorable than the β-H transfer step.

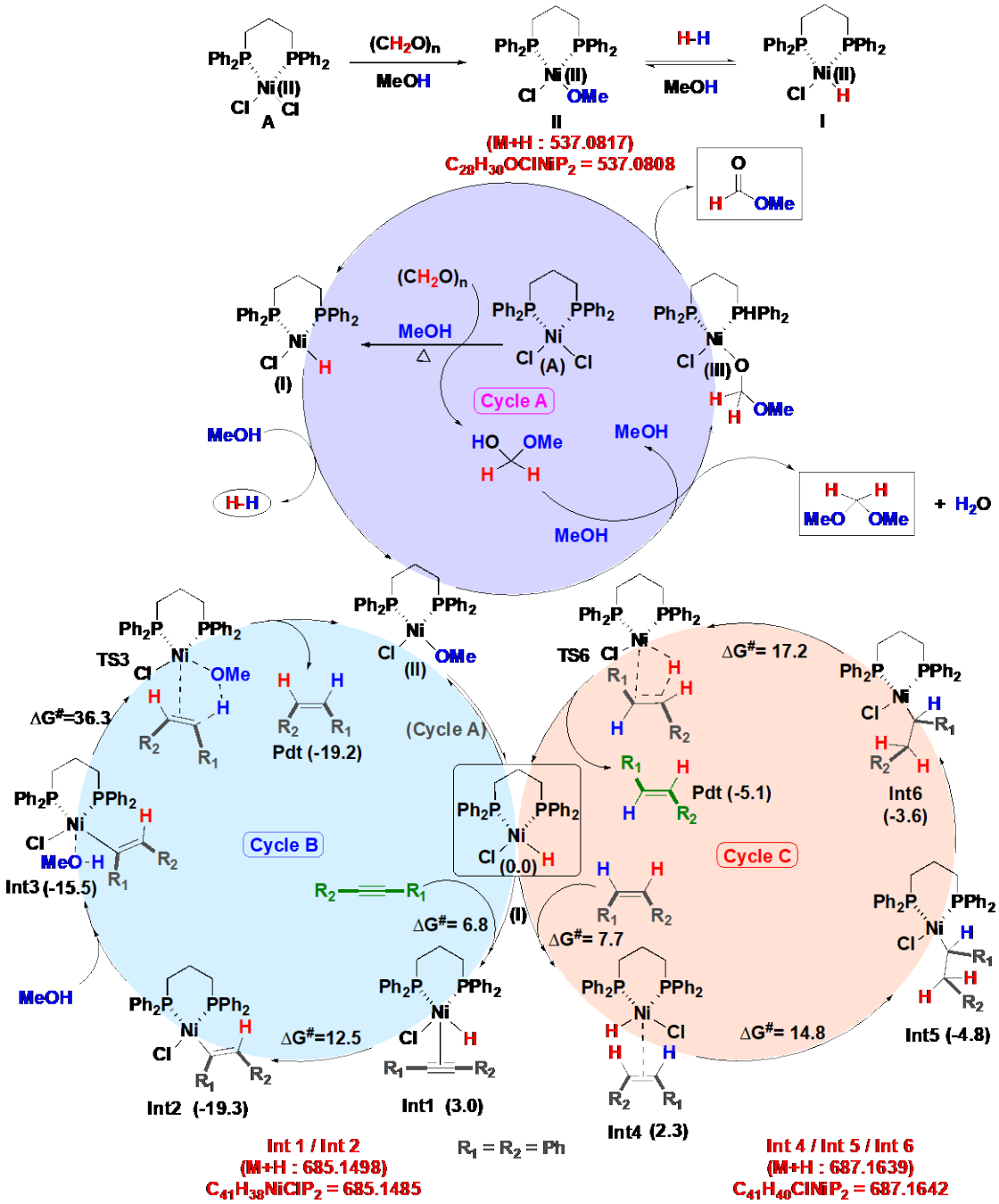


Supplementary Figure S26. The free energy profile for the catalytic semi-hydrogenation of diphenylacetylene by $NiCl_2$.dppp.



Supplementary Figure S27. The free energy profile for the catalytic isomerization of (*Z*)-stilbene into (*E*)-stilbene by $NiCl_2$.dppp.

In DFT, it is a common issue to observe an overestimation of energy barriers when compared to experimentally calculated values, primarily due to its approximation-based nature. As a result, the absolute values obtained from DFT may not be entirely accurate. The exact energy barriers can be calculated using methods such as coupled cluster and full CI. However, these approaches are computationally intensive and are usually feasible only for small systems that are computationally less expensive to handle. Unfortunately, our reaction mechanisms involve complex steps in large systems, demanding high computational costs and time-consuming simulations. As a result, employing the more accurate but computationally demanding methods is not practical for our current study. However, for the current computational investigation's objective, which involves comparing relative barriers, DFT values serve their purpose.



Supplementary Figure S28.

7. References

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(7). Ahlrichs, R., Bär, M., Häser, M., Horn, H. & Kölmel, C. Electronic structure calculations on workstation computers: the program system turbomole, *Chem. Phys. Lett*. **1989**, *162*, 165−169.

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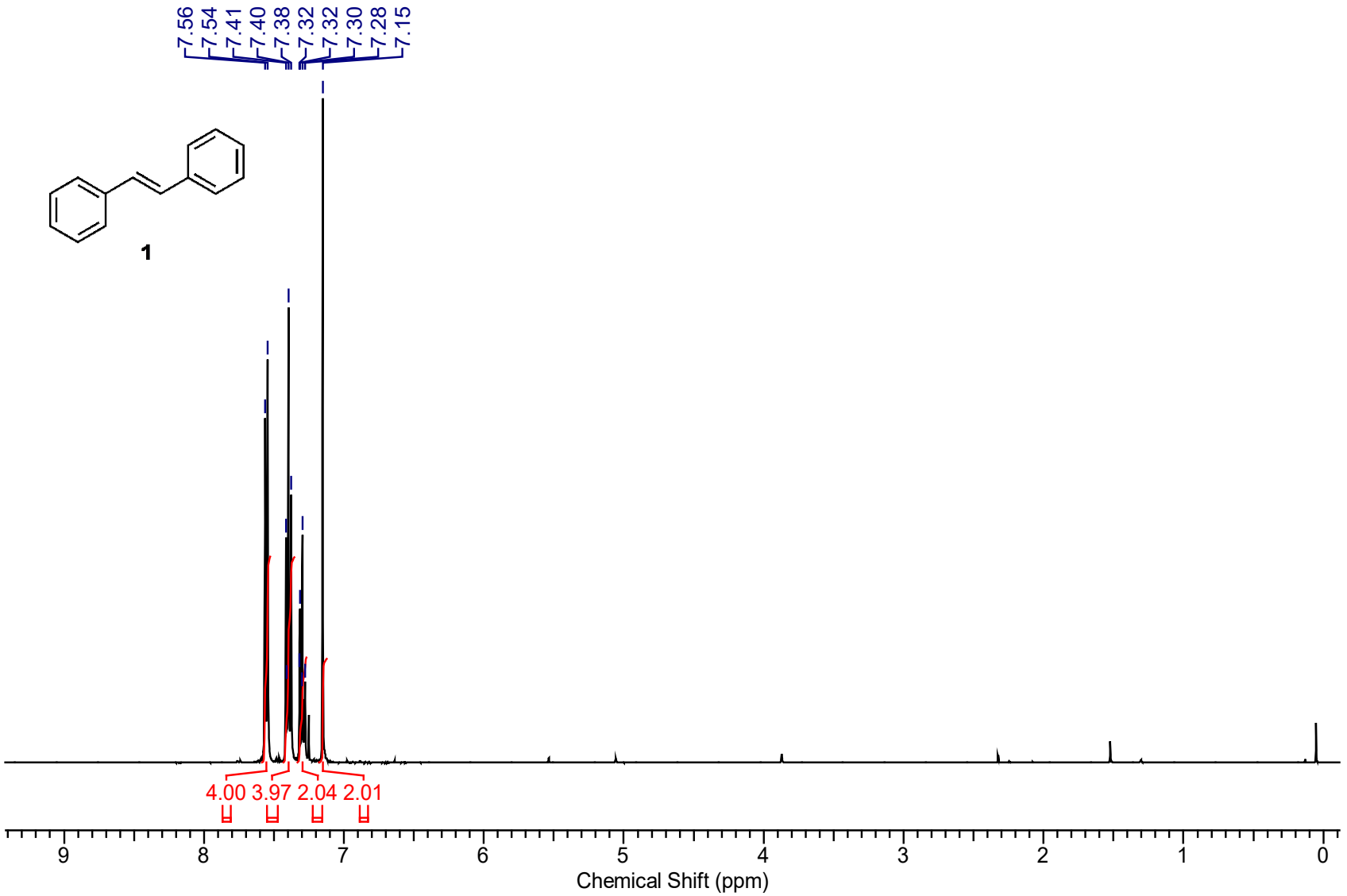
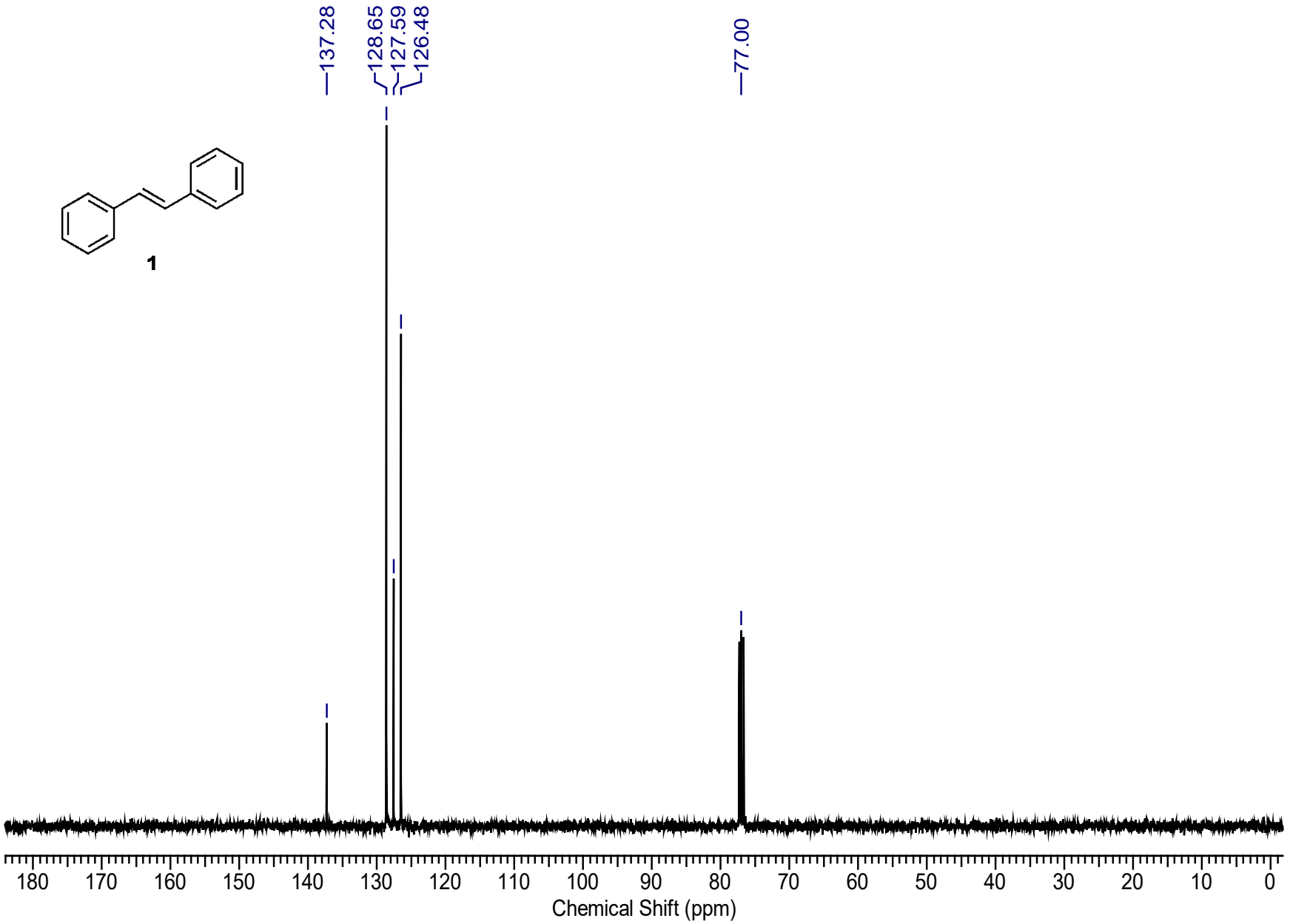
(12) M.T. Nguyen, V.S. Nguyen, M.H. Matus, G. Gopakumar, D.A. Dixon, Molecular mechanism for H_2 release from BH_3NH_3, including the catalytic role of the lewis acid BH_3, *J. Phys. Chem. A* **2007**, *111*, 679-690.

8. ^{1}H and ^{13}C Spectra

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70
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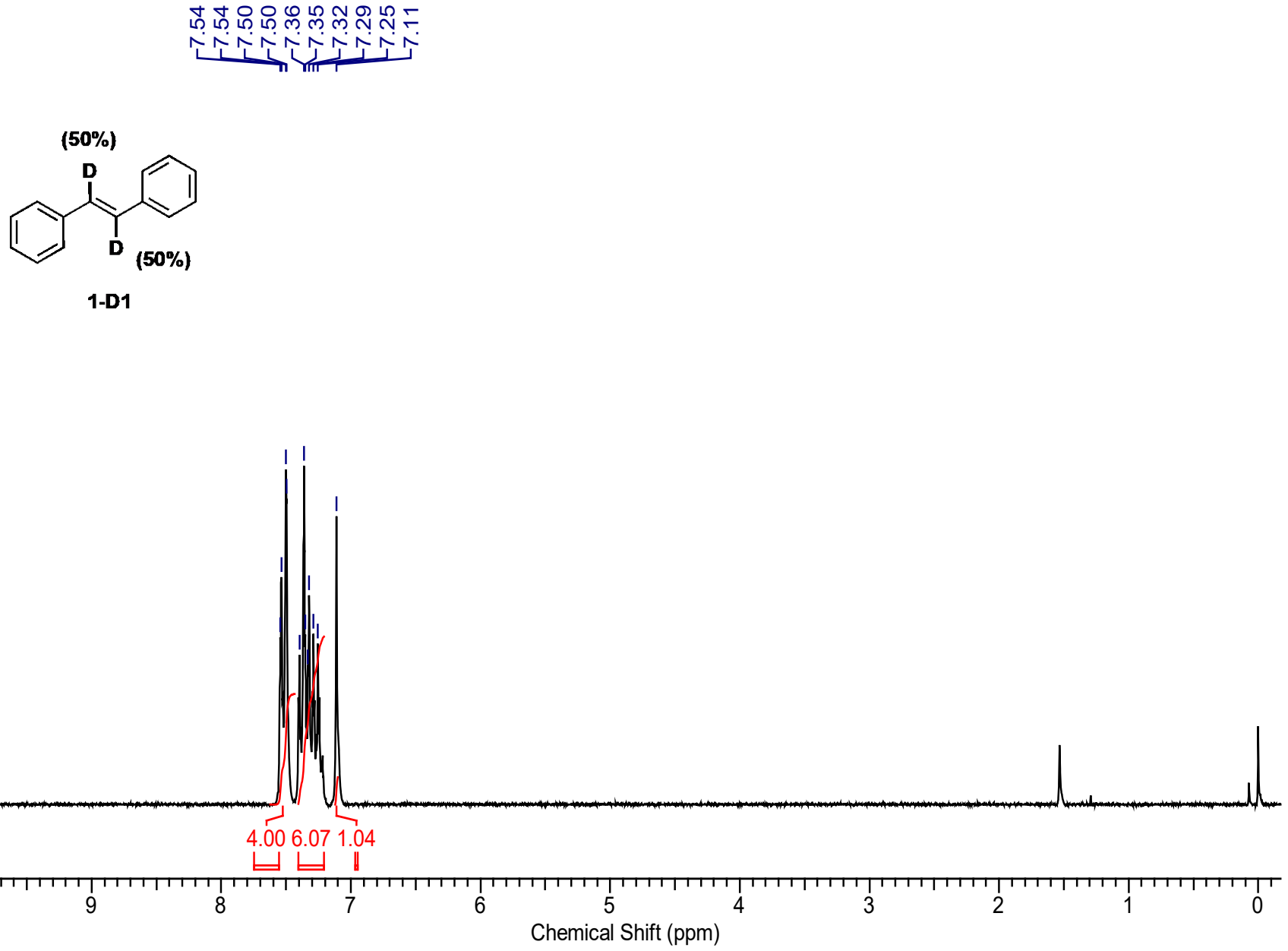
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(50%)
D
D
(50%)
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8
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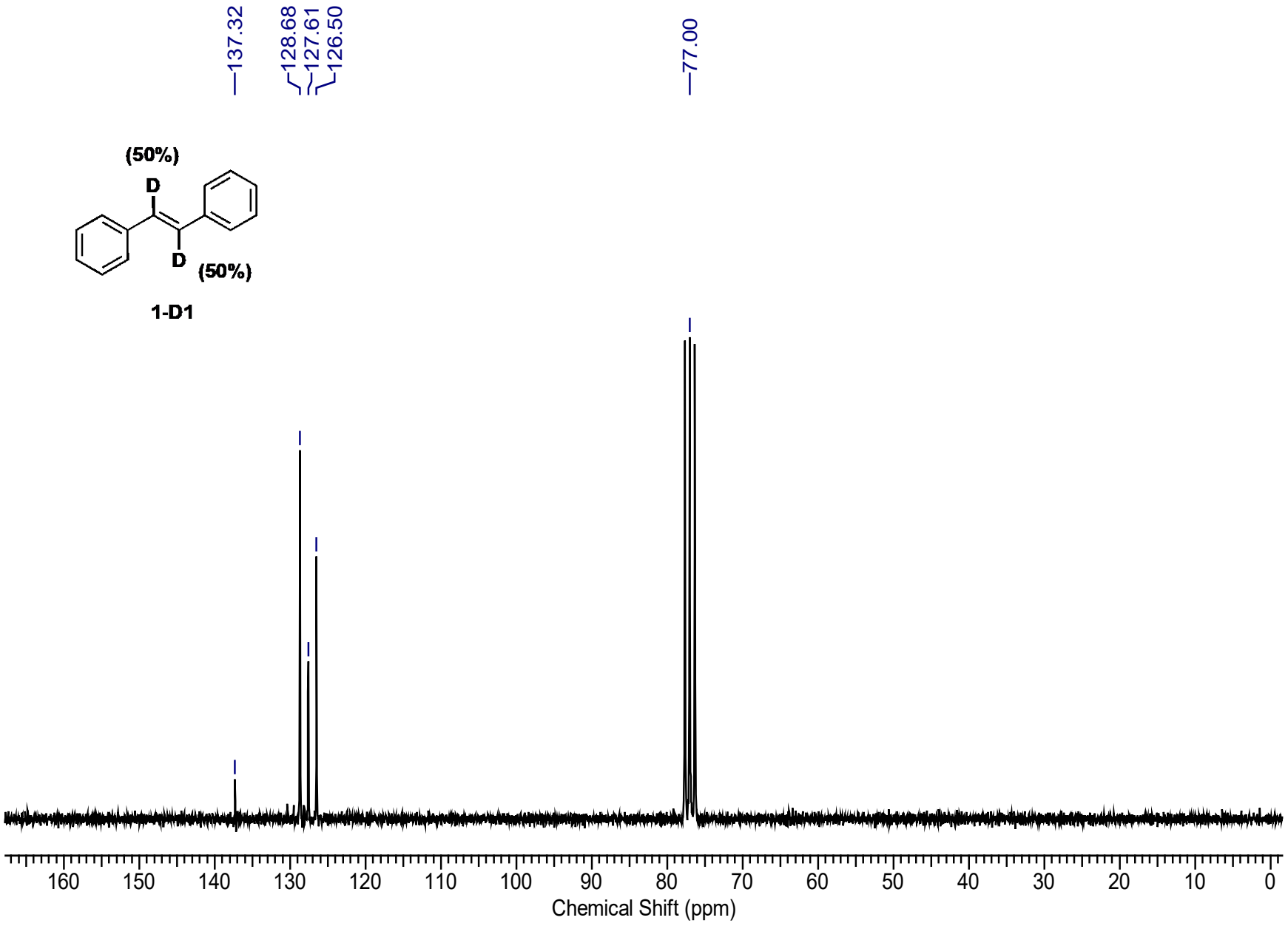
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(50%)
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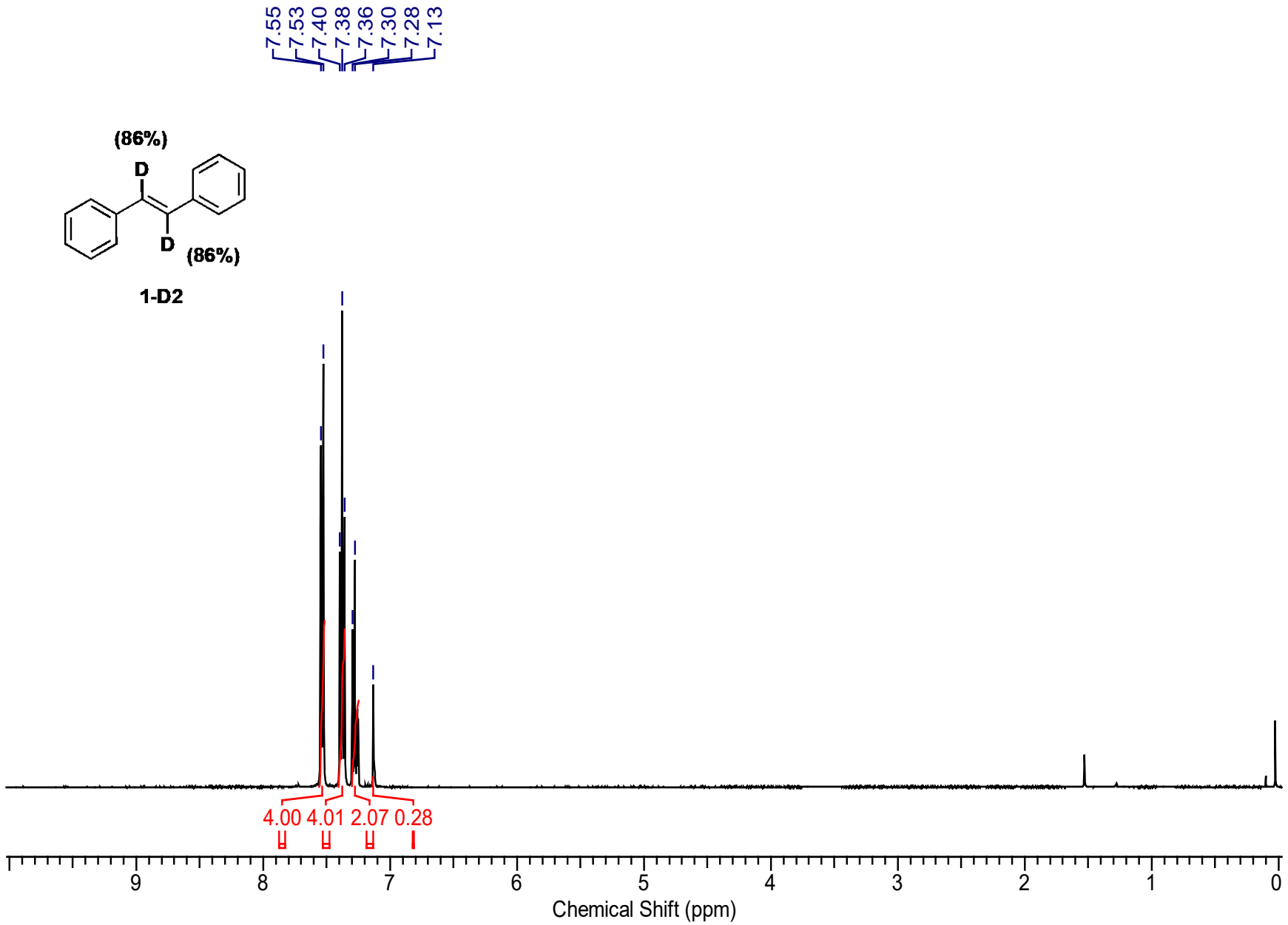
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D
(86%)
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4
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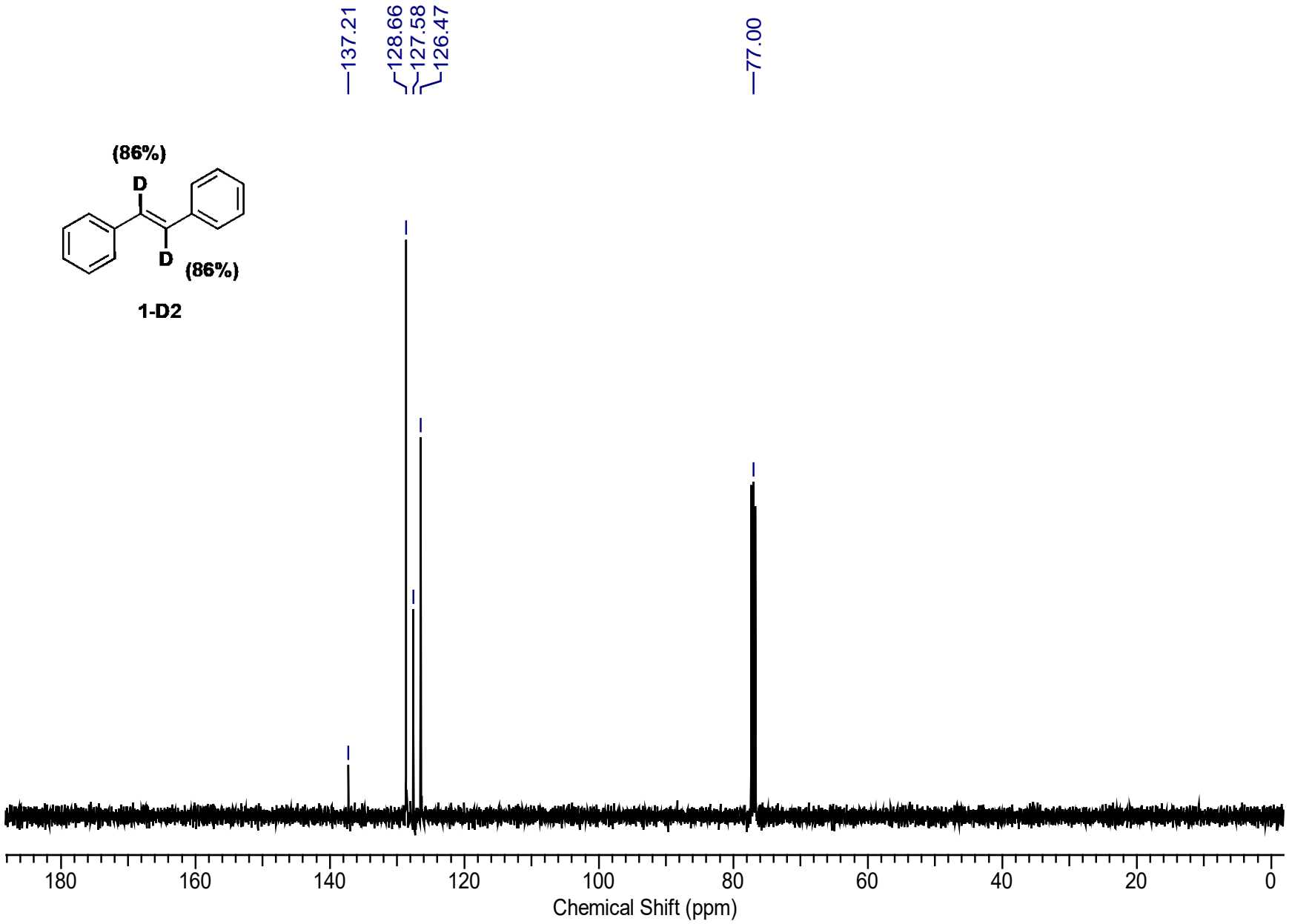
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(86%)
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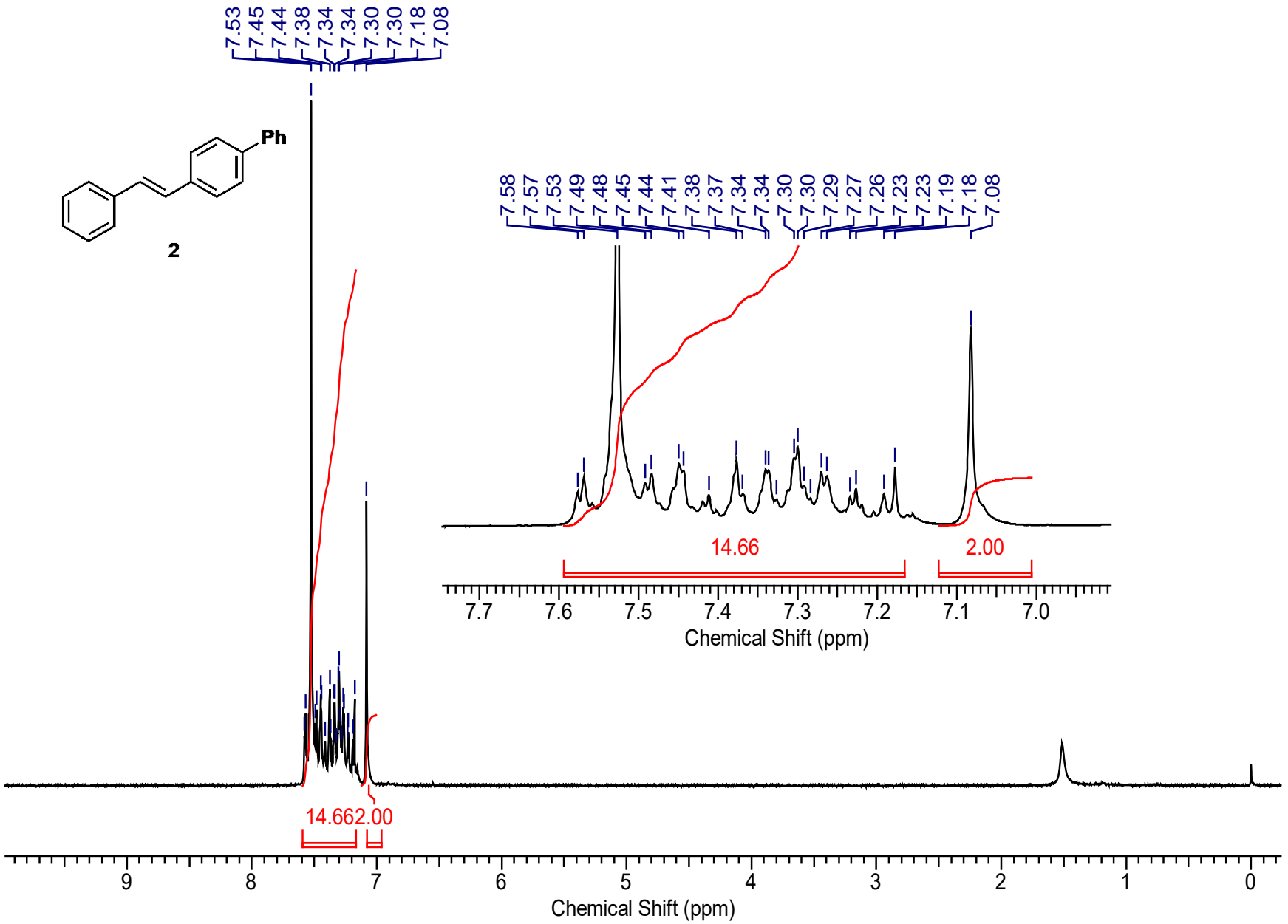
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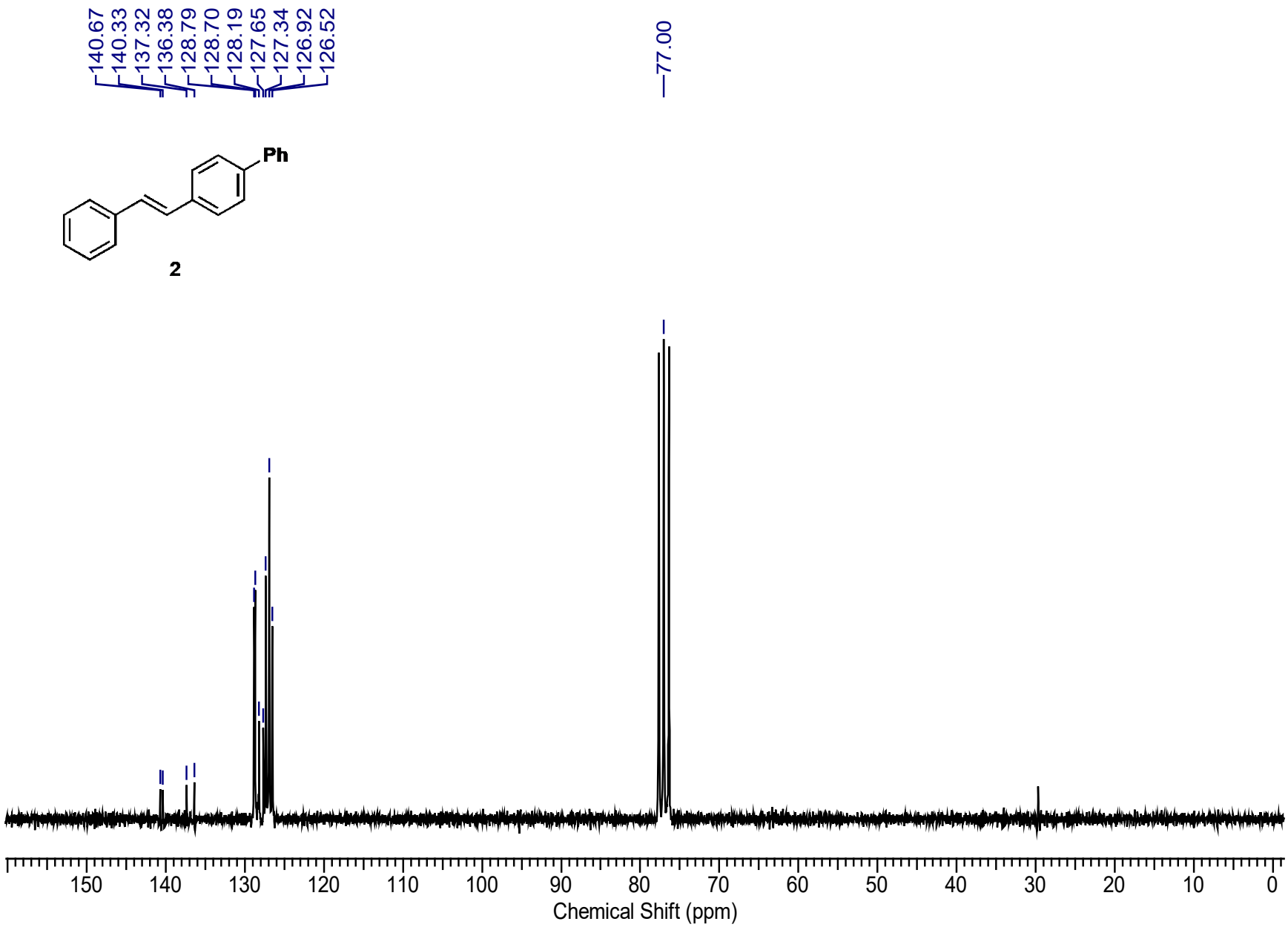
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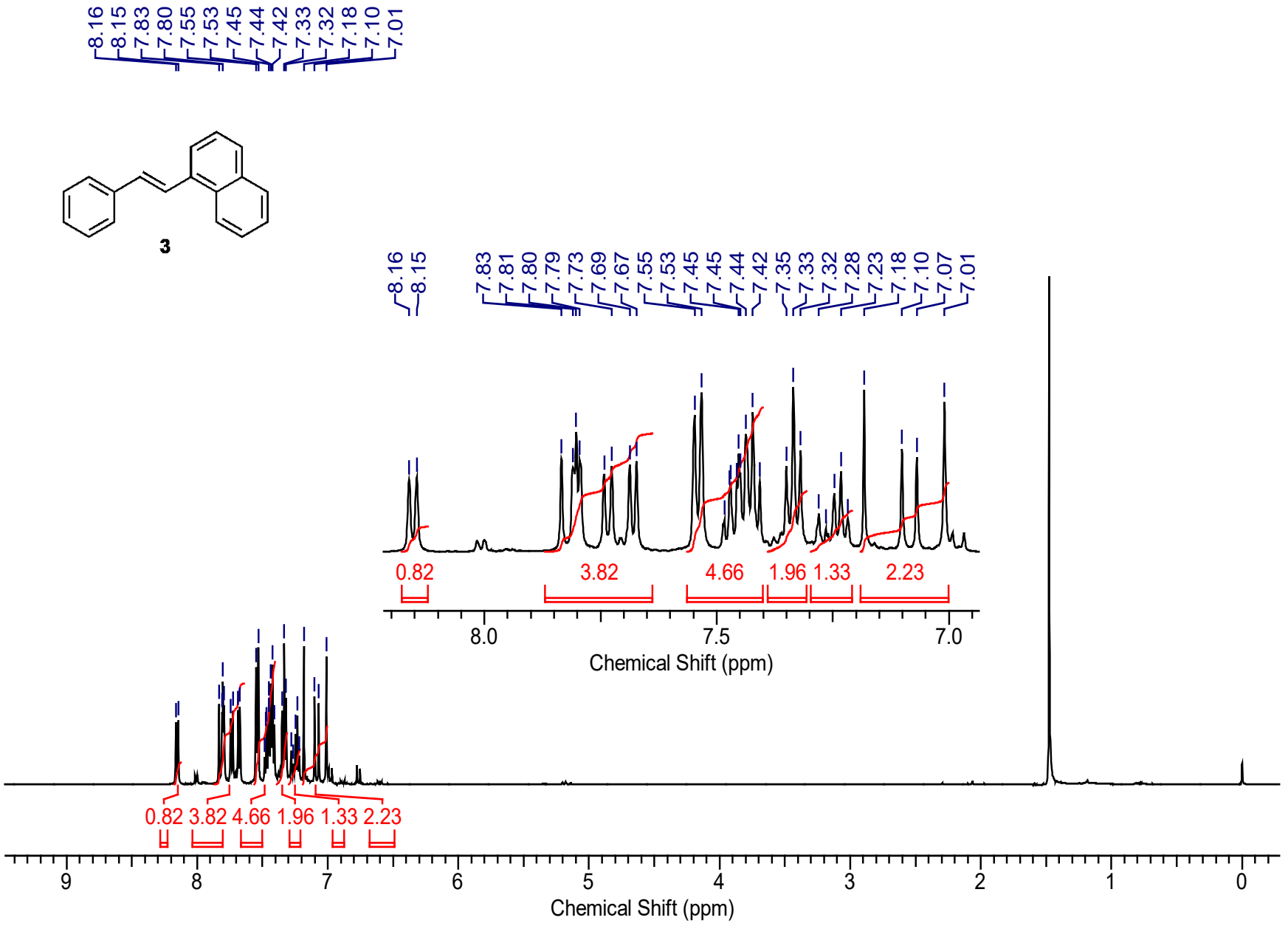
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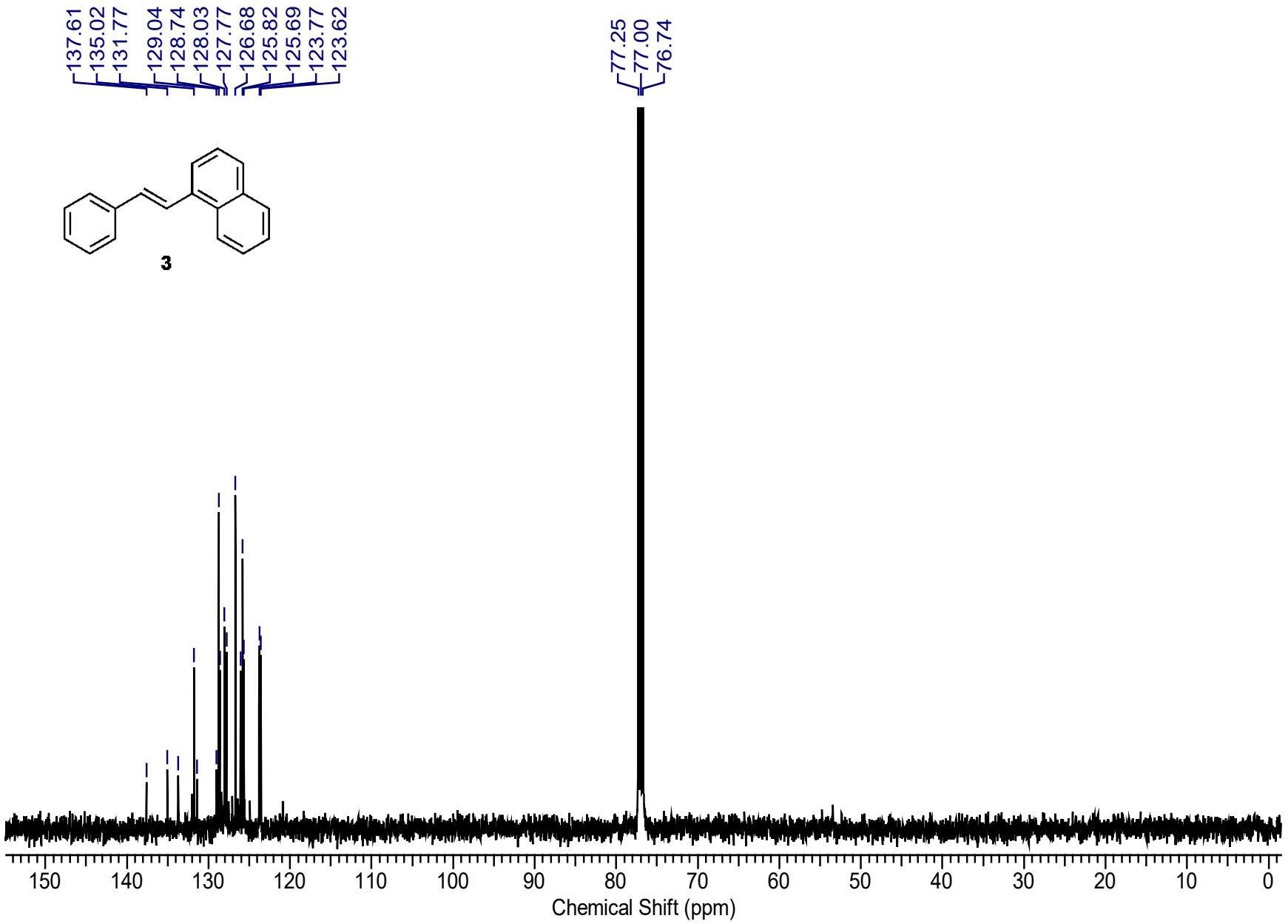
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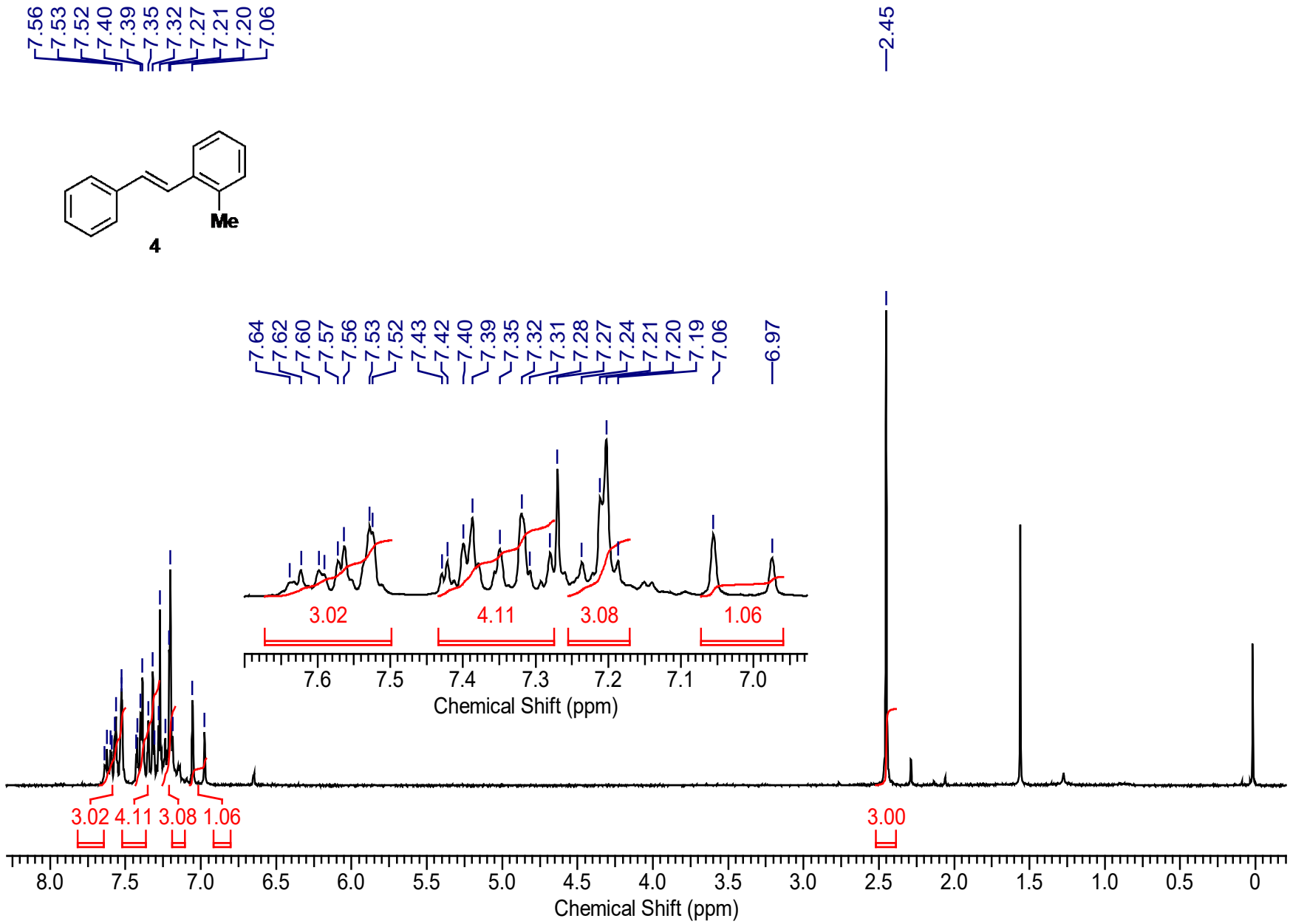
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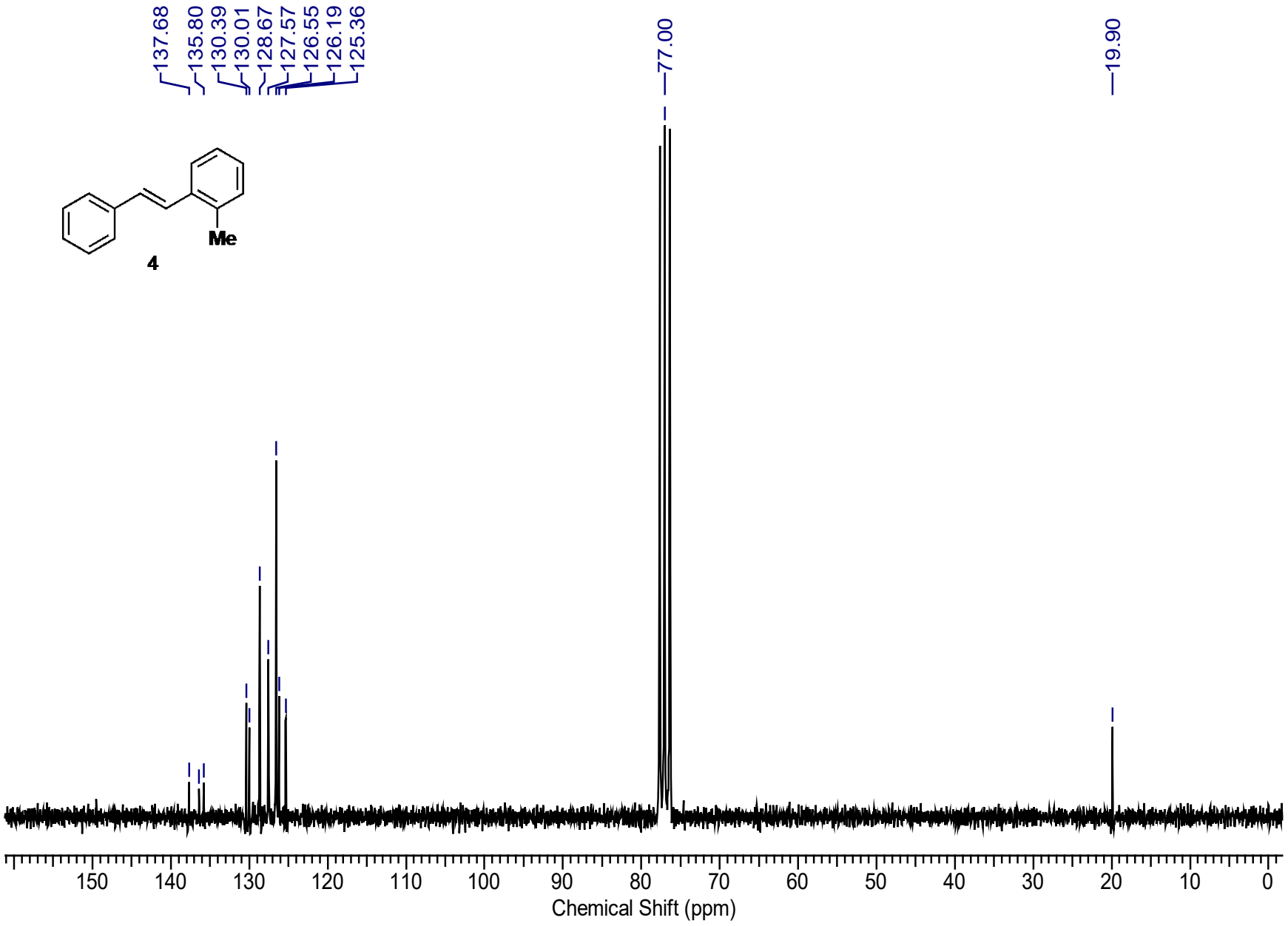
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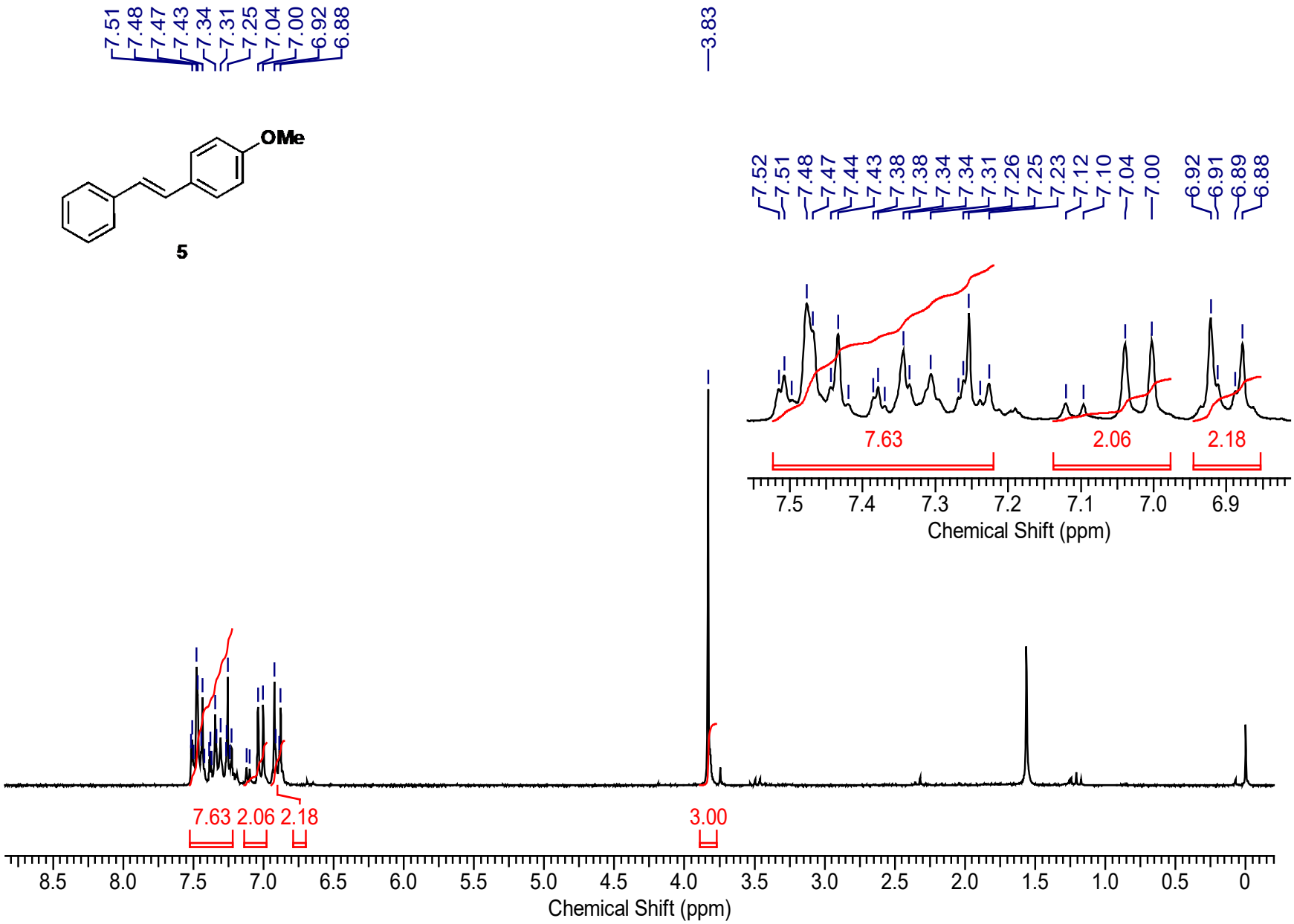
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7.63
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2.18
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7.4
7.3
7.2
7.1
7.0
6.9
Chemical Shift (ppm)
7.63 2.06 2.18
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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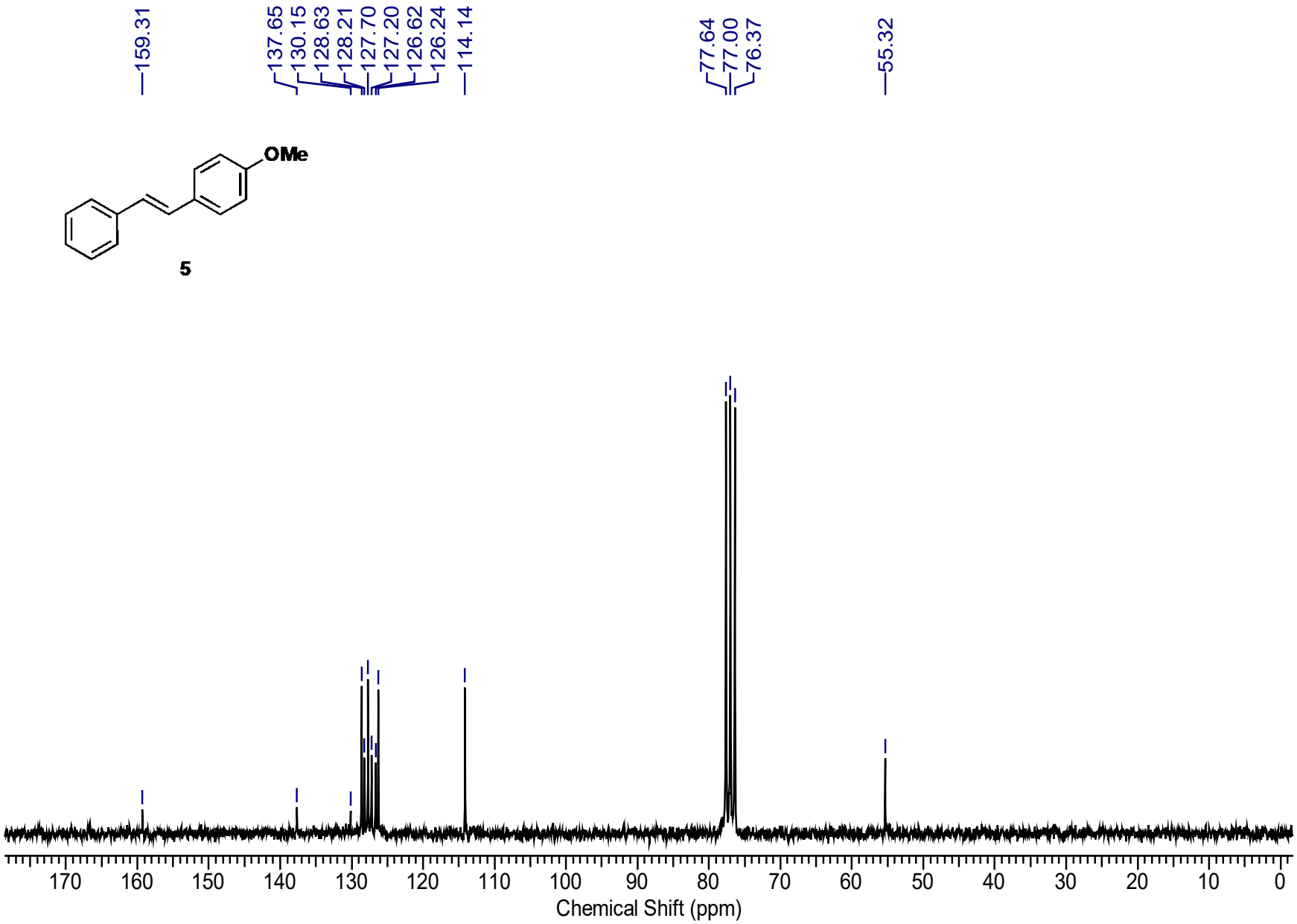
Chemical Shift (ppm)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OMe
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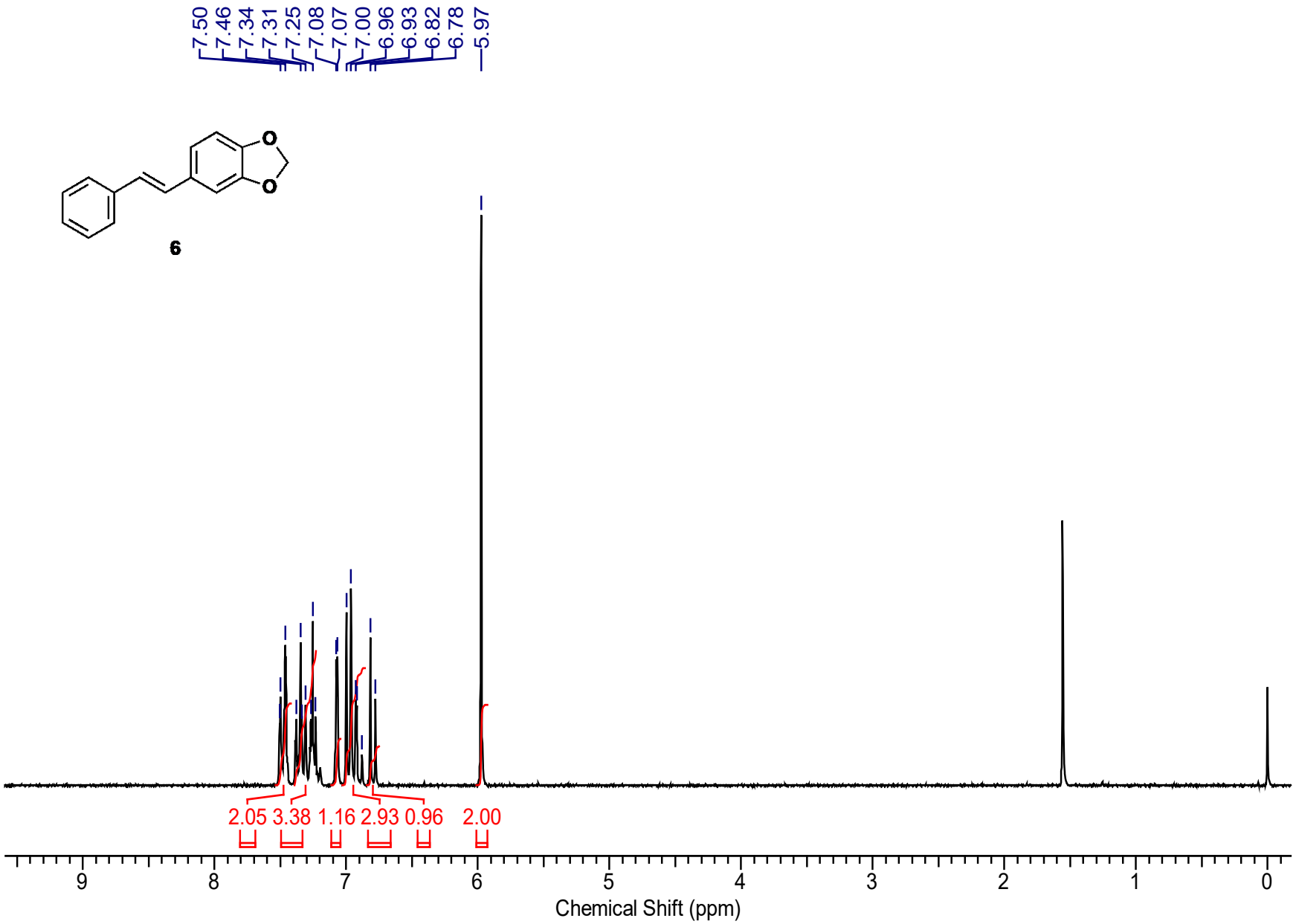
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6.93
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5.97
O
O
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4
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2
1
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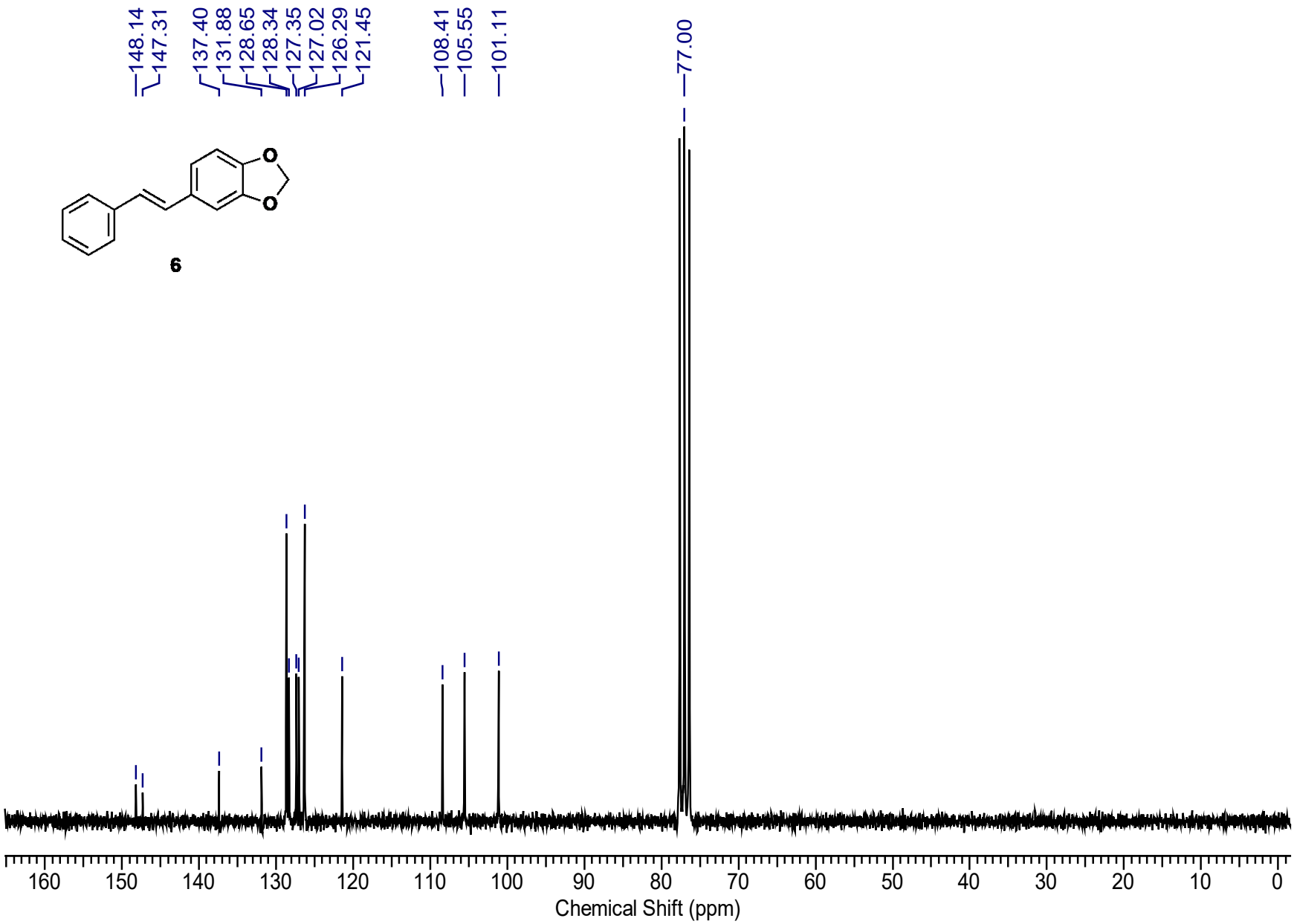
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121.45
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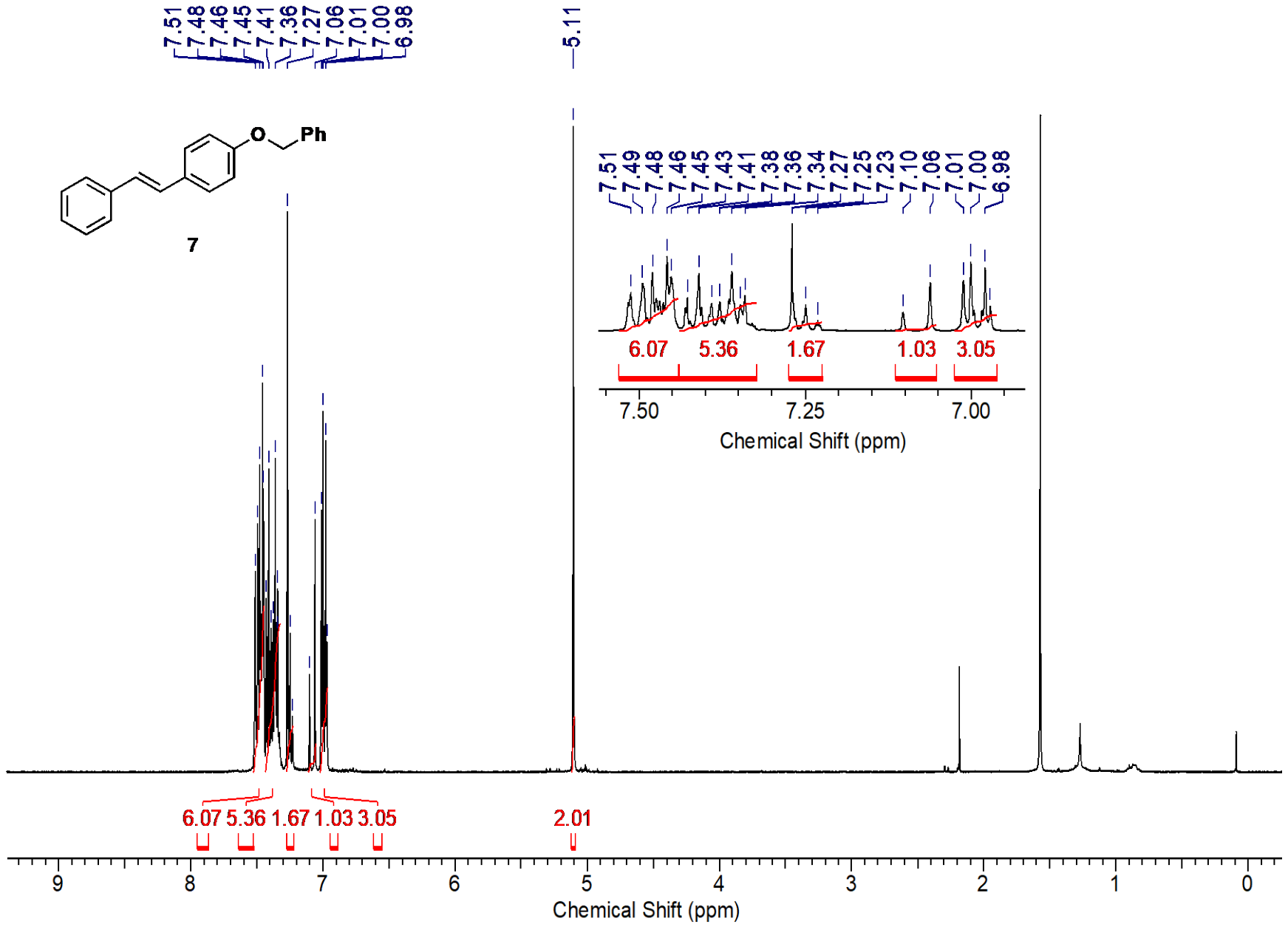
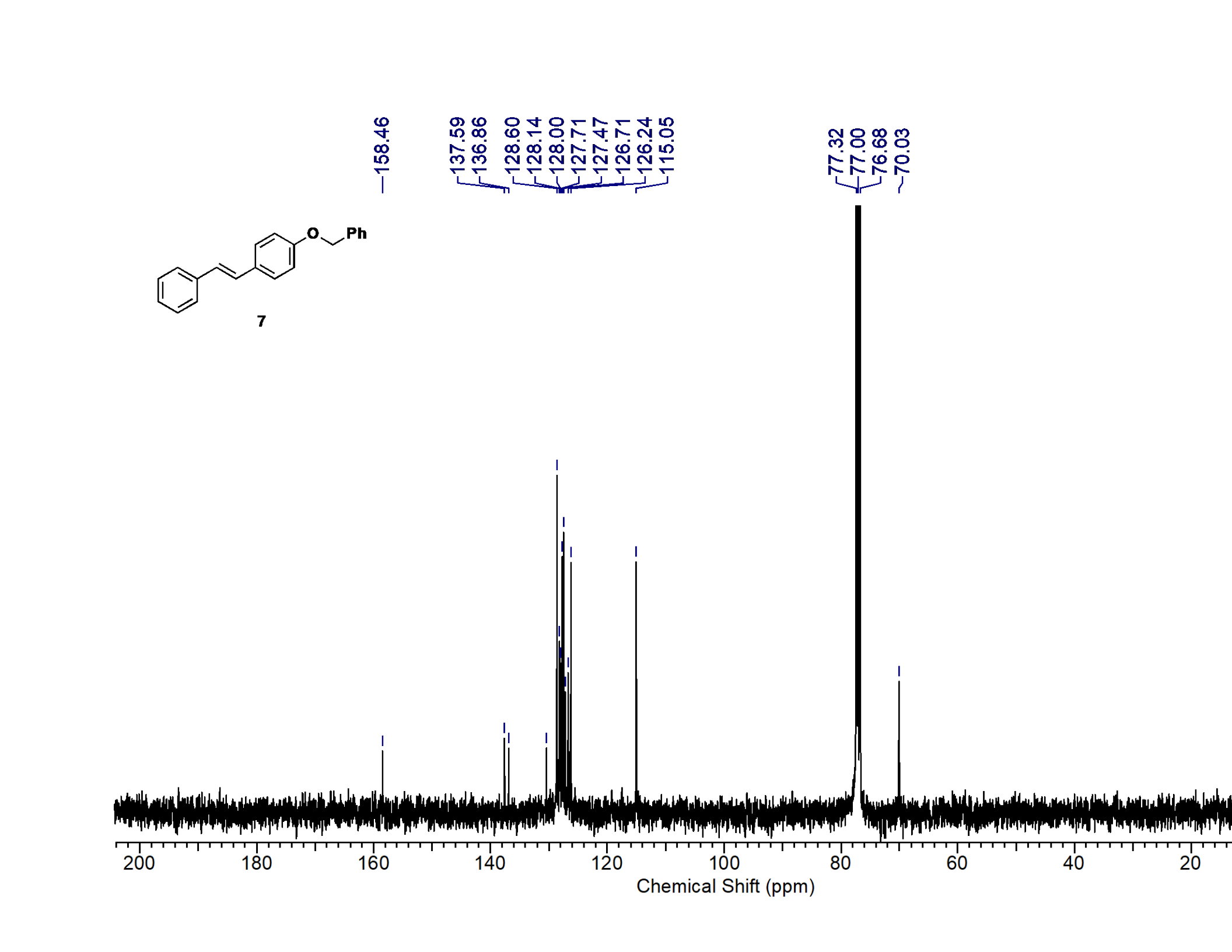
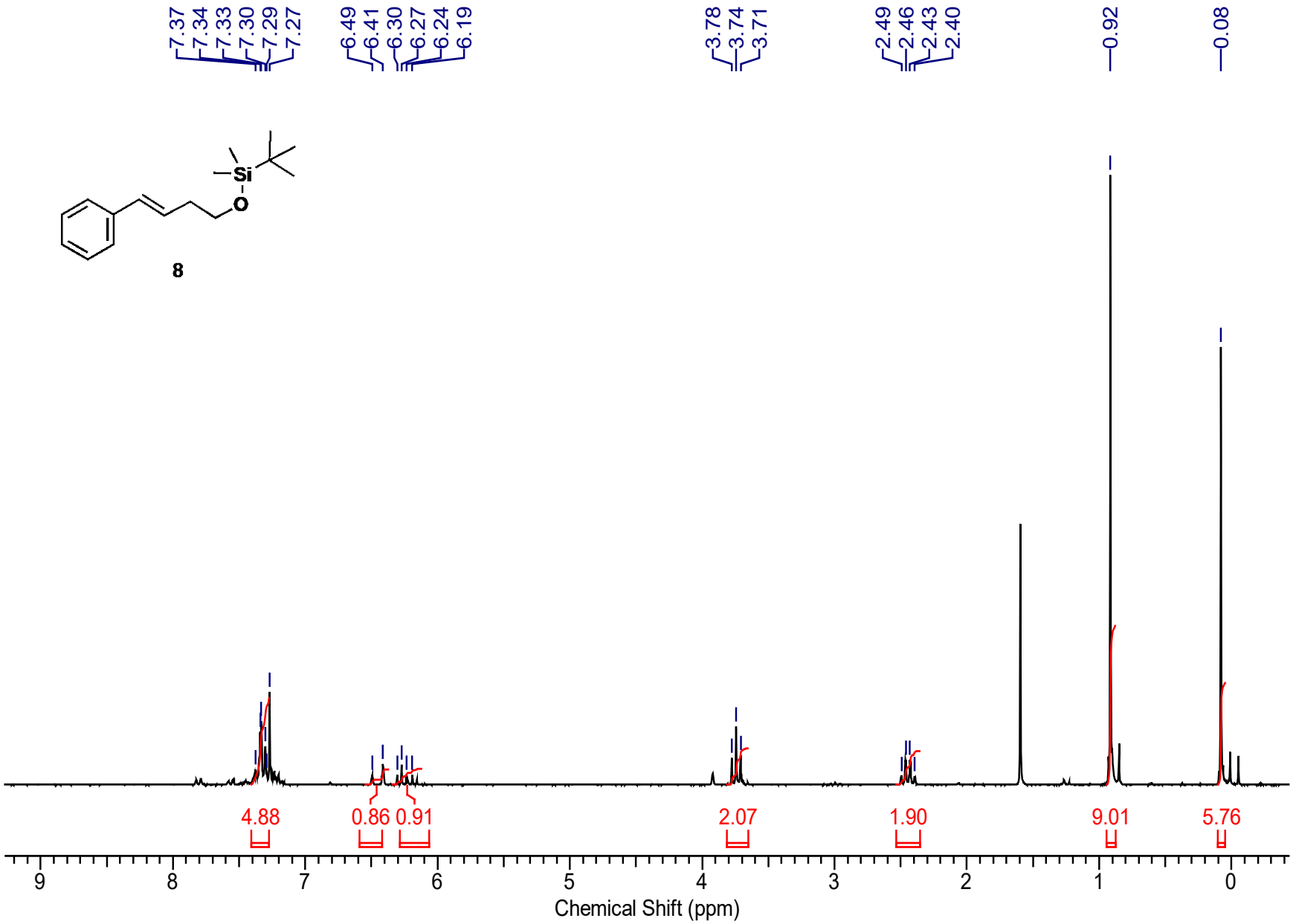
O
6
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)


7.51
7.48
7.46
7.45
7.41
7.36
7.27
7.06
7.01
7.00
6.98
5.11
O
Ph
7
7.51
7.49
7.48
7.46
7.45
7.43
7.41
7.38
7.36
7.34
7.27
7.25
7.23
7.10
7.06
7.01
7.00
6.98
6.07
5.36
1.67
1.03
3.05
7.50
7.25
7.00
Chemical Shift (ppm)
6.07 5.36 1.67 1.03 3.05
2.01
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


158.46
137.59
136.86
128.60
128.14
128.00
127.71
127.47
126.71
126.24
115.05
77.32
77.00
76.68
70.03
O
Ph
7
200
180
160
140
120
100
80
60
40
20
Chemical Shift (ppm)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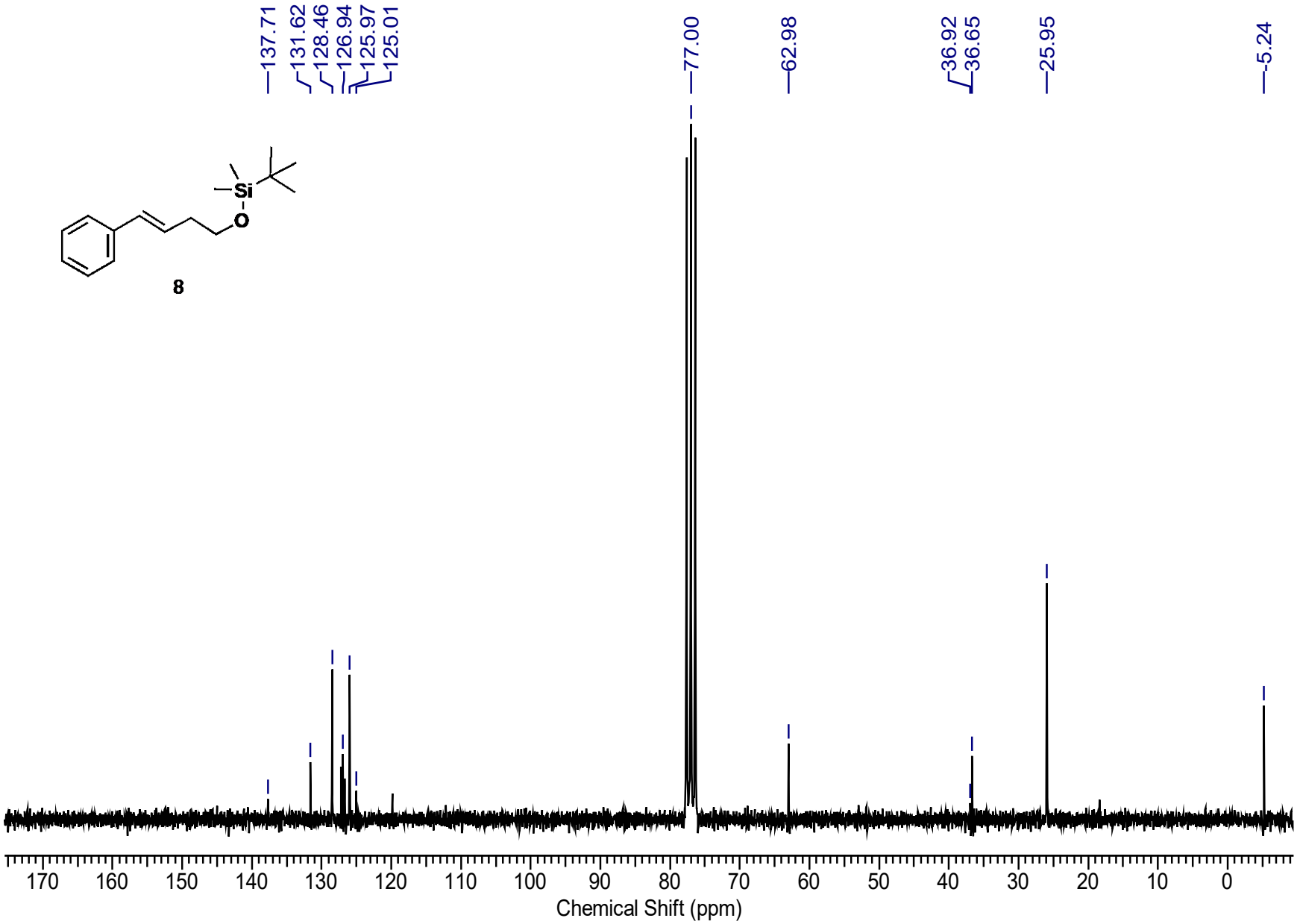
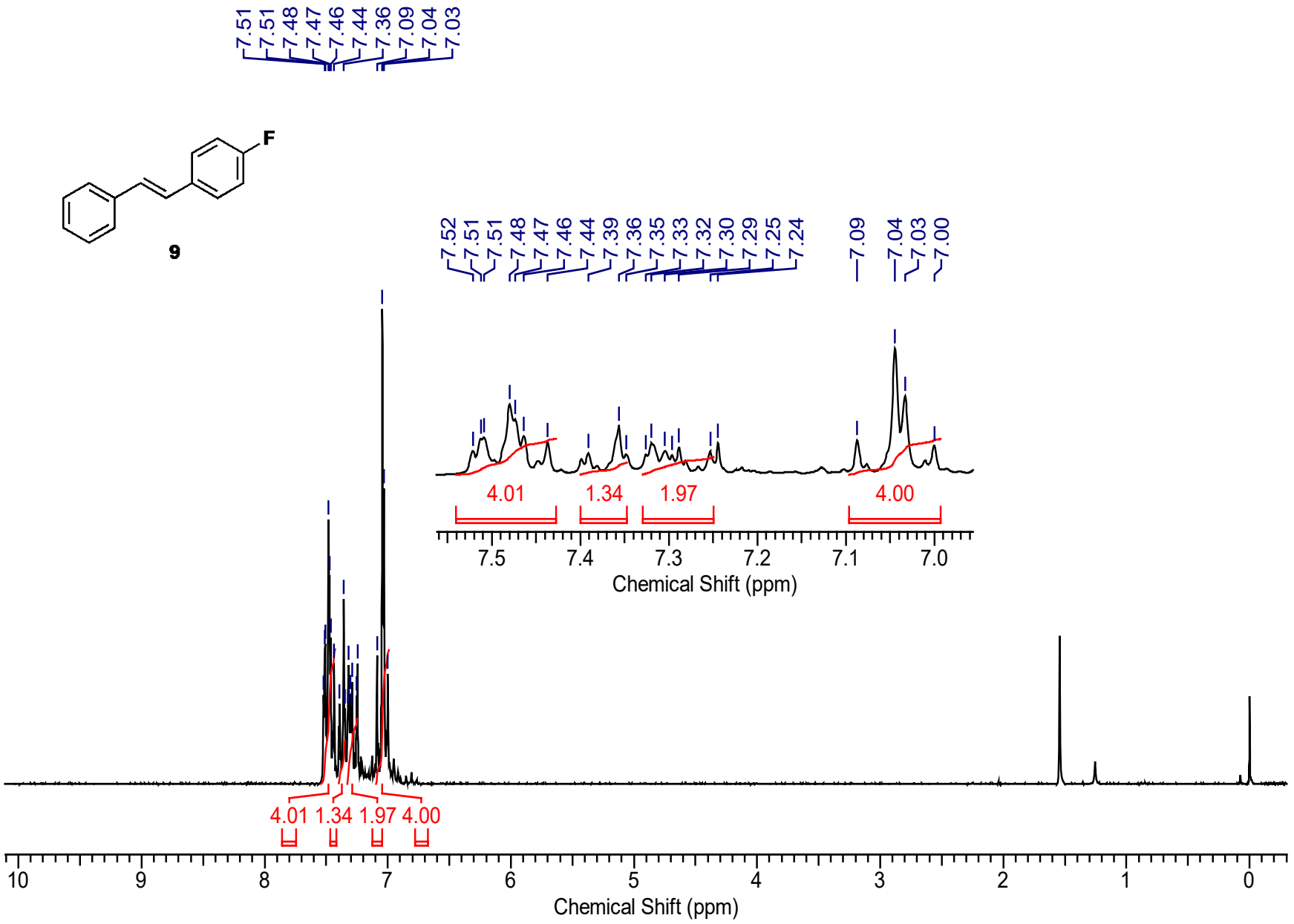
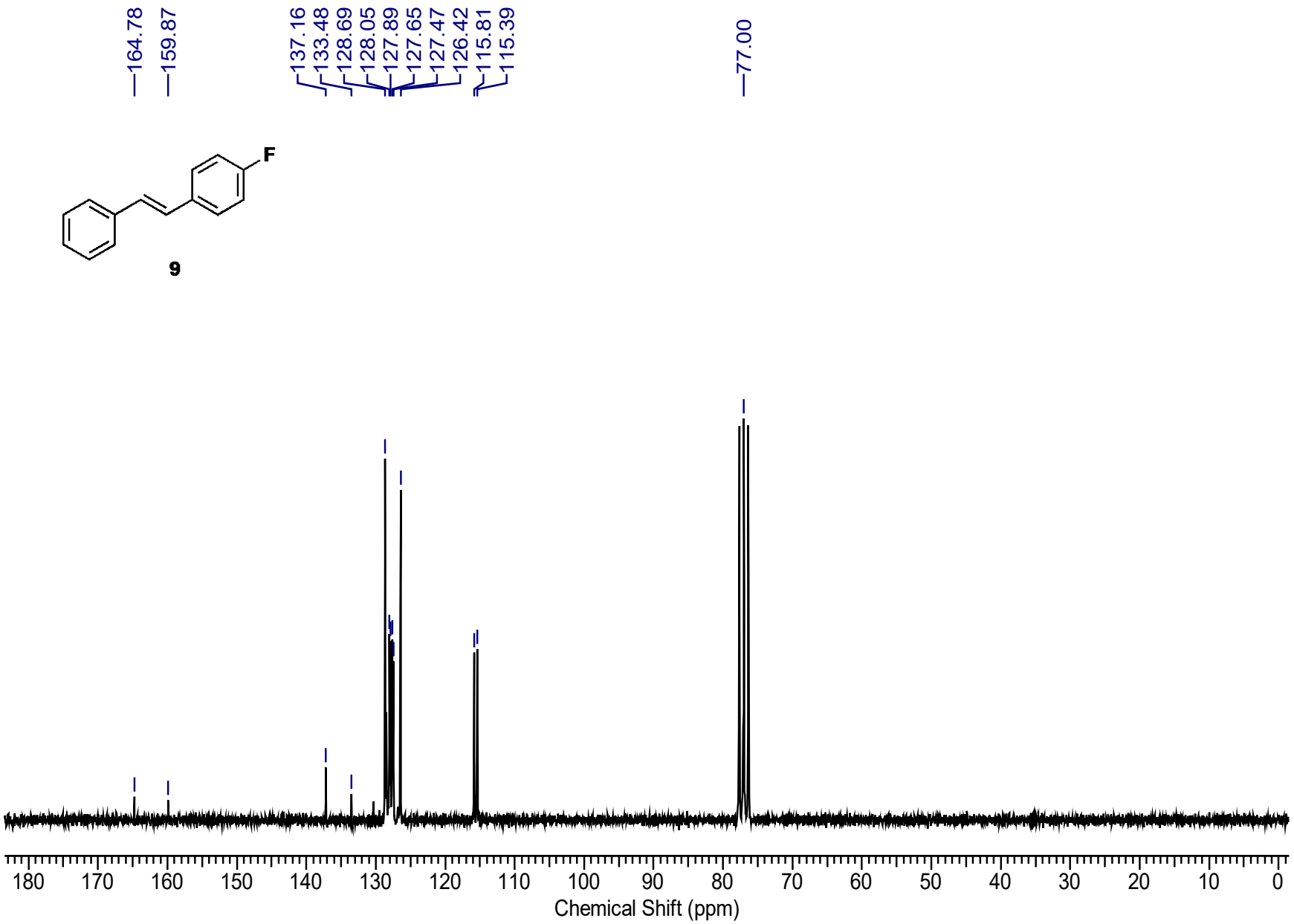
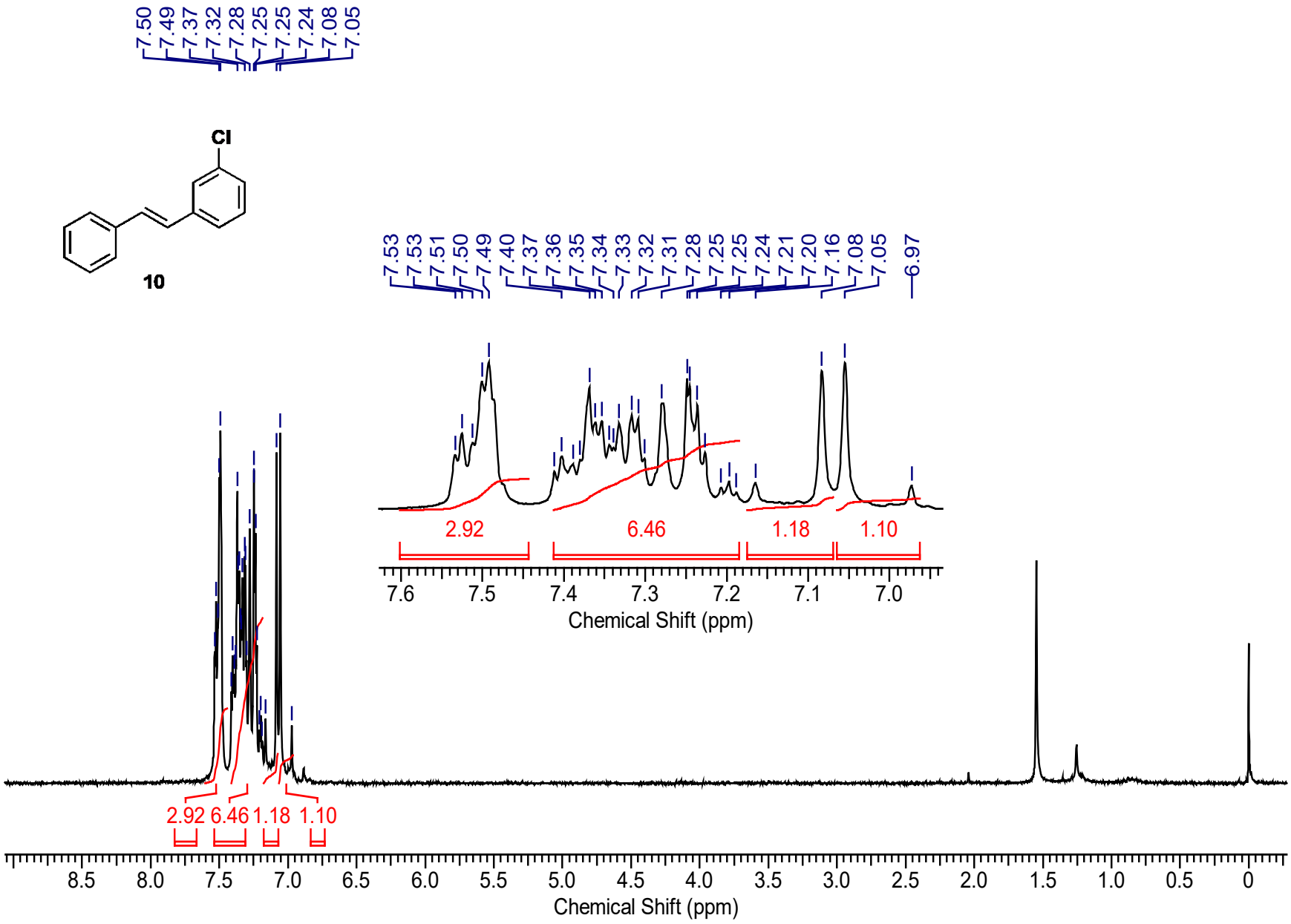
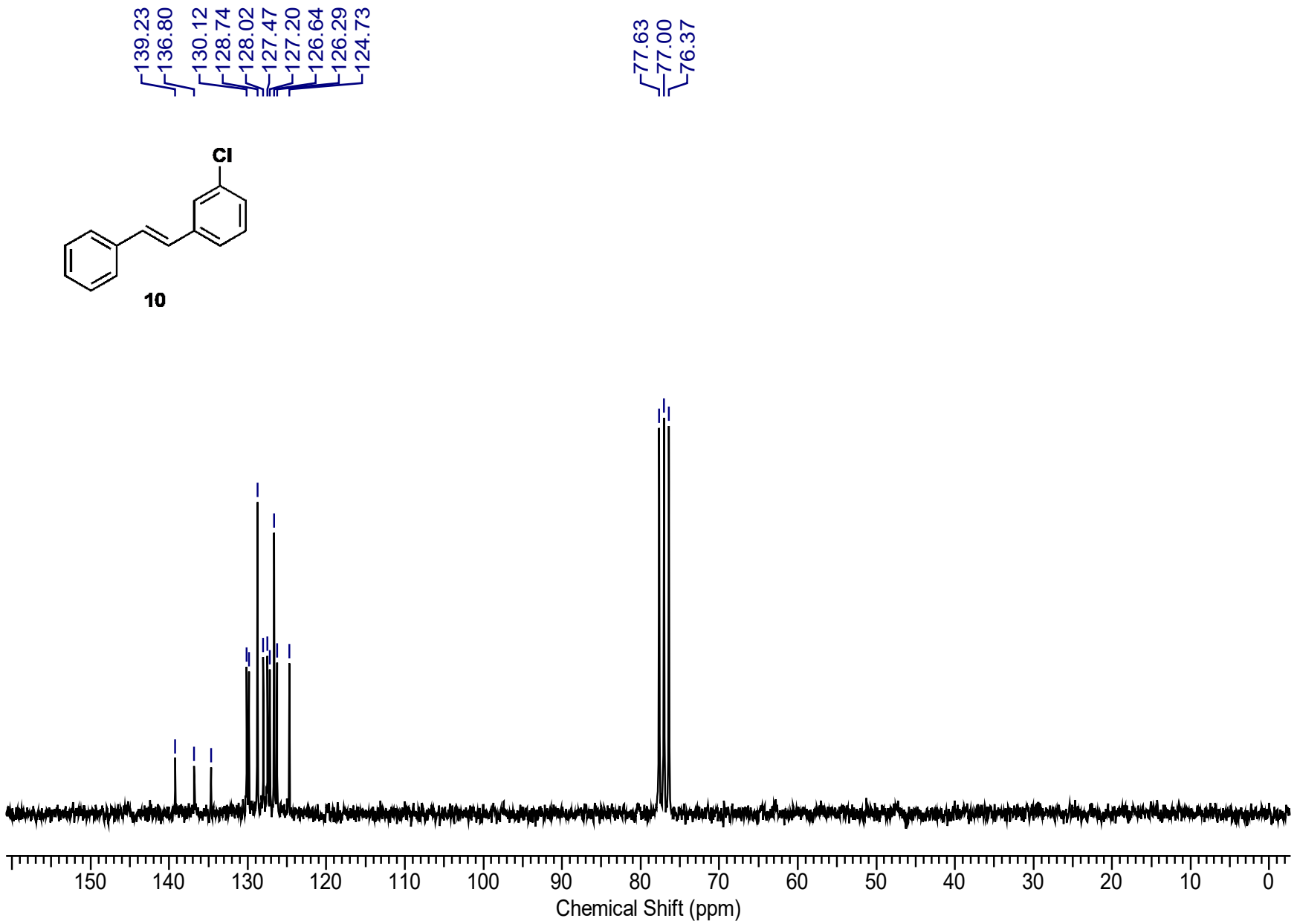
7.34
7.33
7.30
7.29
7.27
6.49
6.41
6.30
6.27
6.24
6.19
3.78
3.74
3.71
2.49
2.46
2.43
2.40
0.92
0.08
Si
O
8
4.88
0.86
0.91
2.07
1.90
9.01
5.76
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

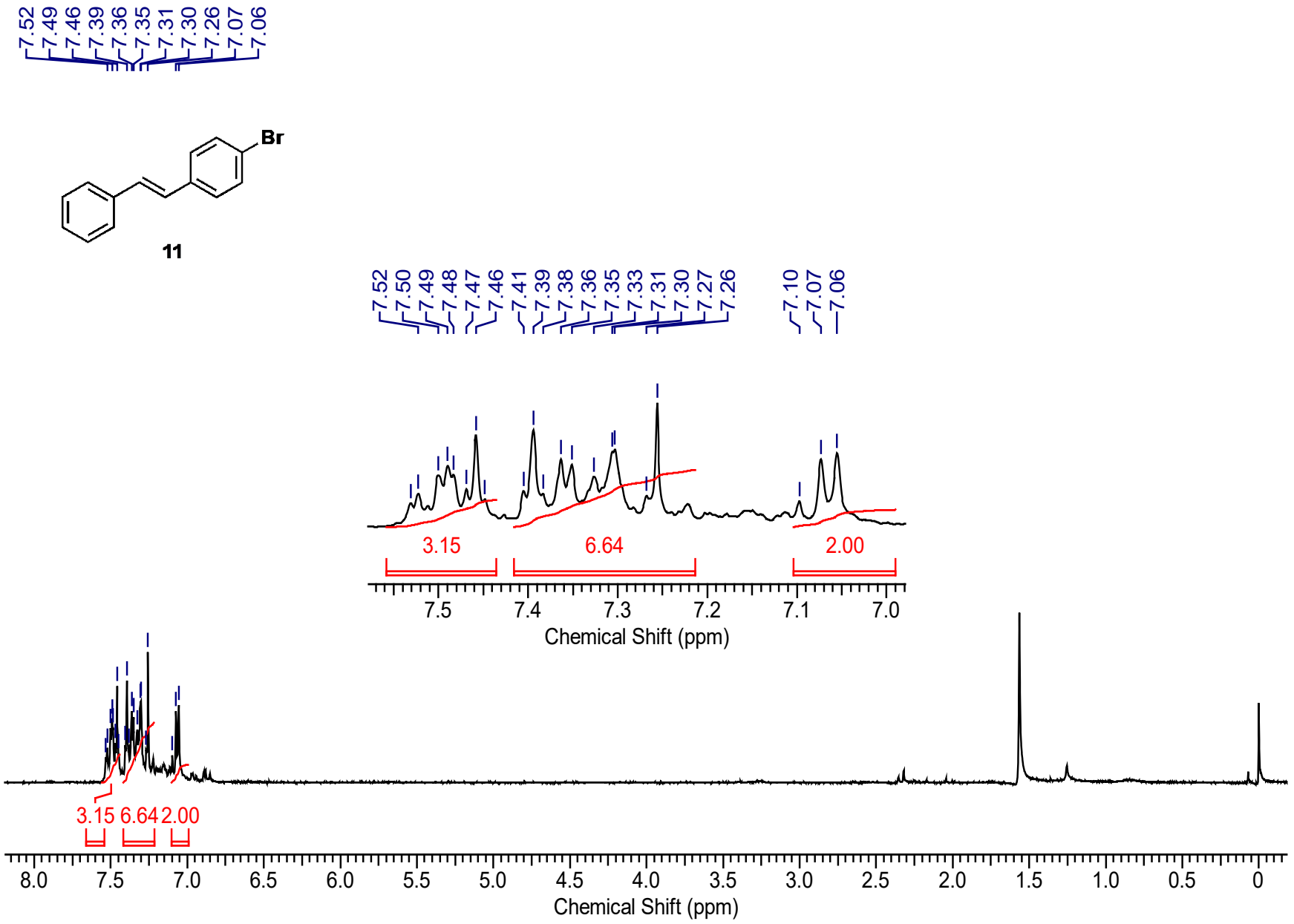

137.71
131.62
128.46
126.94
125.97
125.01
77.00
62.98
36.92
36.65
25.95
5.24
Si
O
8
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

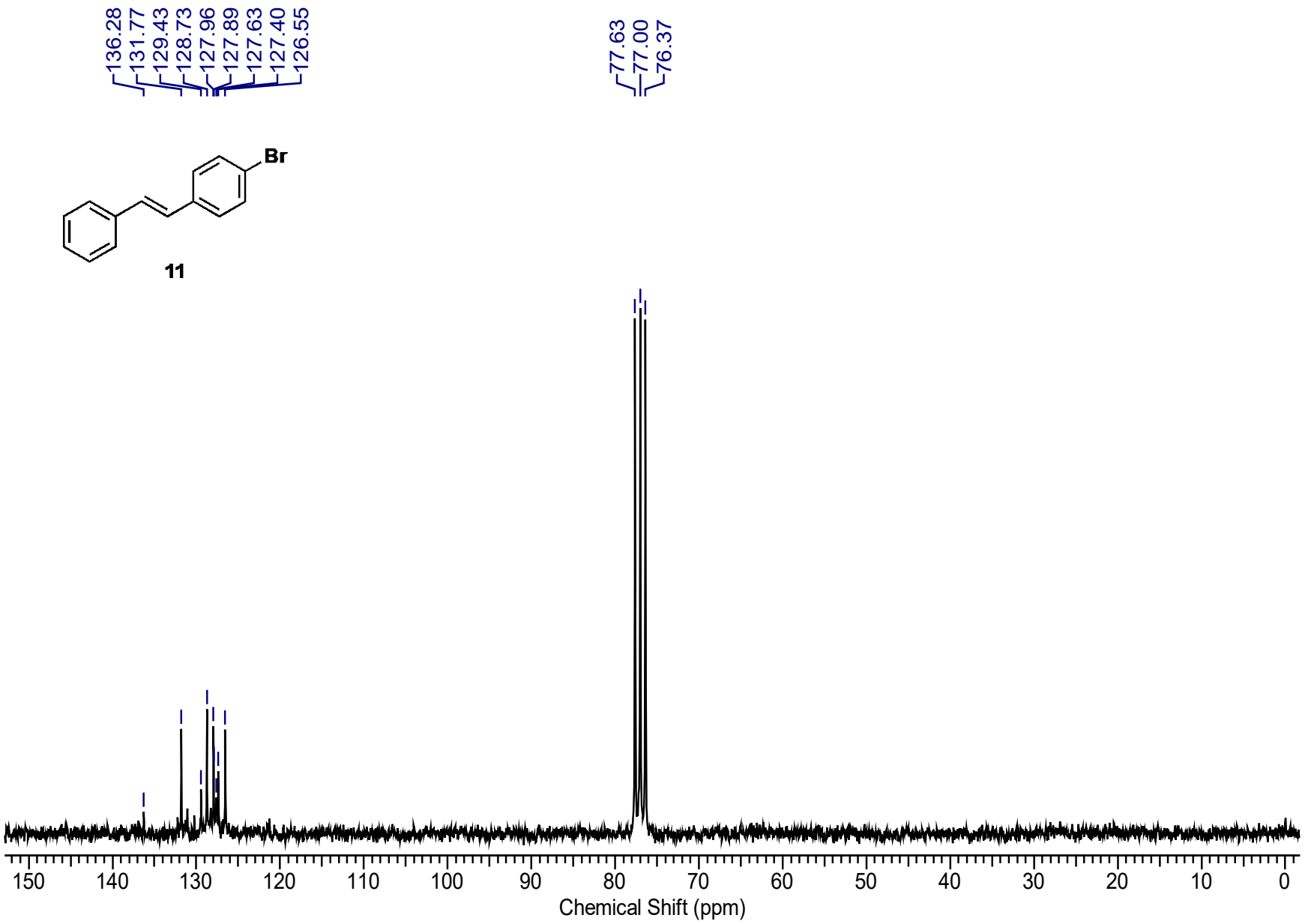

7.51
7.51
7.48
7.47
7.46
7.44
7.36
7.09
7.04
7.03
F
9
7.52
7.51
7.51
7.48
7.47
7.46
7.44
7.39
7.36
7.35
7.33
7.32
7.30
7.29
7.25
7.24
7.09
7.04
7.03
7.00
4.01
1.34
1.97
4.00
7.5
7.4
7.3
7.2
7.1
7.0
Chemical Shift (ppm)
4.01 1.34 1.97 4.00
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

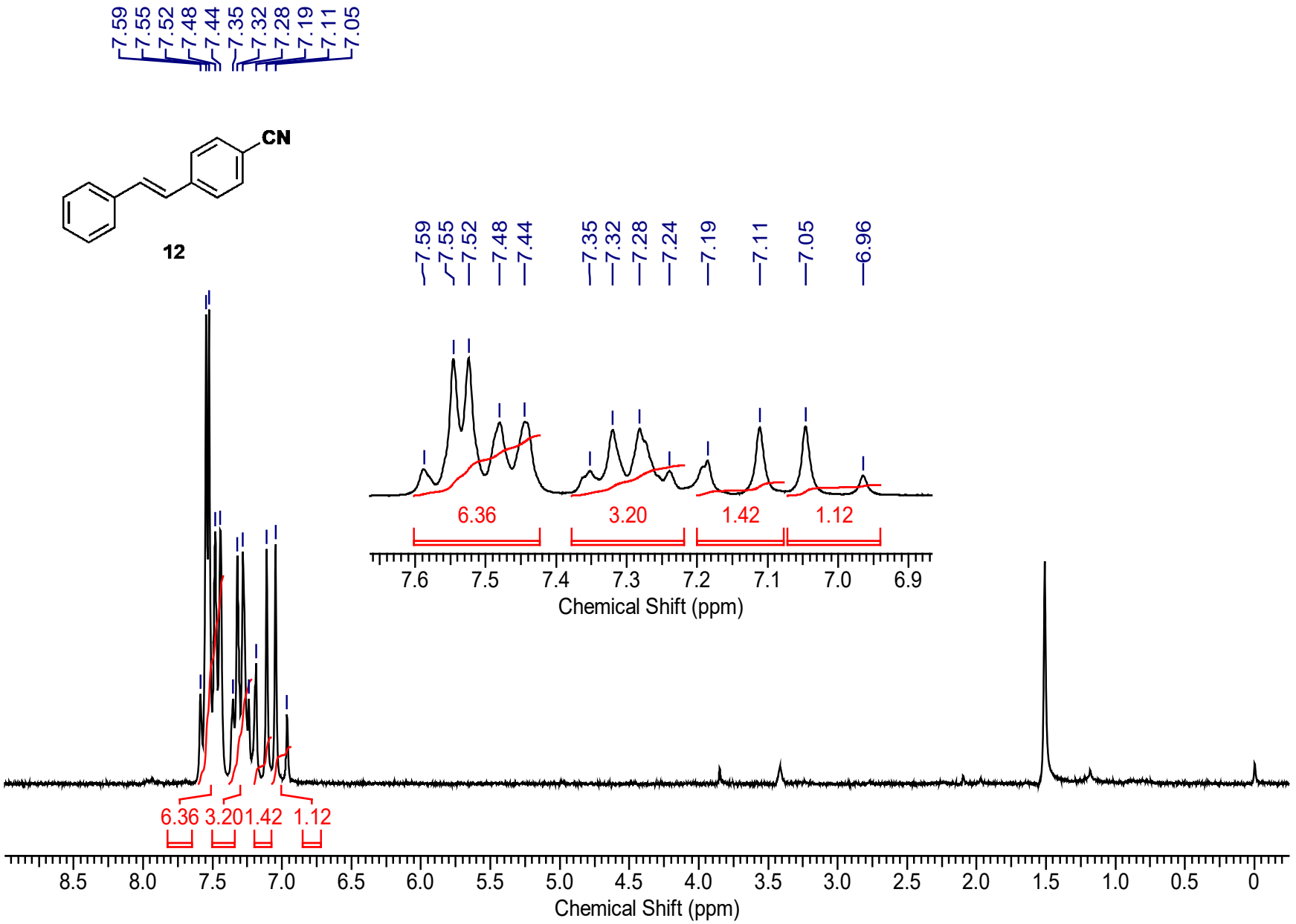

164.78
159.87
137.16
133.48
128.69
128.05
127.89
127.65
127.47
126.42
115.81
115.39
77.00
F
9
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

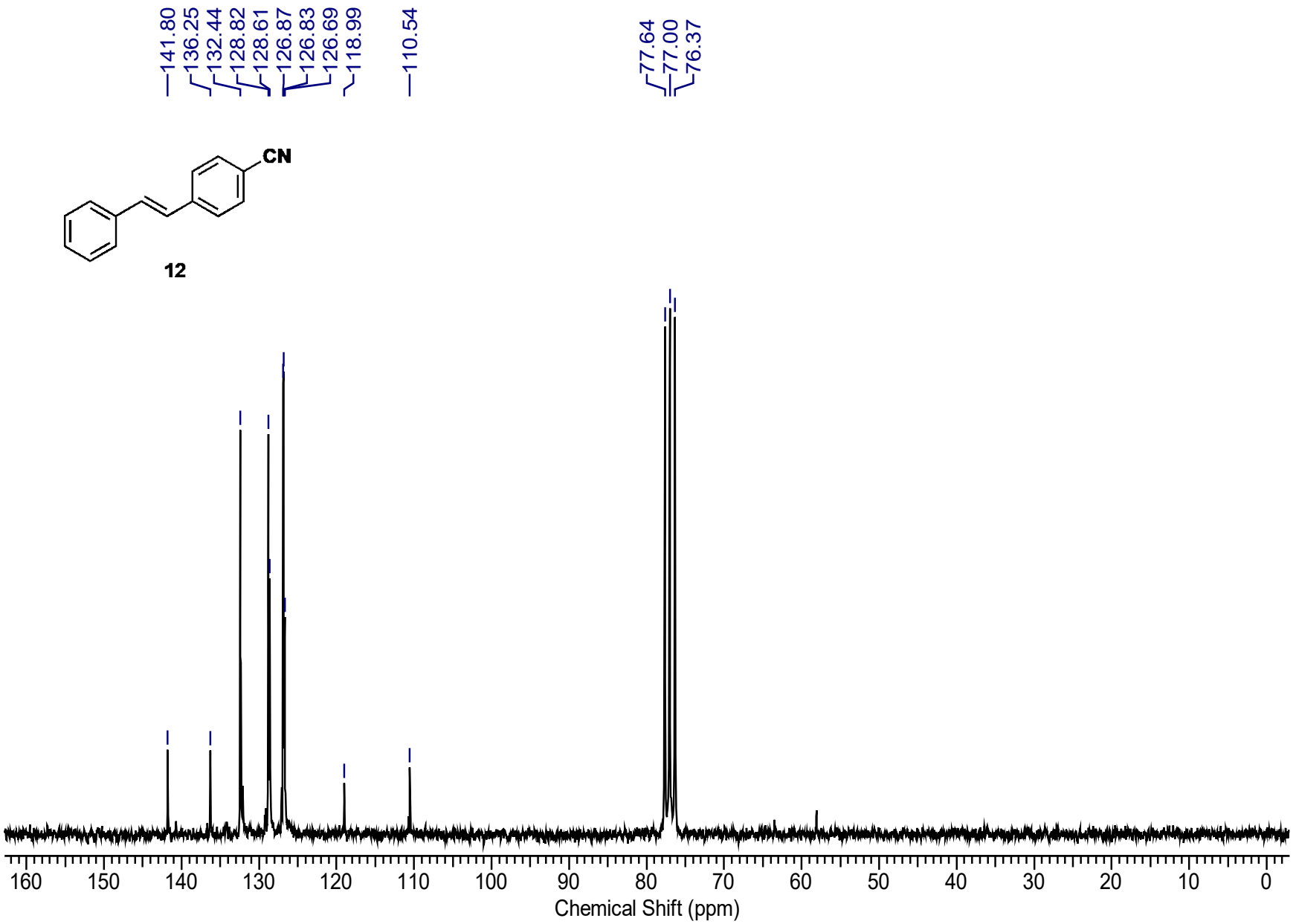

7.50
7.49
7.37
7.32
7.28
7.25
7.25
7.24
7.08
7.05
Cl
10
7.53
7.53
7.51
7.50
7.49
7.40
7.37
7.36
7.35
7.34
7.33
7.32
7.31
7.28
7.25
7.25
7.24
7.21
7.20
7.16
7.08
7.05
6.97
2.92
6.46
1.18
1.10
7.6
7.5
7.4
7.3
7.2
7.1
7.0
Chemical Shift (ppm)
2.92 6.46 1.18 1.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

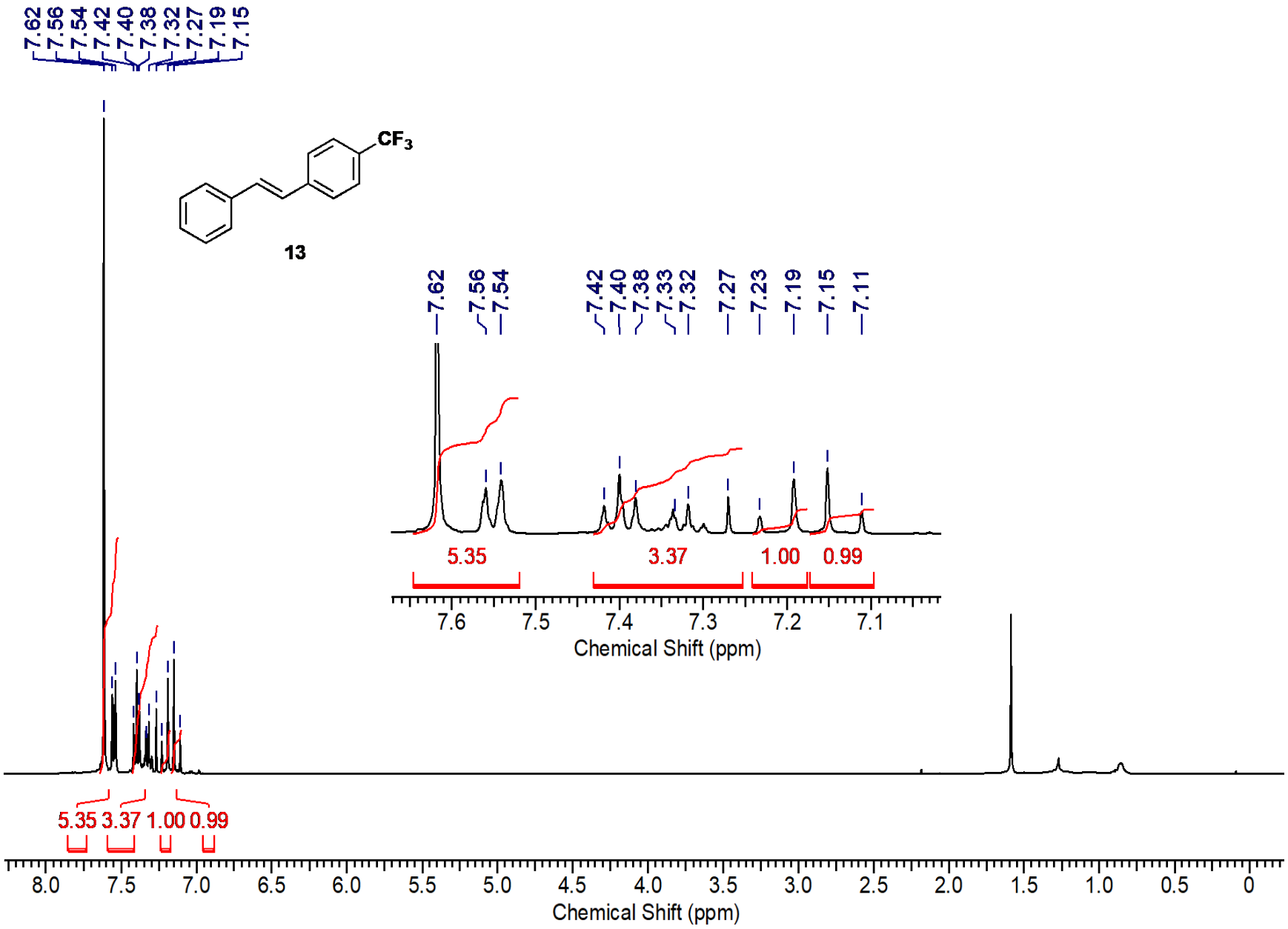

139.23
136.80
130.12
128.74
128.02
127.47
127.20
126.64
126.29
124.73
77.63
77.00
76.37
Cl
10
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

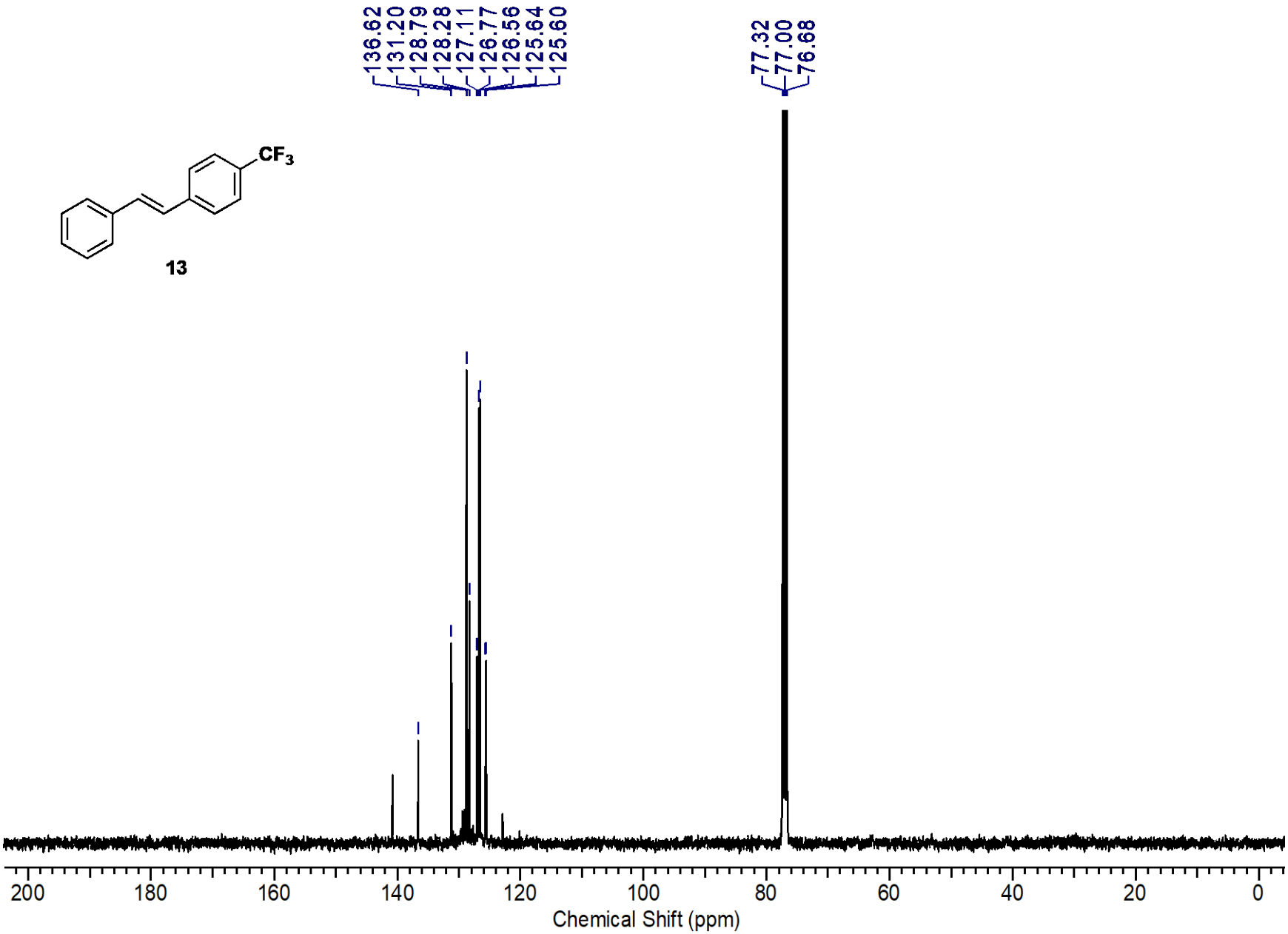

7.52
7.49
7.46
7.39
7.36
7.35
7.31
7.30
7.26
7.07
7.06
Br
11
7.52
7.50
7.49
7.48
7.47
7.46
7.41
7.39
7.38
7.36
7.35
7.33
7.31
7.30
7.27
7.26
7.10
7.07
7.06
3.15
6.64
2.00
7.5
7.4
7.3
7.2
7.1
7.0
Chemical Shift (ppm)
3.15
6.64
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

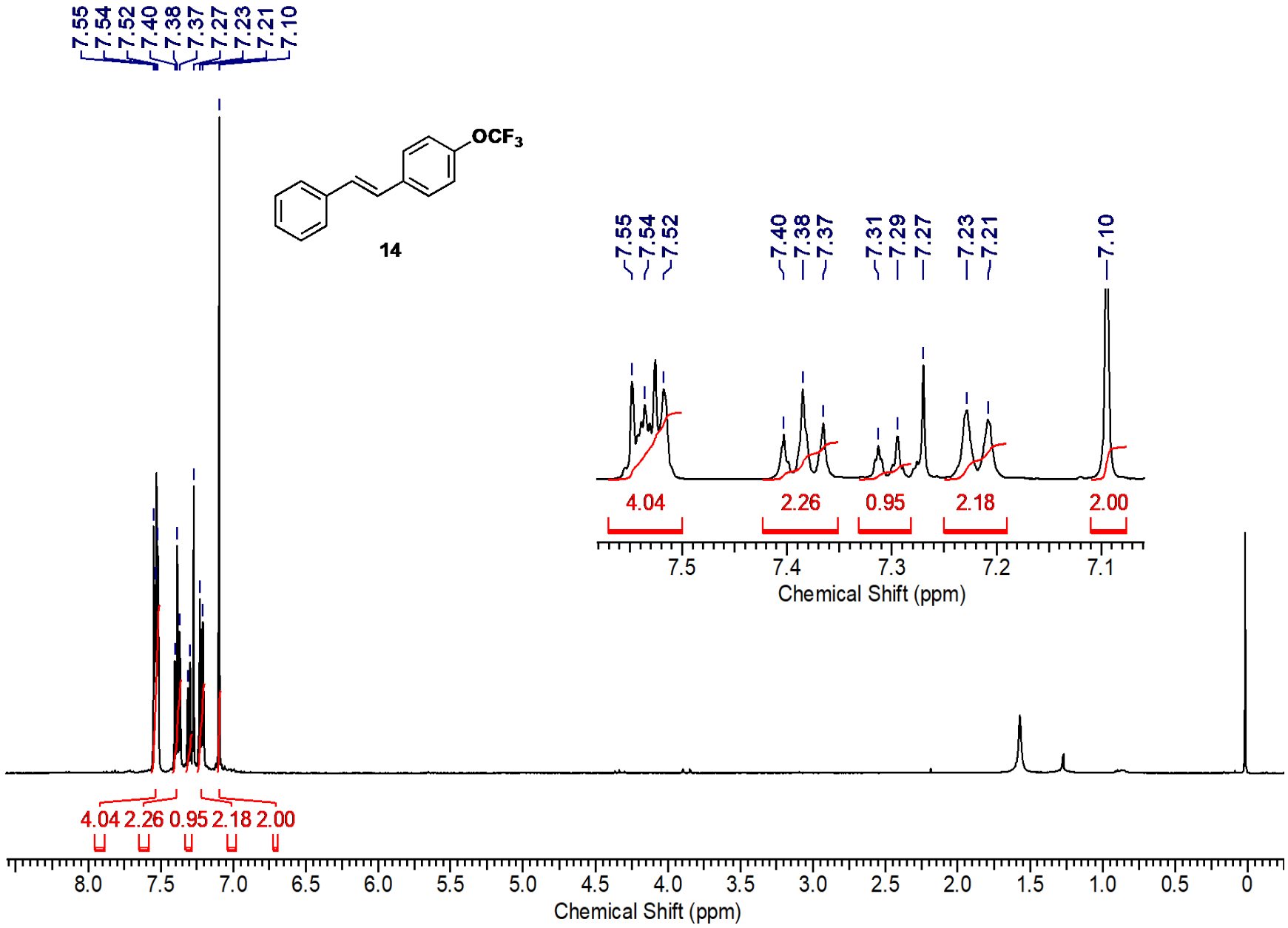

136.28
131.77
129.43
128.73
127.96
127.89
127.63
127.40
126.55
77.63
77.00
76.37
Br
11
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

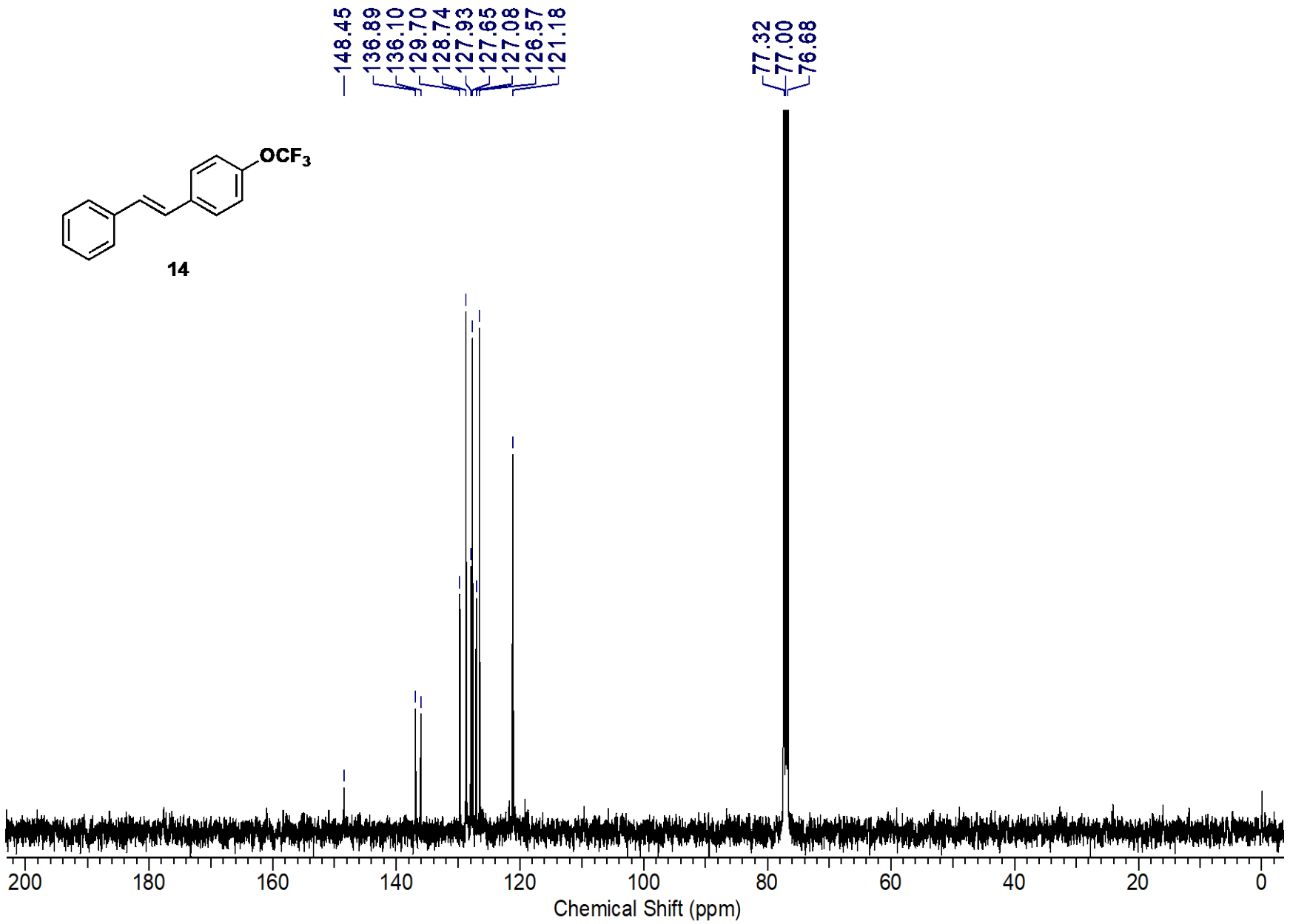

7.59
7.55
7.52
7.48
7.44
7.35
7.32
7.28
7.19
7.11
7.05
CN
12
7.59
7.55
7.52
7.48
7.44
7.35
7.32
7.28
7.24
7.19
7.11
7.05
6.96
6.36
3.20
1.42
1.12
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
Chemical Shift (ppm)
6.36
3.20
1.42
1.12
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

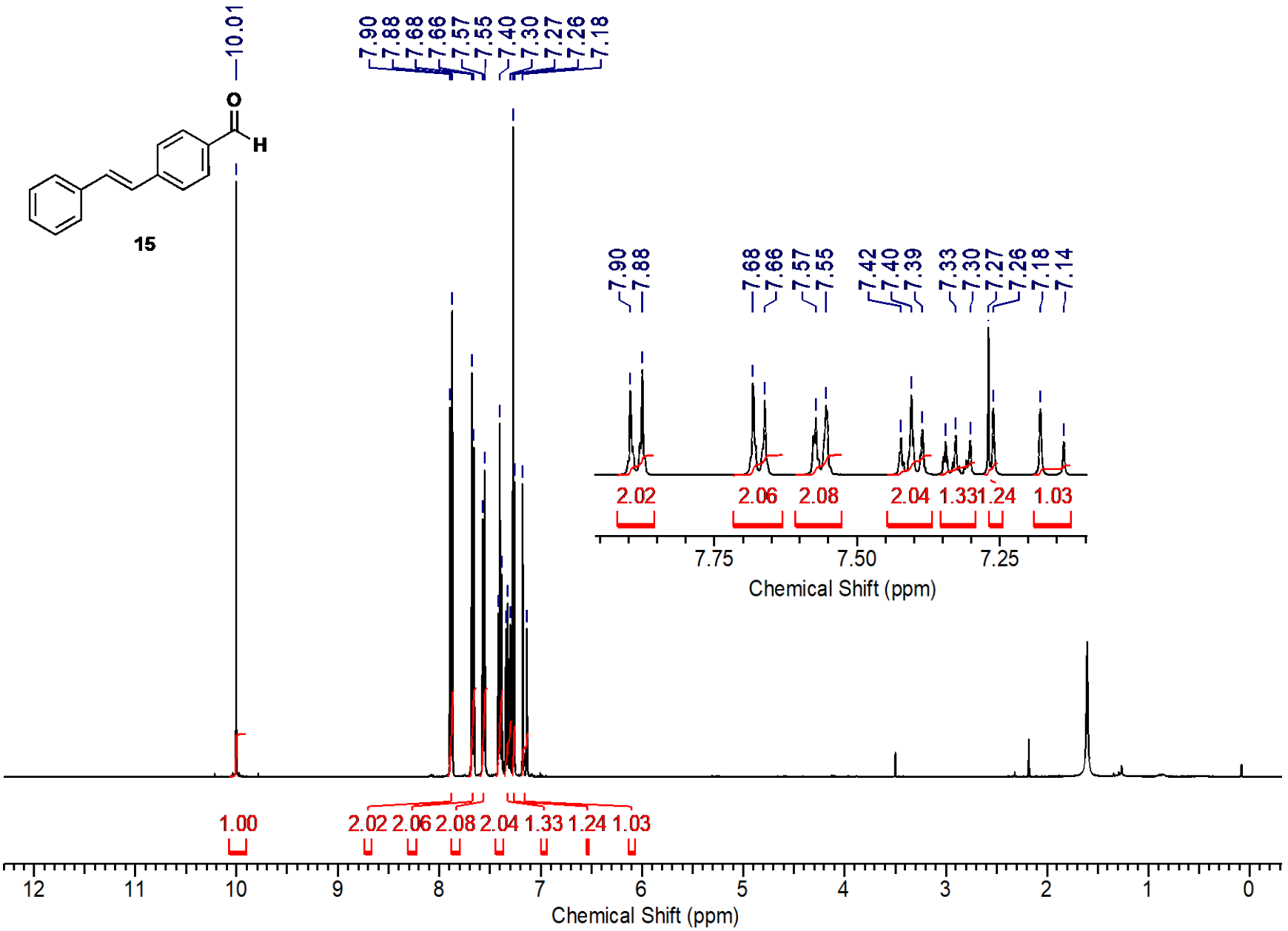

141.80
136.25
132.44
128.82
128.61
126.87
126.83
126.69
118.99
110.54
77.64
77.00
76.37
CN
12
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

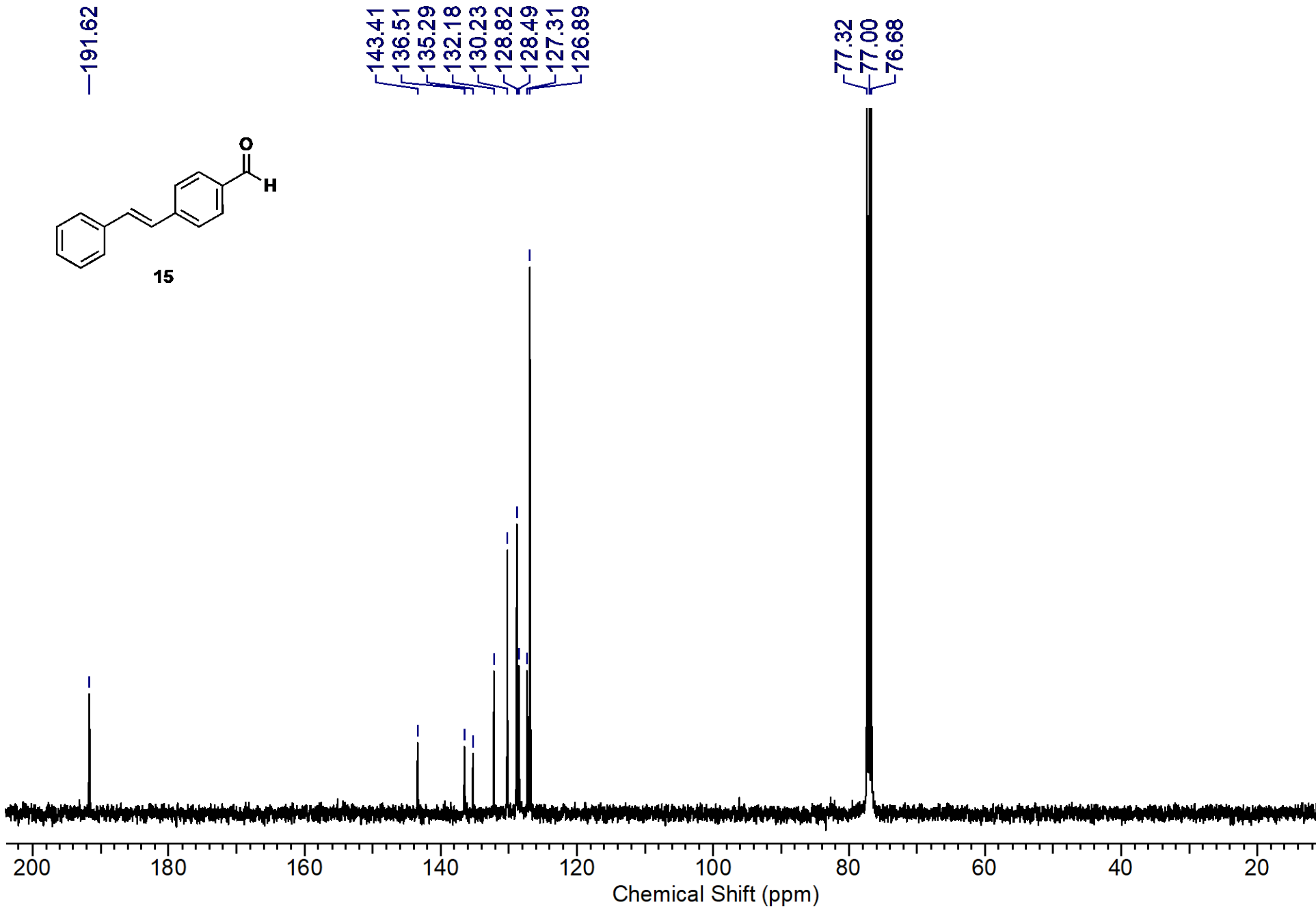

7.62
7.56
7.54
7.42
7.40
7.38
7.32
7.27
7.19
7.15
CF3
13
7.62
7.56
7.54
7.42
7.40
7.38
7.33
7.32
7.27
7.23
7.19
7.15
7.11
5.35
3.37
1.00
0.99
7.6
7.5
7.4
7.3
7.2
7.1
Chemical Shift (ppm)
5.35 3.37 1.00 0.99
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

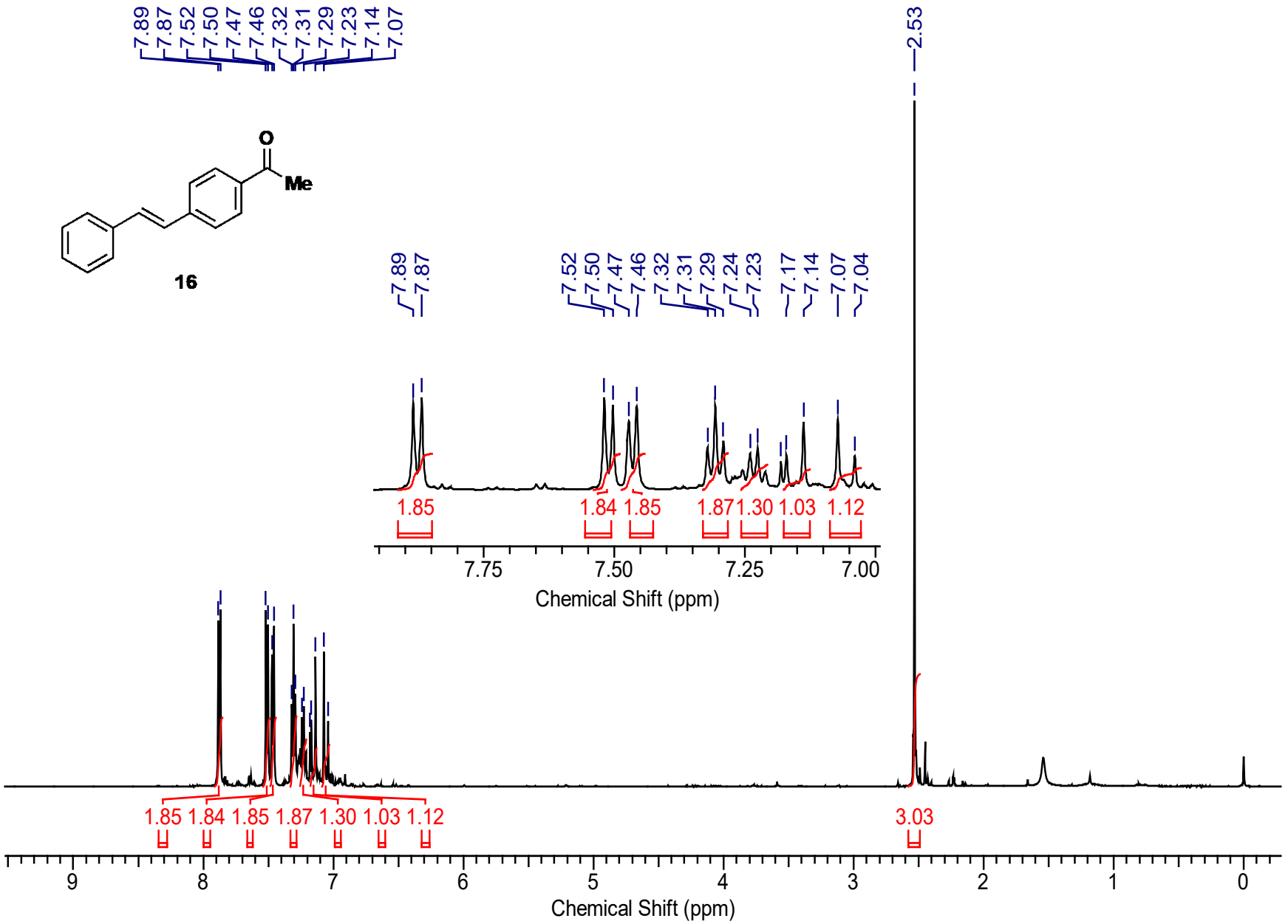

136.62
131.20
128.79
128.28
127.11
126.77
126.56
125.64
125.60
77.32
77.00
76.68
CF3
13
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)


7.55
7.54
7.52
7.40
7.38
7.37
7.27
7.23
7.21
7.10
OCF3
14
4.04 2.26 0.95 2.18 2.00
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
Chemical Shift (ppm)
7.55
7.54
7.52
7.40
7.38
7.37
7.31
7.29
7.27
7.23
7.21
7.10
4.04
2.26
0.95
2.18
2.00
7.5 7.4 7.3 7.2 7.1
Chemical Shift (ppm)


148.45
136.89
136.10
129.70
128.74
127.93
127.65
127.08
126.57
121.18
77.32
77.00
76.68
OCF3
14
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)


10.01
7.90
7.88
7.68
7.66
7.57
7.55
7.40
7.30
7.27
7.26
7.18
O
H
15
7.90
7.88
7.68
7.66
7.57
7.55
7.42
7.40
7.39
7.33
7.30
7.27
7.26
7.18
7.14
2.02
2.06
2.08
2.04
1.33
1.24
1.03
7.75
7.50
7.25
Chemical Shift (ppm)
1.00
2.02 2.06 2.08 2.04 1.33 1.24 1.03
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


191.62
143.41
136.51
135.29
132.18
130.23
128.82
128.49
127.31
126.89
77.32
77.00
76.68
O
H
15
200
180
160
140
120
100
80
60
40
20
Chemical Shift (ppm)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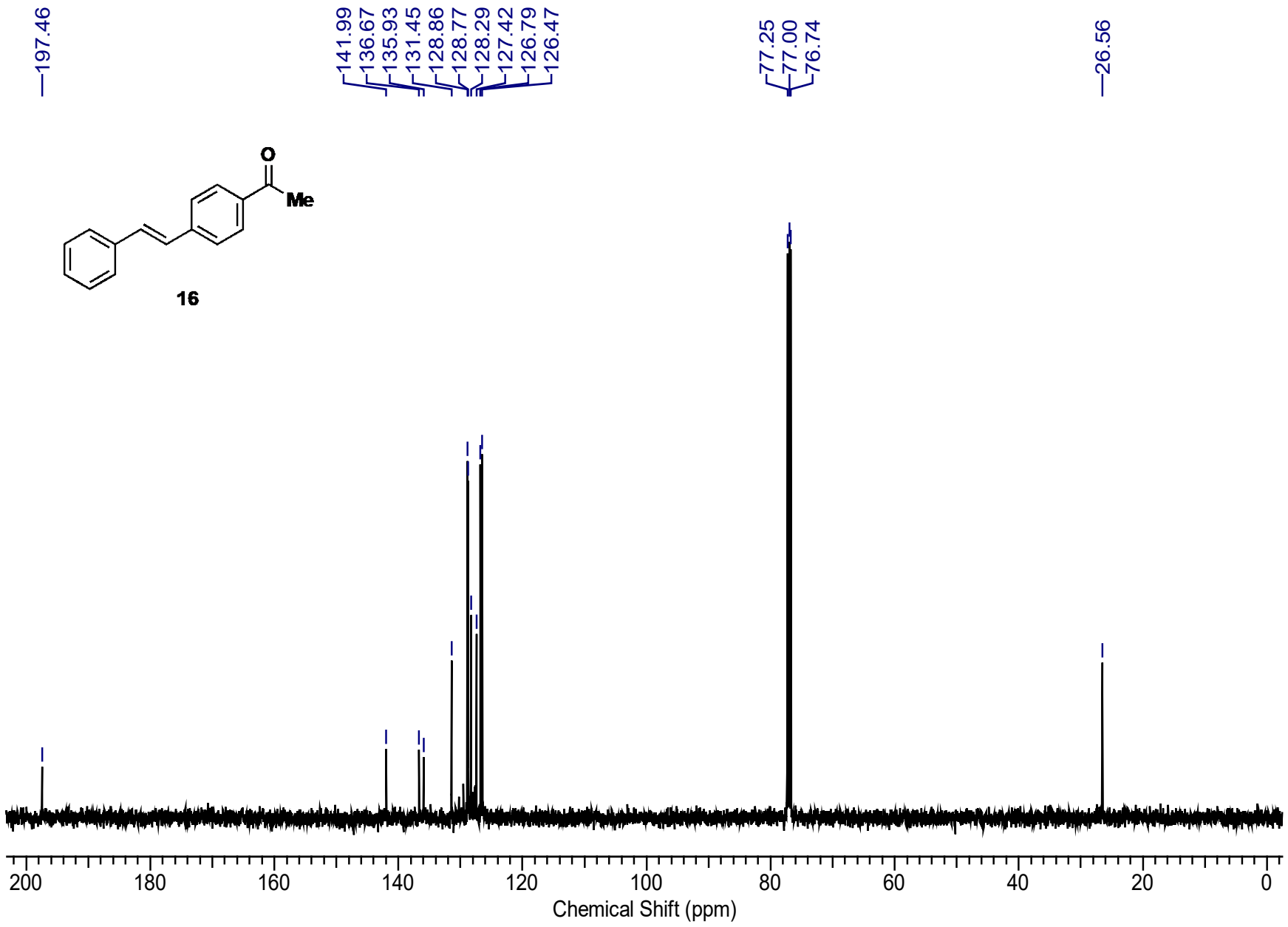
7.87
7.52
7.50
7.47
7.46
7.32
7.31
7.29
7.23
7.14
7.07
2.53
O
Me
16
7.89
7.87
7.52
7.50
7.47
7.46
7.32
7.31
7.29
7.24
7.23
7.17
7.14
7.07
7.04
1.85
1.84
1.85
1.87
1.30
1.03
1.12
7.75
7.50
7.25
7.00
Chemical Shift (ppm)
1.85
1.84
1.85
1.87
1.30
1.03
1.12
3.03
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


197.46
141.99
136.67
135.93
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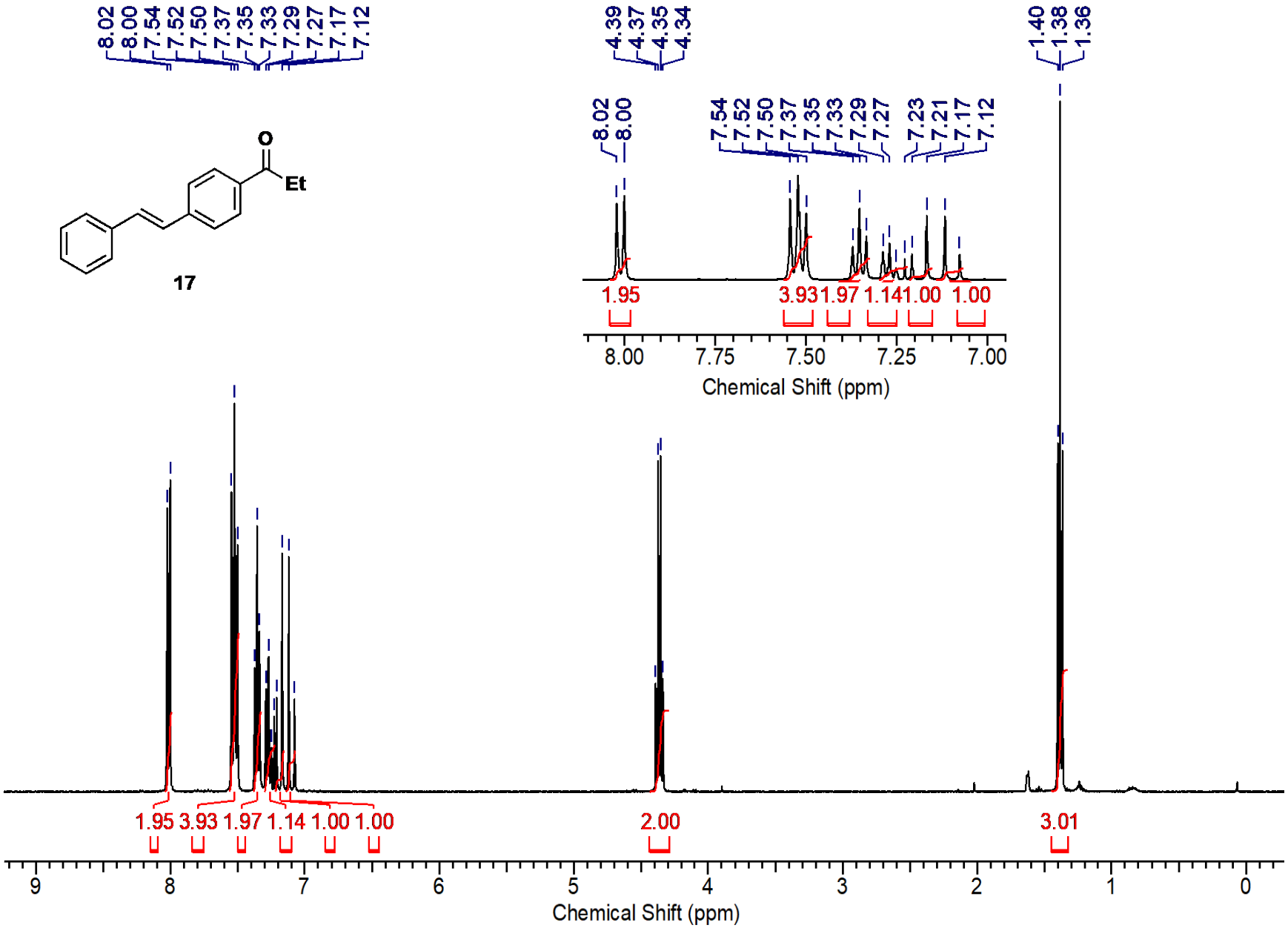
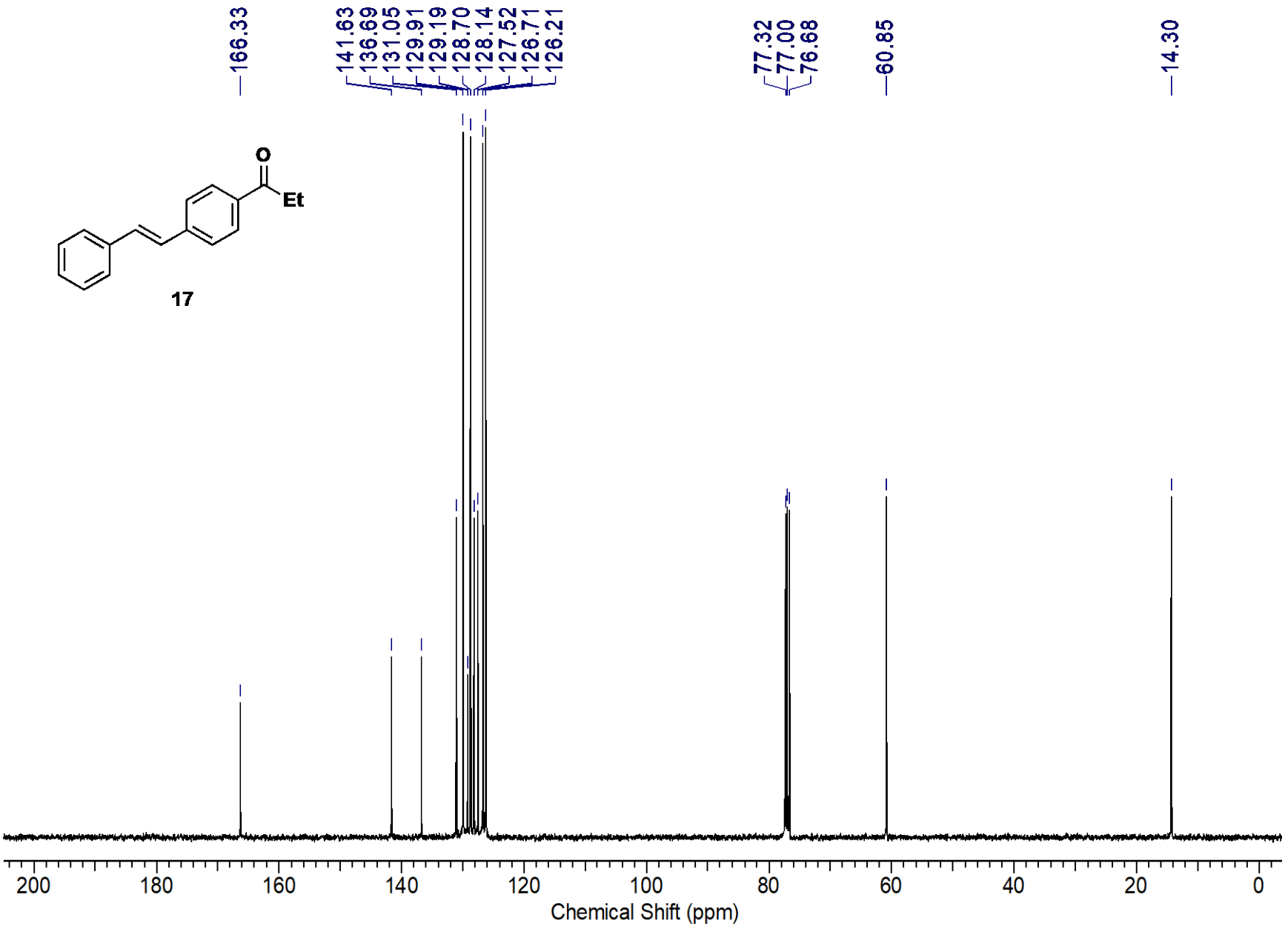
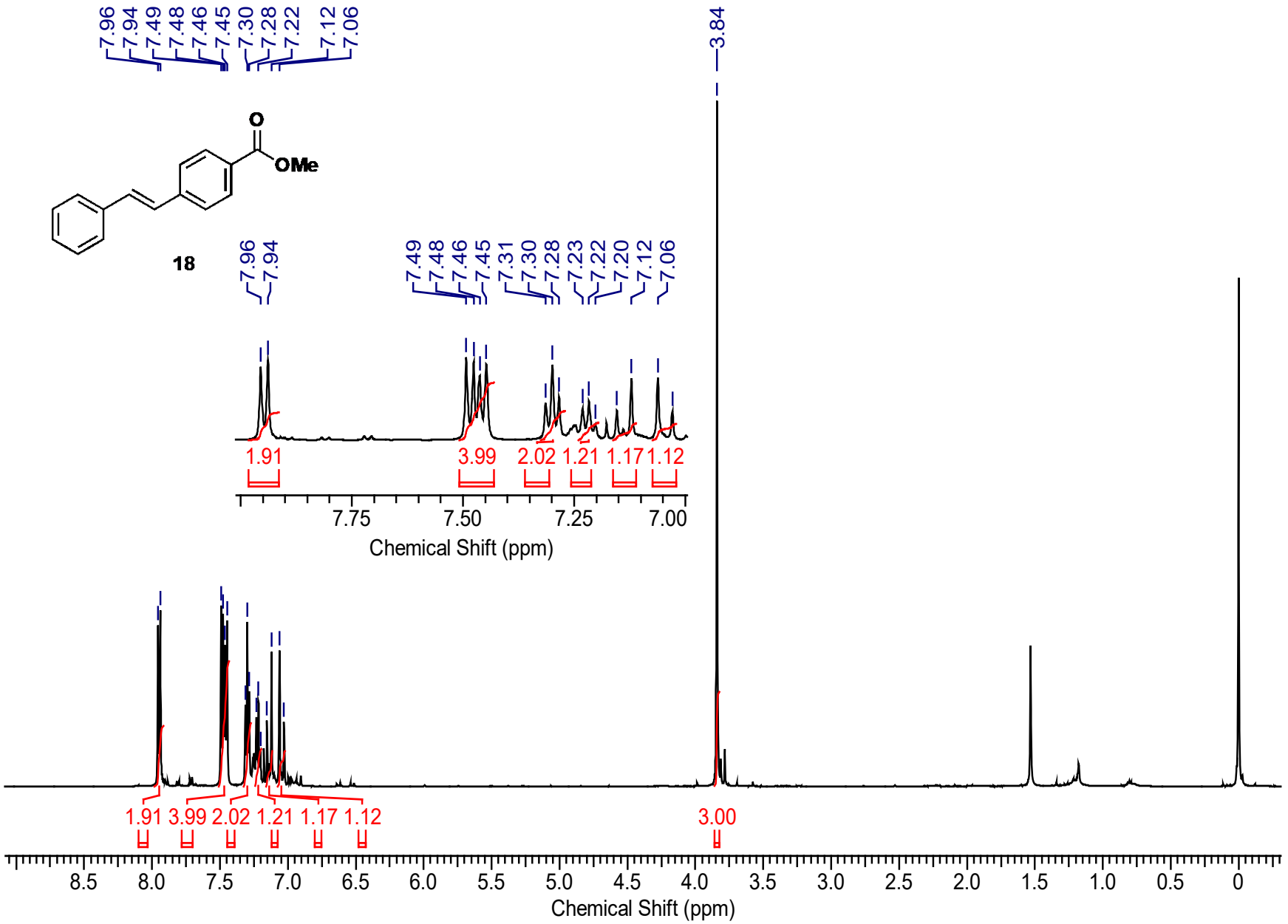
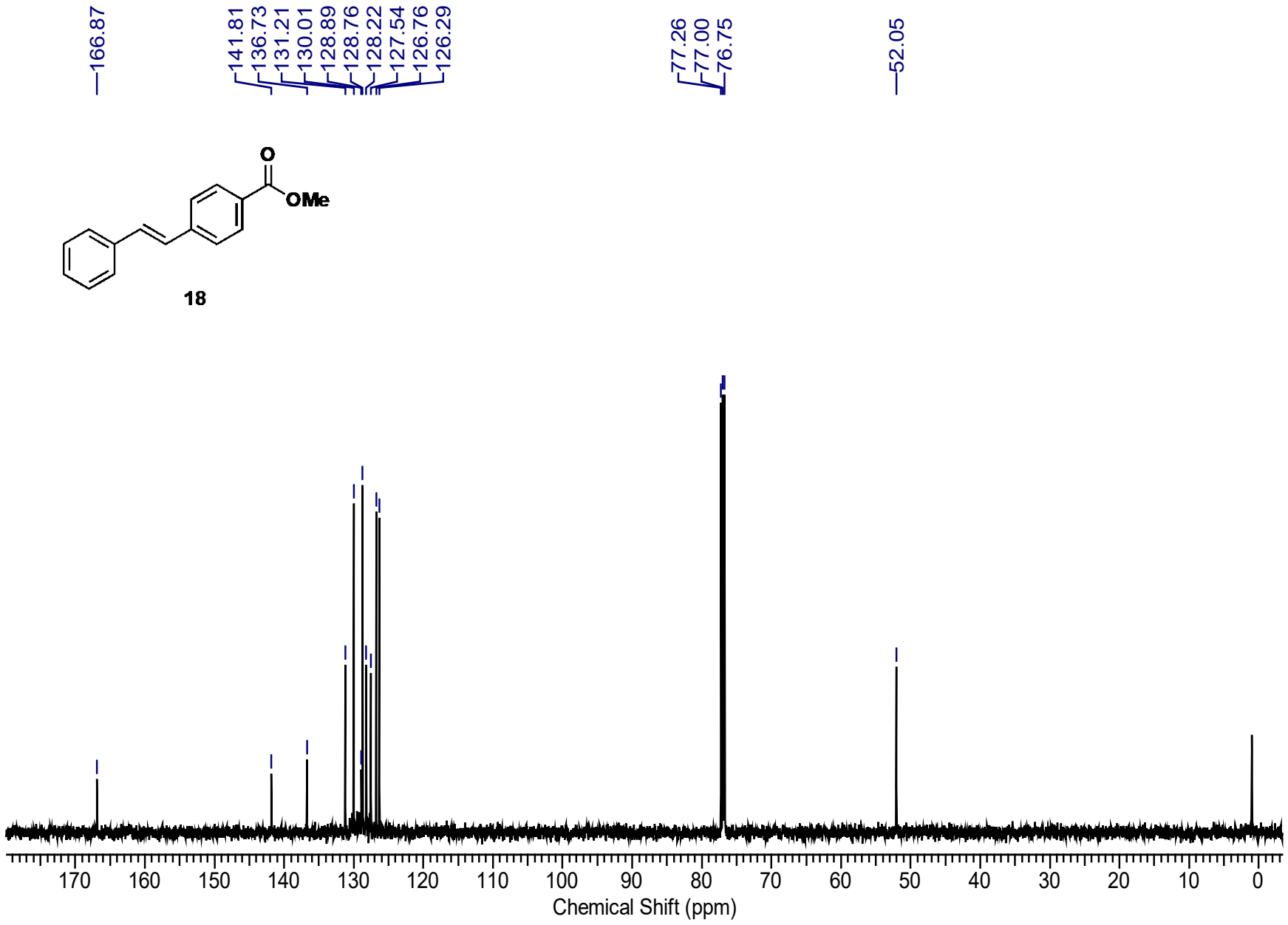
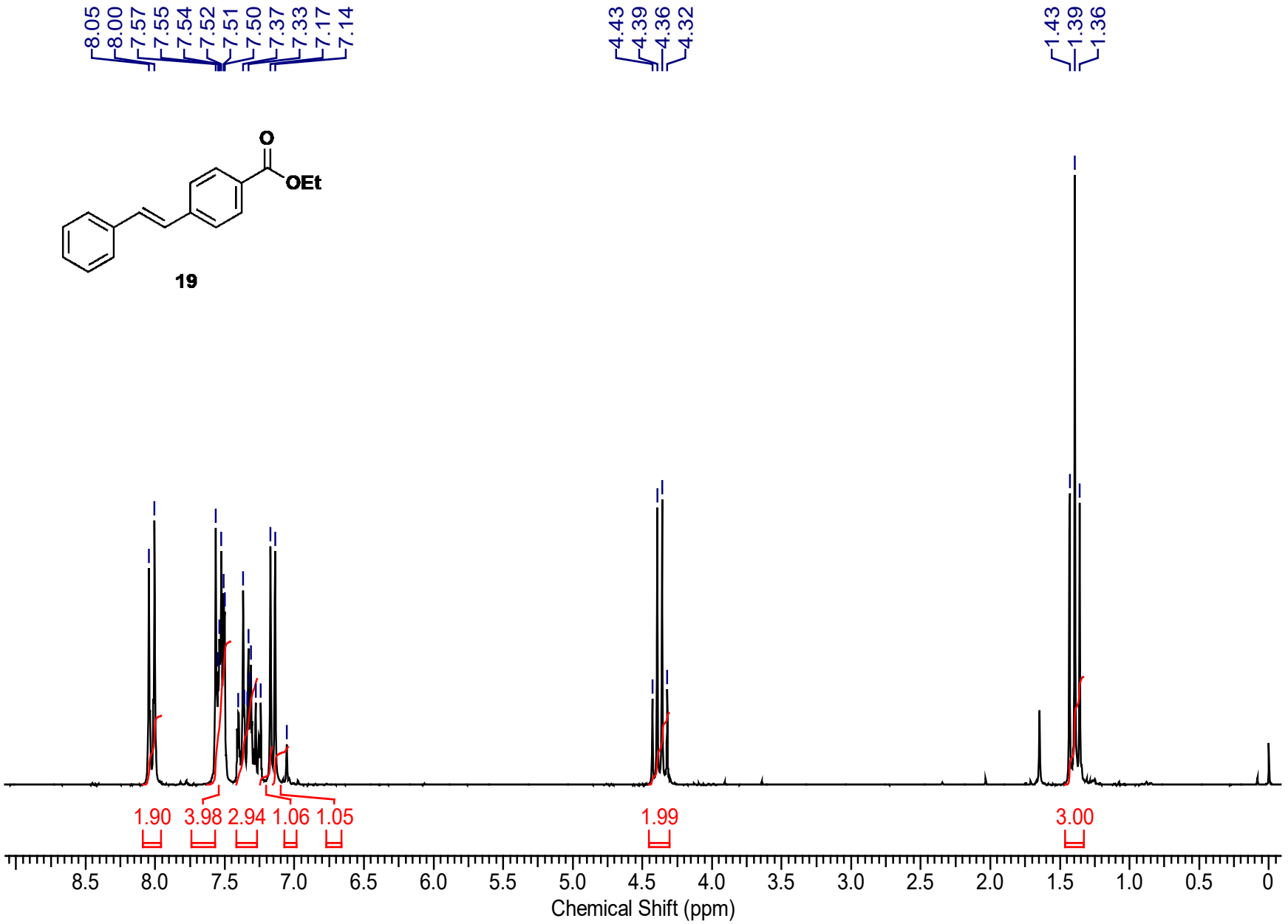
128.86
128.77
128.29
127.42
126.79
126.47
77.25
77.00
76.74
26.56
O
Me
16
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

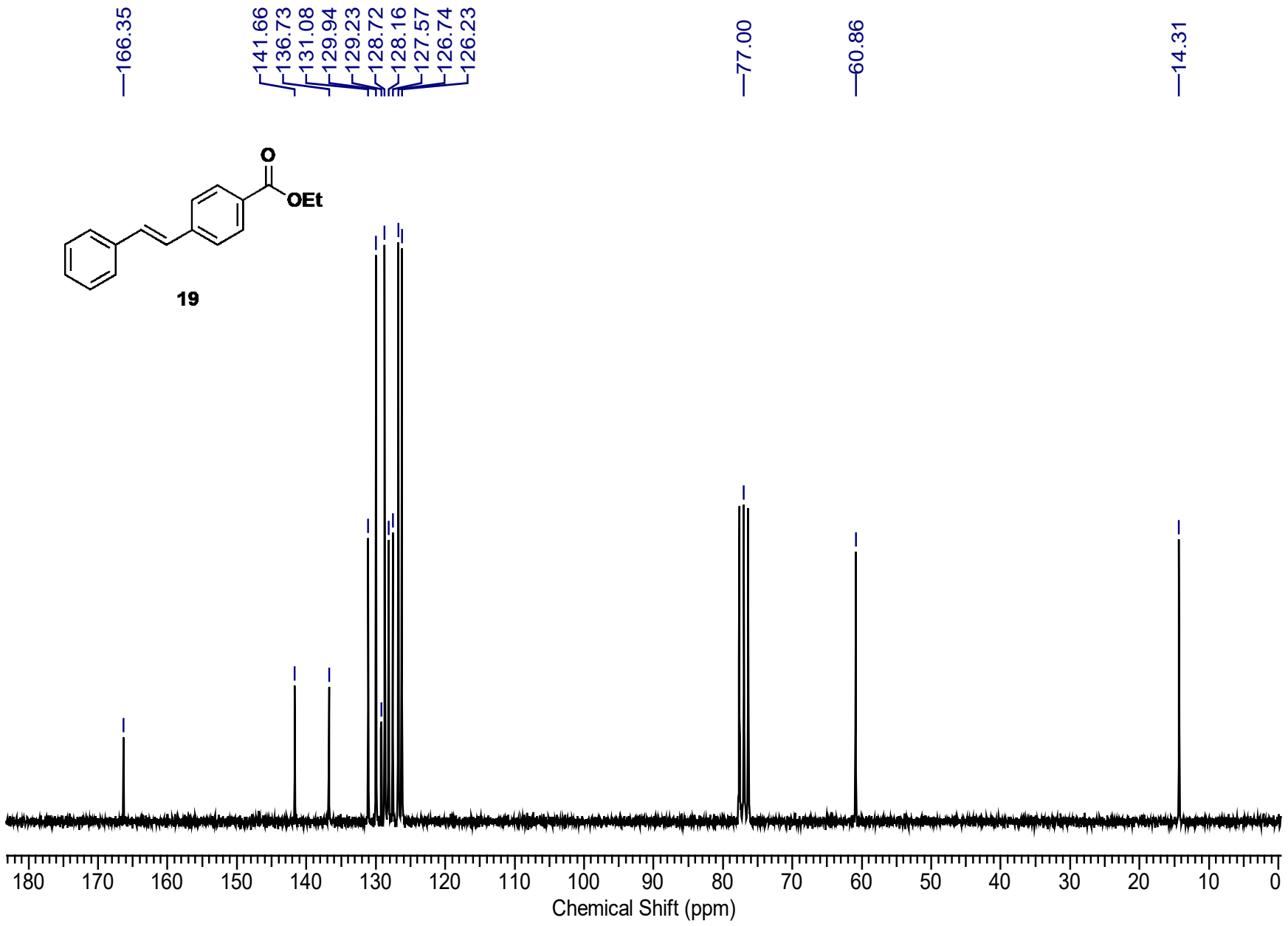

8.02
8.00
7.54
7.52
7.50
7.37
7.35
7.33
7.29
7.27
7.17
7.12
4.39
4.37
4.35
4.34
1.40
1.38
1.36
O
Et
17
1.95
3.93
1.97
1.14
1.00
1.00
2.00
3.01
Chemical Shift (ppm)

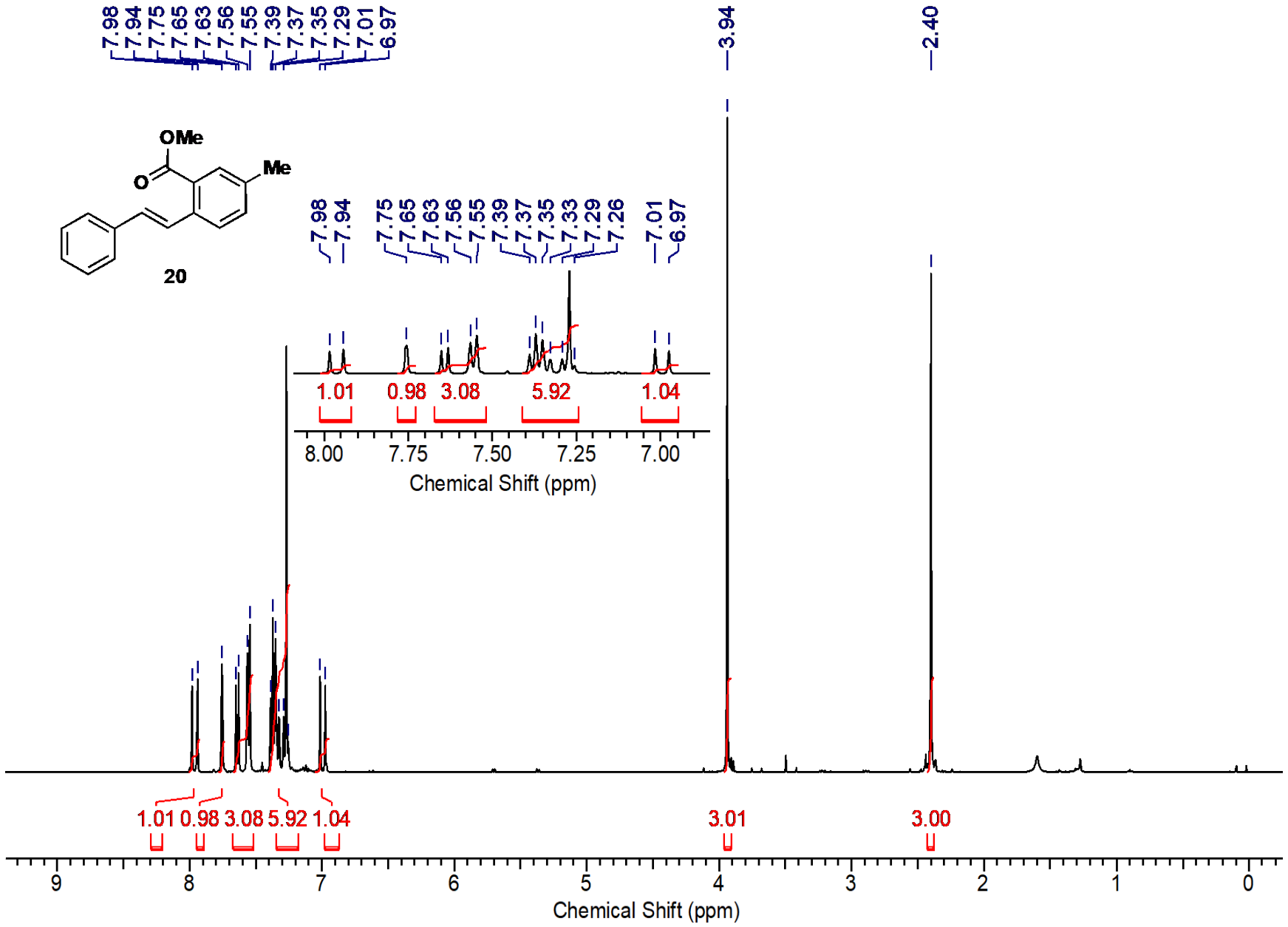

166.33
141.63
136.69
131.05
129.91
129.19
128.70
128.14
127.52
126.71
126.21
77.32
77.00
76.68
60.85
14.30
O
Et
17
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

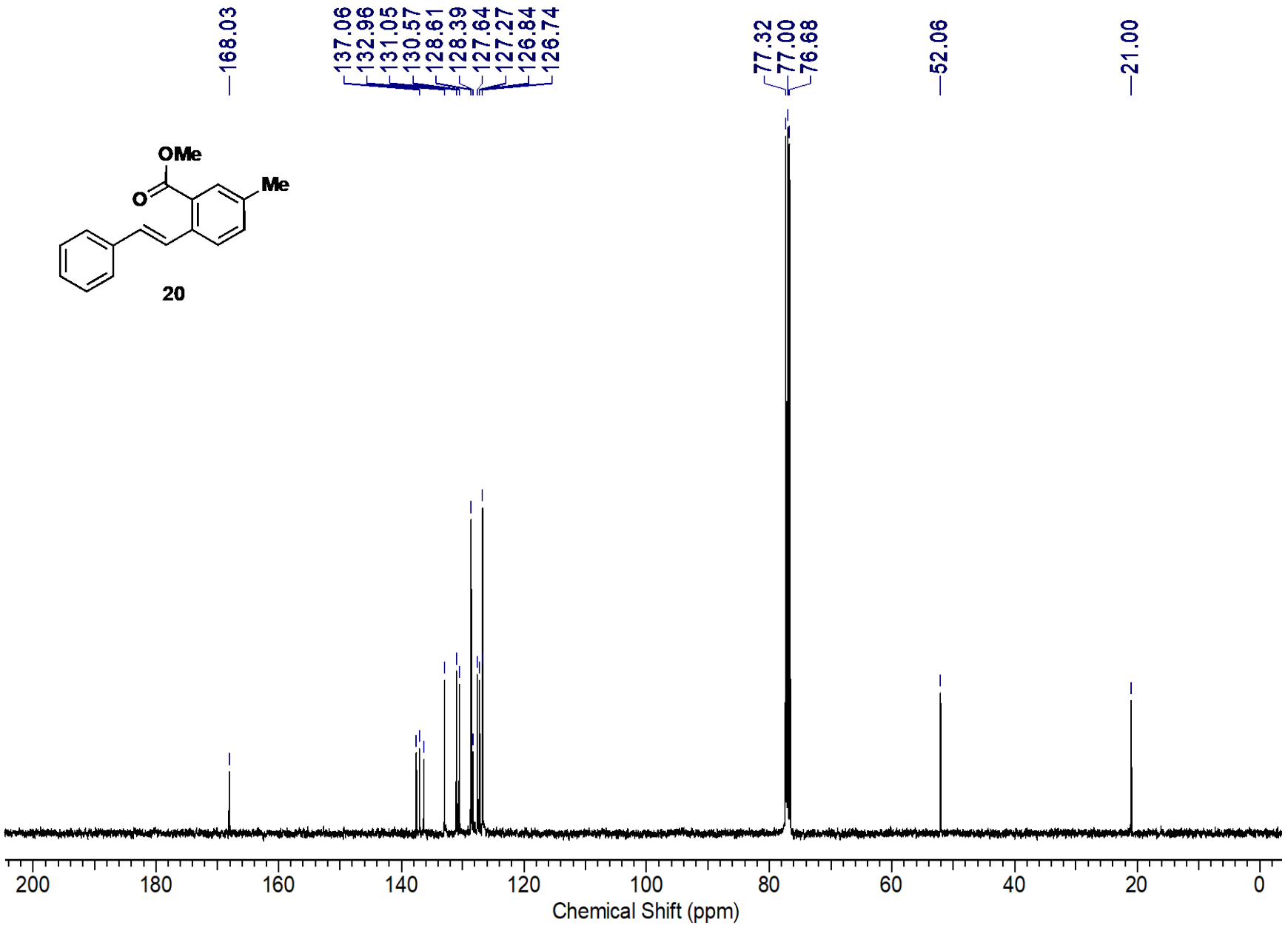

7.96
7.94
7.49
7.48
7.46
7.45
7.30
7.28
7.22
7.12
7.06
3.84
O
OMe
18
7.96
7.94
7.49
7.48
7.46
7.45
7.31
7.30
7.28
7.23
7.22
7.20
7.12
7.06
1.91
3.99
2.02
1.21
1.17
1.12
7.75
7.50
7.25
7.00
Chemical Shift (ppm)
1.91
3.99
2.02
1.21
1.17
1.12
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

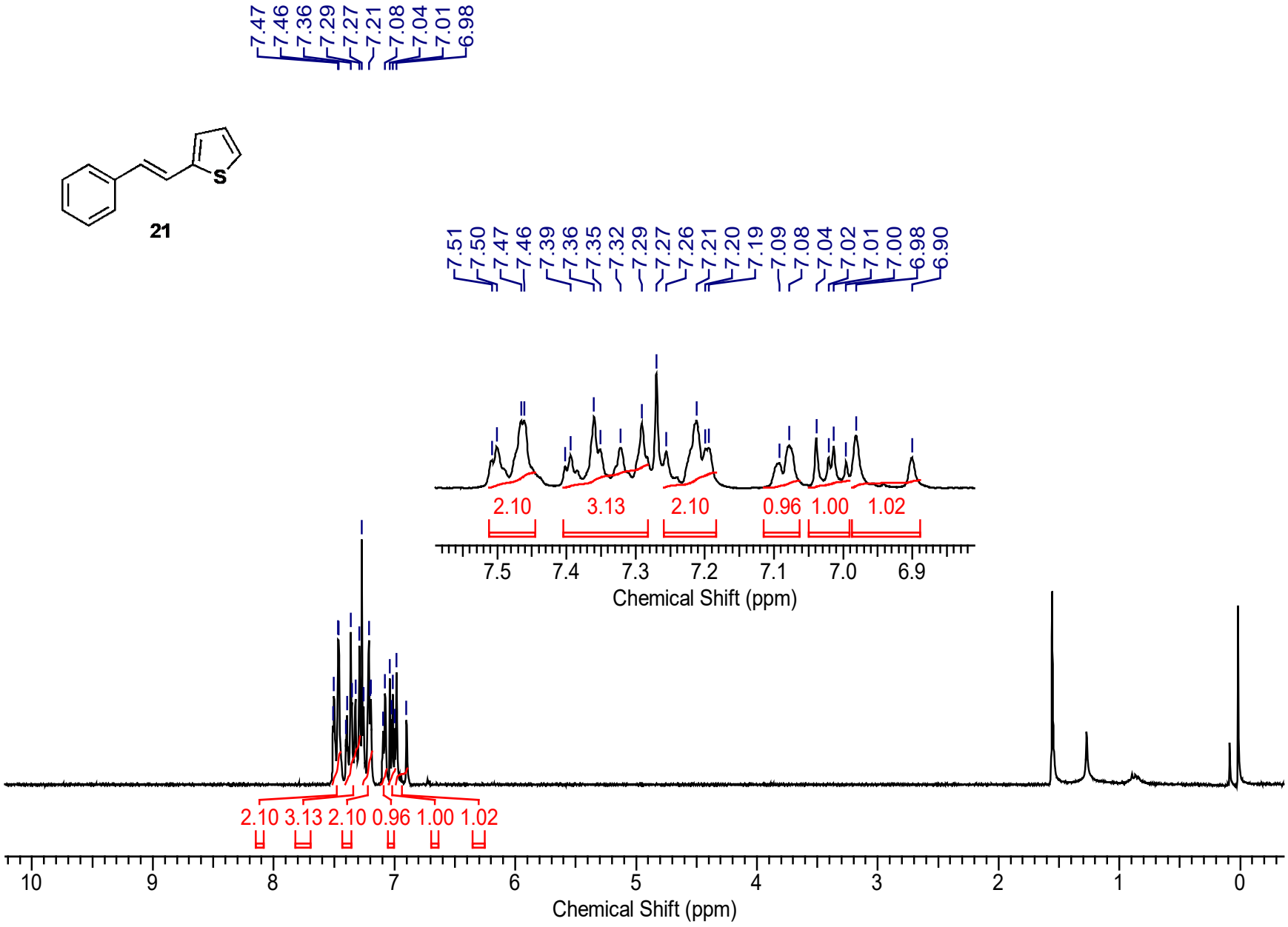

166.87
141.81
136.73
131.21
130.01
128.89
128.76
128.22
127.54
126.76
126.29
77.26
77.00
76.75
52.05
O
OMe
18
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

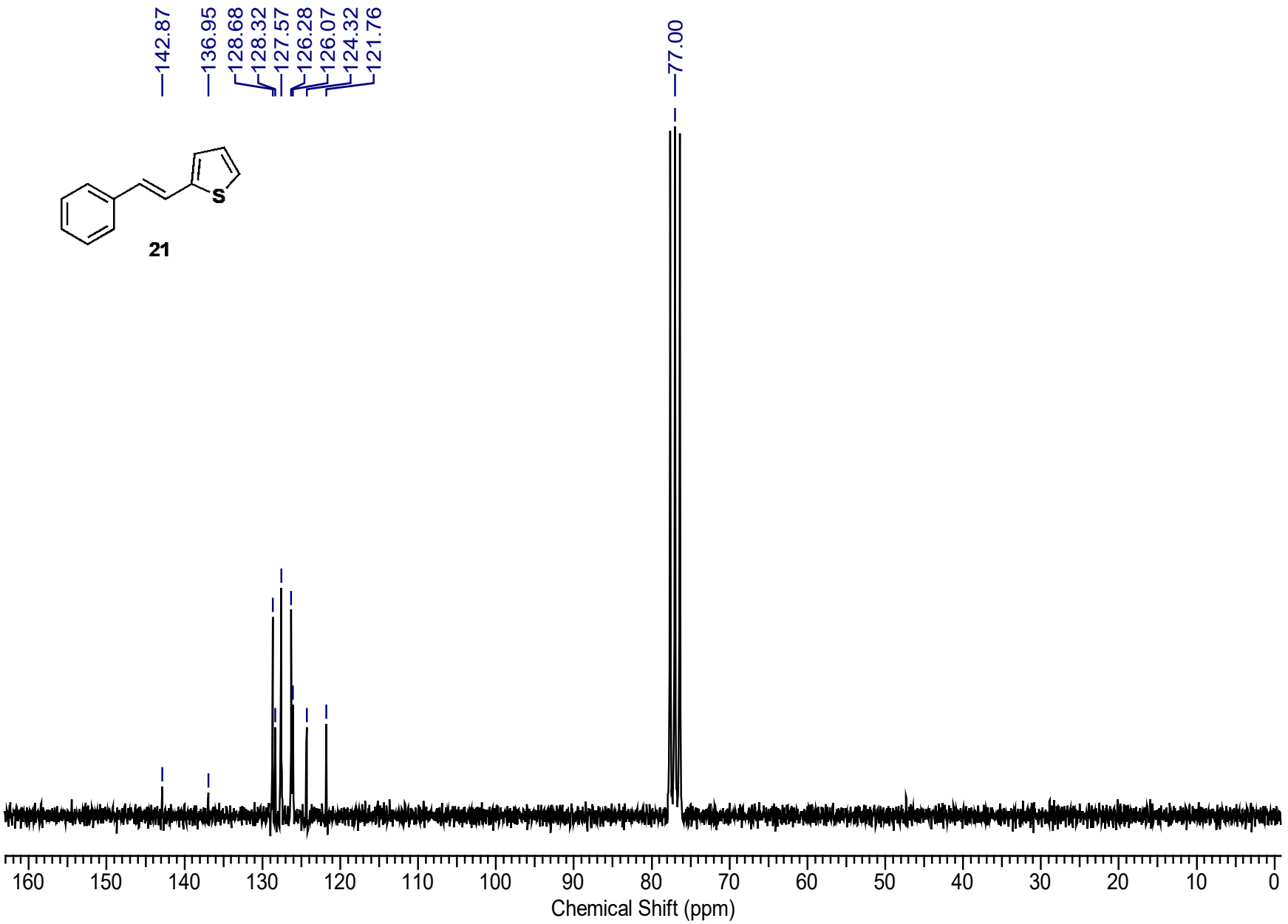

8.05
8.00
7.57
7.55
7.54
7.52
7.51
7.50
7.37
7.33
7.17
7.14
4.43
4.39
4.36
4.32
1.43
1.39
1.36
O
OEt
19
1.90
3.98
2.94
1.06
1.05
1.99
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

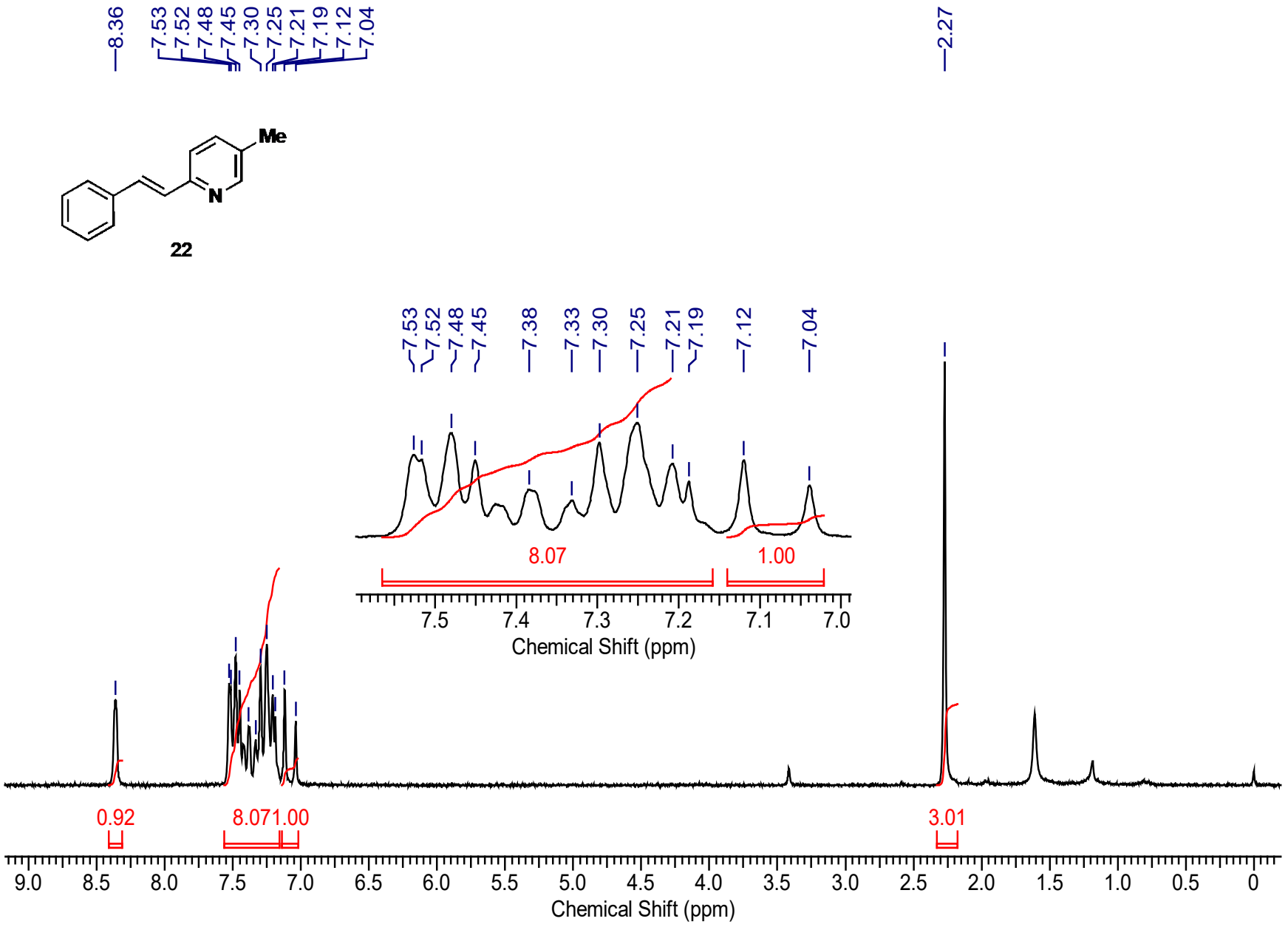

166.35
141.66
136.73
131.08
129.94
129.23
128.72
128.16
127.57
126.74
126.23
77.00
60.86
14.31
O
OEt
19
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

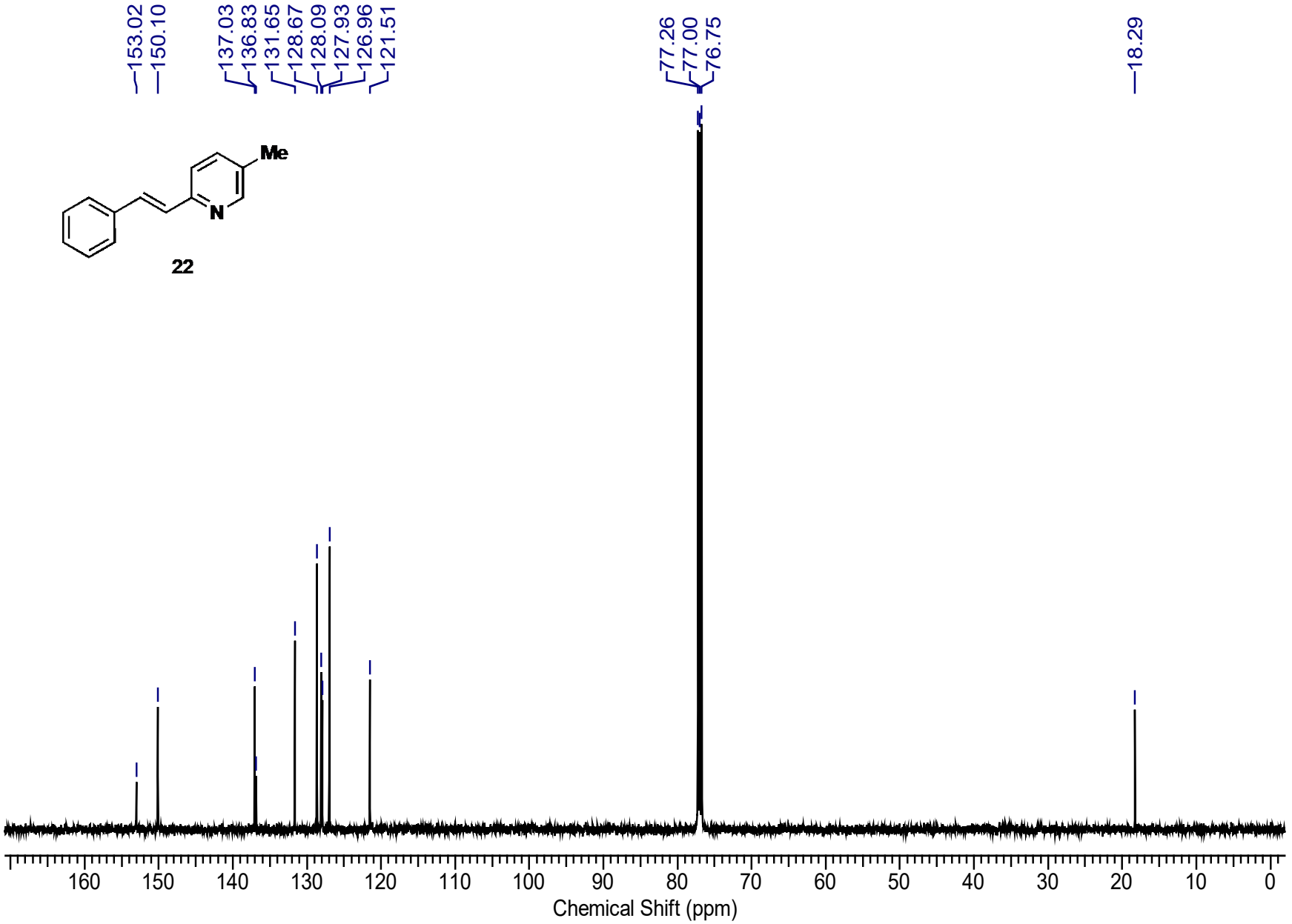

7.98
7.94
7.75
7.65
7.63
7.56
7.55
7.39
7.37
7.35
7.29
7.01
6.97
3.94
2.40
OMe
O
Me
20
7.98
7.94
7.75
7.65
7.63
7.56
7.55
7.39
7.37
7.35
7.33
7.29
7.26
7.01
6.97
1.01
0.98
3.08
5.92
1.04
8.00
7.75
7.50
7.25
7.00
Chemical Shift (ppm)
1.01
0.98
3.08
5.92
1.04
3.01
3.00
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

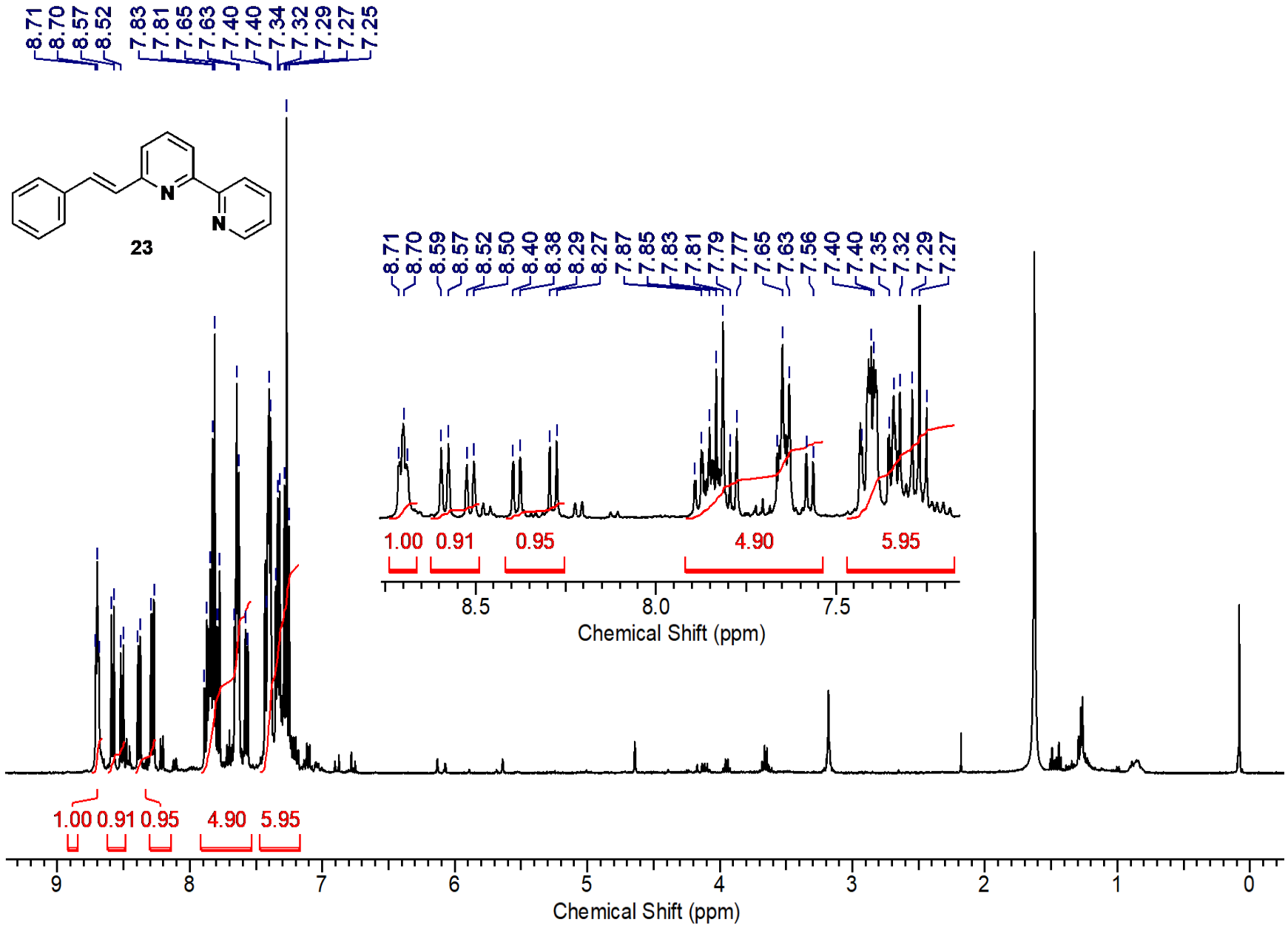

168.03
137.06
132.96
131.05
130.57
128.61
128.39
127.64
127.27
126.84
126.74
77.32
77.00
76.68
52.06
21.00
OMe
O
Me
20
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

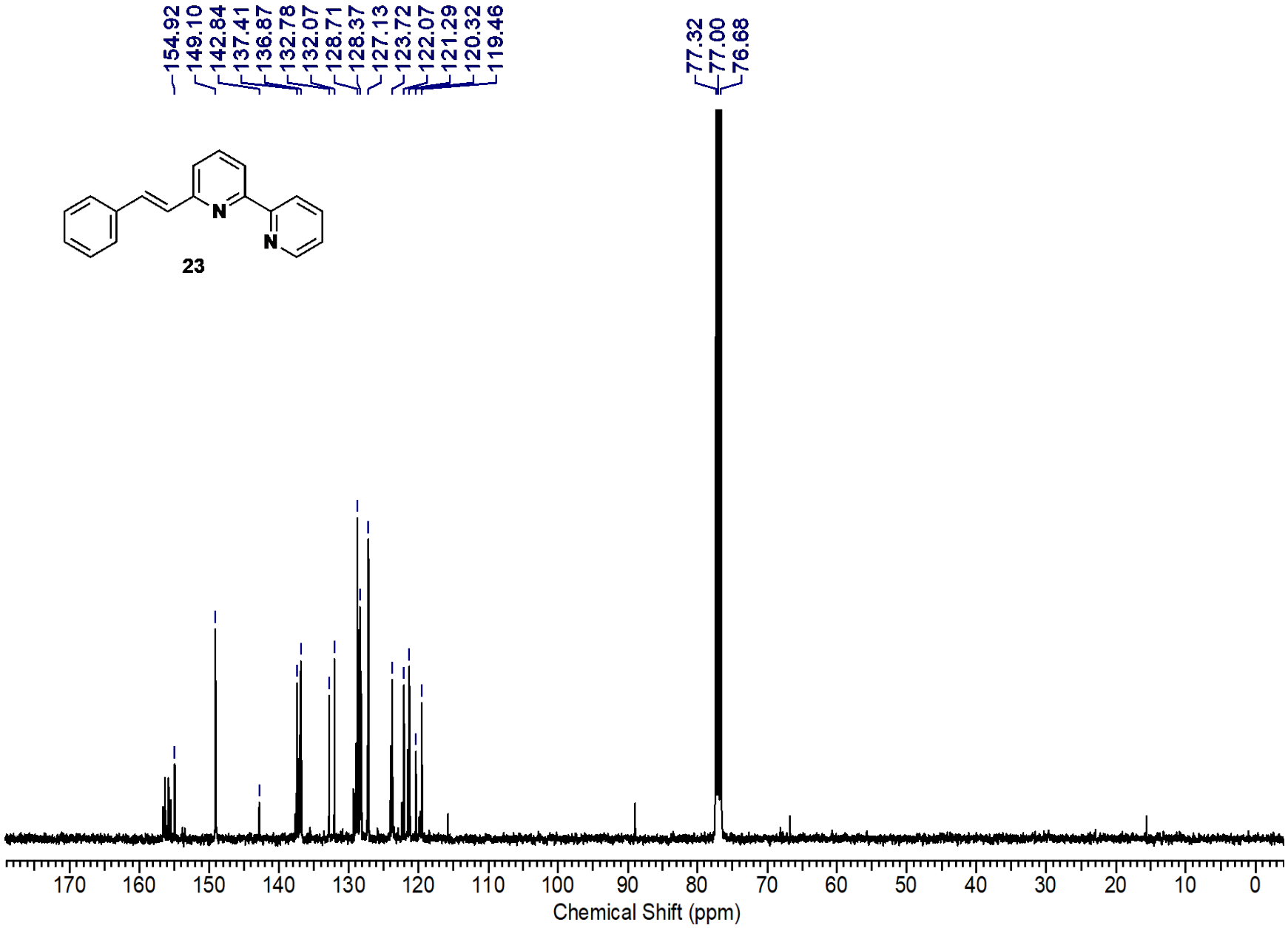

7.47
7.46
7.36
7.29
7.27
7.21
7.08
7.04
7.01
6.98
S
21
7.51
7.50
7.47
7.46
7.39
7.36
7.35
7.32
7.29
7.27
7.26
7.21
7.20
7.19
7.09
7.08
7.04
7.02
7.01
7.00
6.98
6.90
2.10
3.13
2.10
0.96
1.00
1.02
7.5
7.4
7.3
7.2
7.1
7.0
6.9
Chemical Shift (ppm)
2.10 3.13 2.10 0.96 1.00 1.02
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

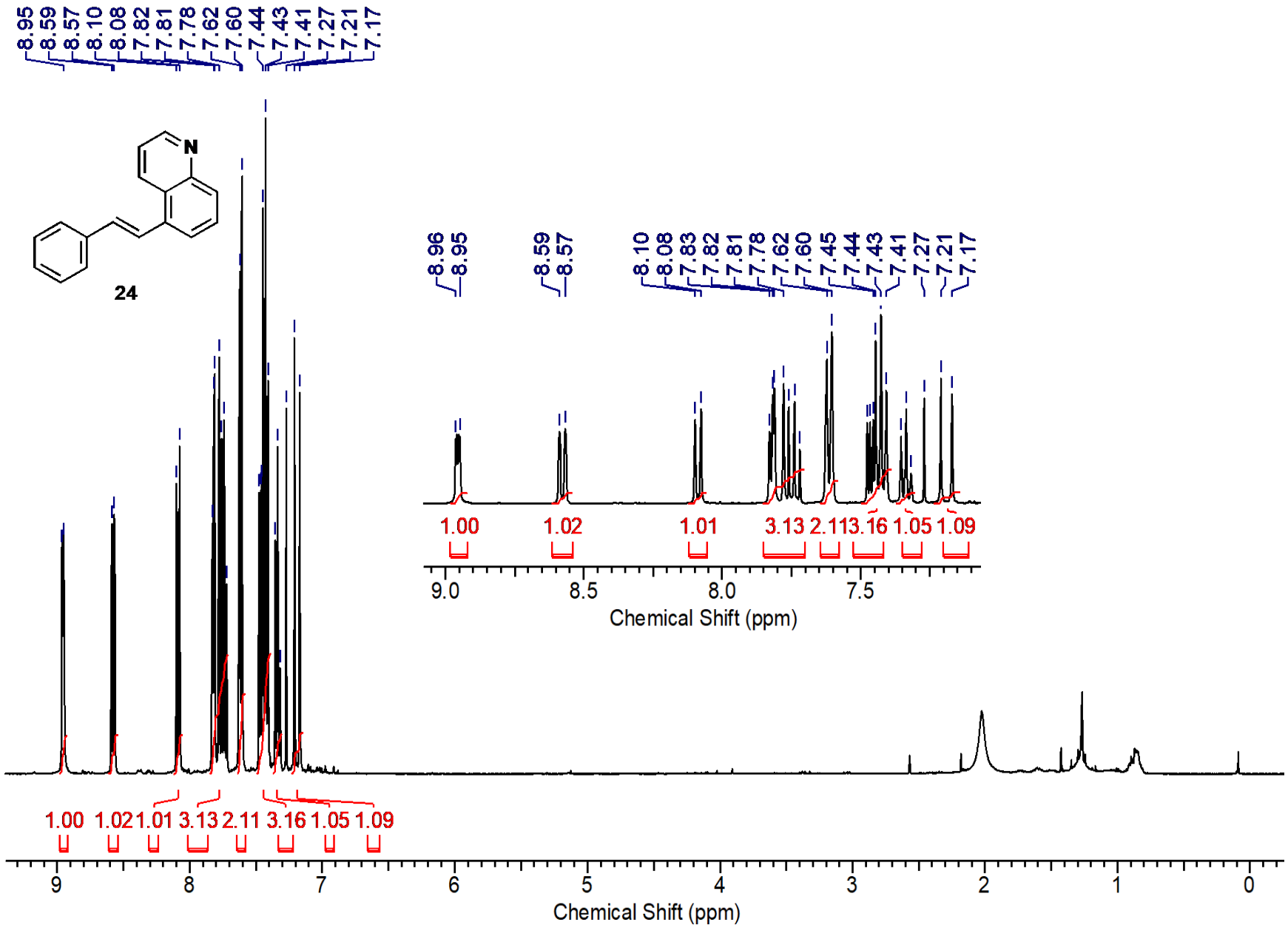

142.87
136.95
128.68
128.32
127.57
126.28
126.07
124.32
121.76
77.00
S
21
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

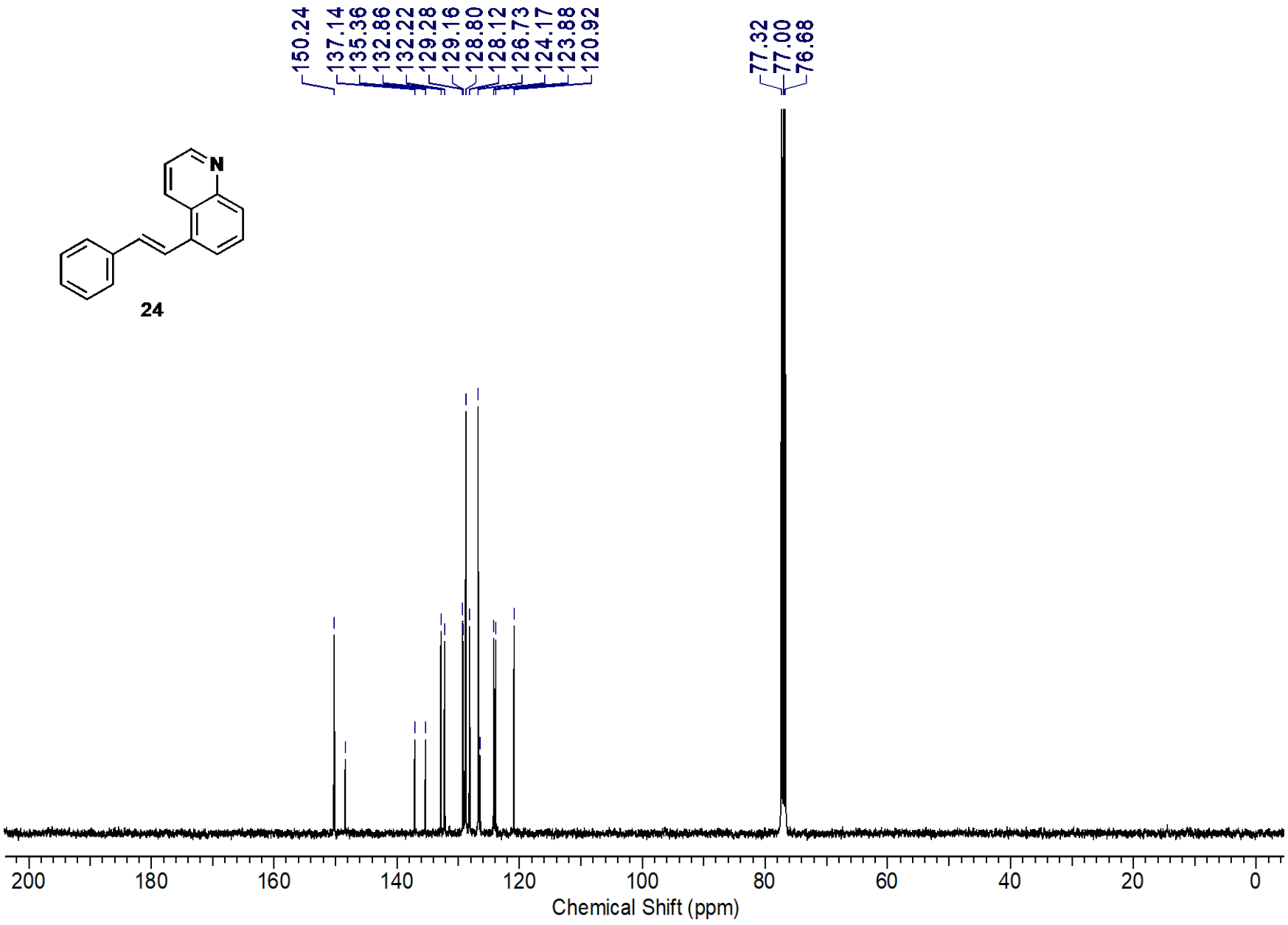

8.36
7.53
7.52
7.48
7.45
7.30
7.25
7.21
7.19
7.12
7.04
2.27
Me
N
22
7.53
7.52
7.48
7.45
7.38
7.33
7.30
7.25
7.21
7.19
7.12
7.04
8.07
1.00
7.5
7.4
7.3
7.2
7.1
7.0
Chemical Shift (ppm)
0.92
8.07
1.00
3.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

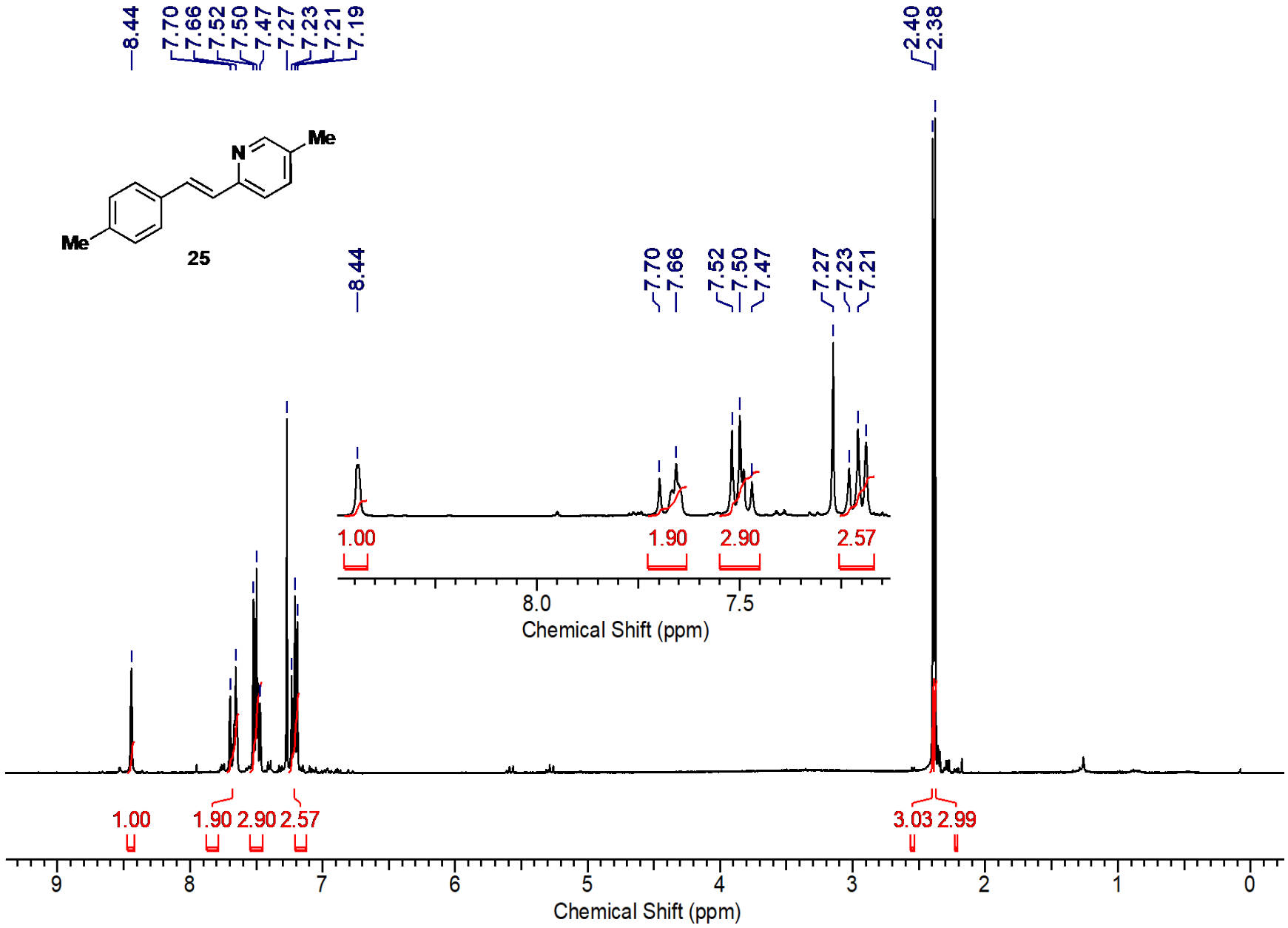

153.02
150.10
137.03
136.83
131.65
128.67
128.09
127.93
126.96
121.51
77.26
77.00
76.75
18.29
Me
N
22
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

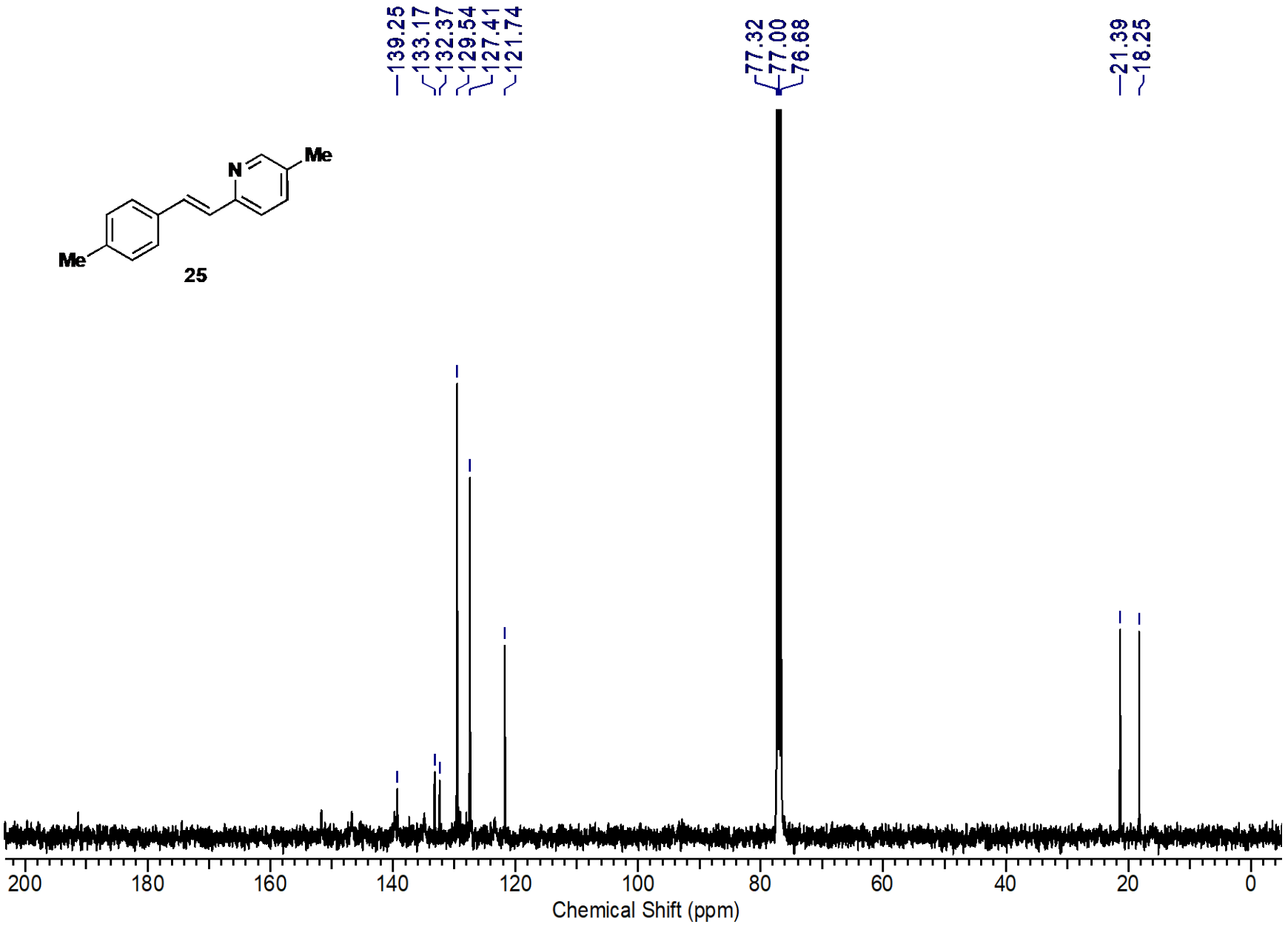

8.71
8.70
8.57
8.52
7.83
7.81
7.65
7.63
7.40
7.40
7.34
7.32
7.29
7.27
7.25
N
N
23
1.00 0.91 0.95 4.90 5.95
9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)
8.71
8.70
8.59
8.57
8.52
8.50
8.40
8.38
8.29
8.27
7.87
7.85
7.83
7.81
7.79
7.77
7.65
7.63
7.56
7.40
7.40
7.35
7.32
7.29
7.27
1.00 0.91 0.95 4.90 5.95
8.5 8.0 7.5
Chemical Shift (ppm)

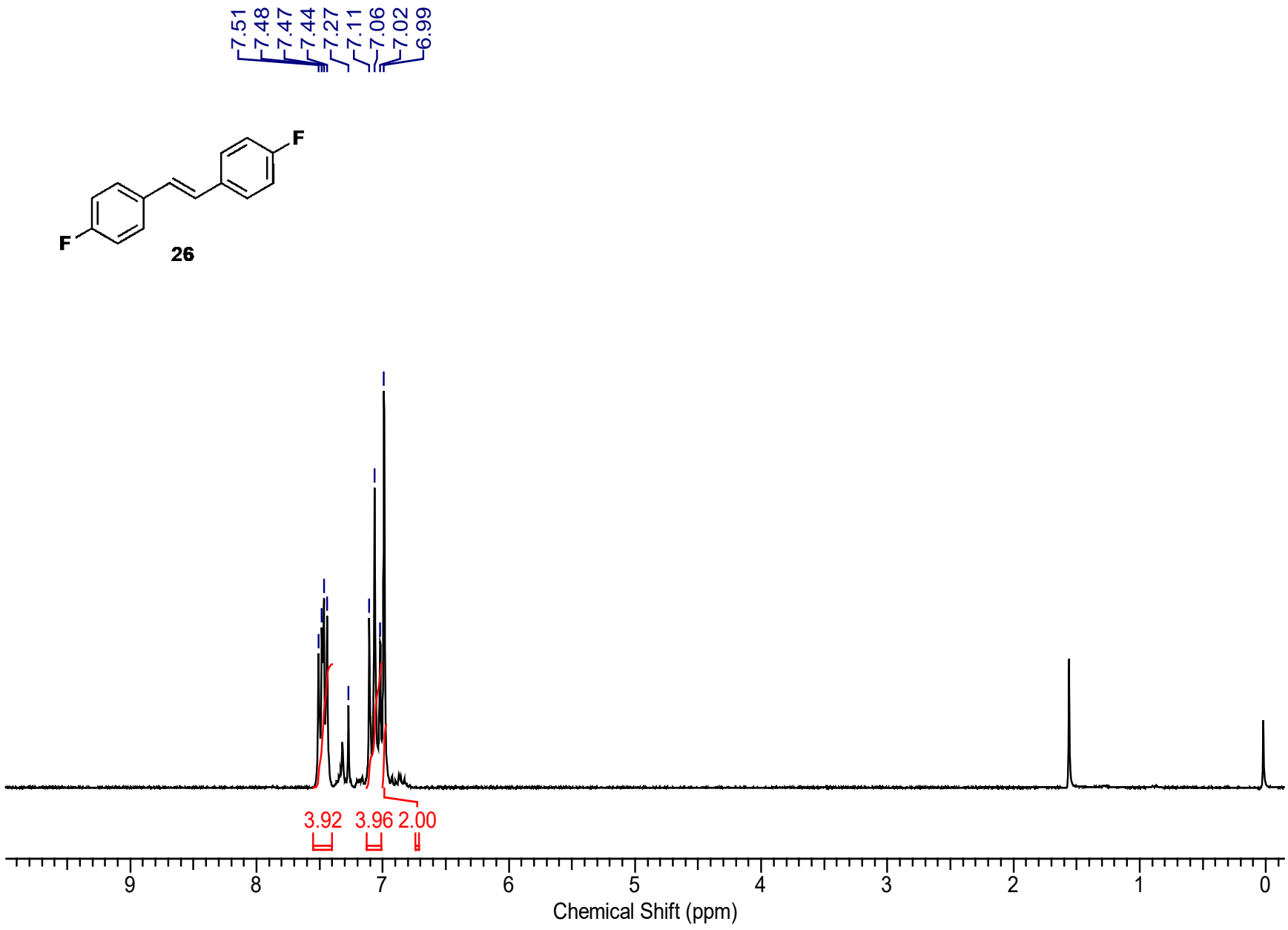

154.92
149.10
142.84
137.41
136.87
132.78
132.07
128.71
128.37
127.13
123.72
122.07
121.29
120.32
119.46
77.32
77.00
76.68
N
N
23
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

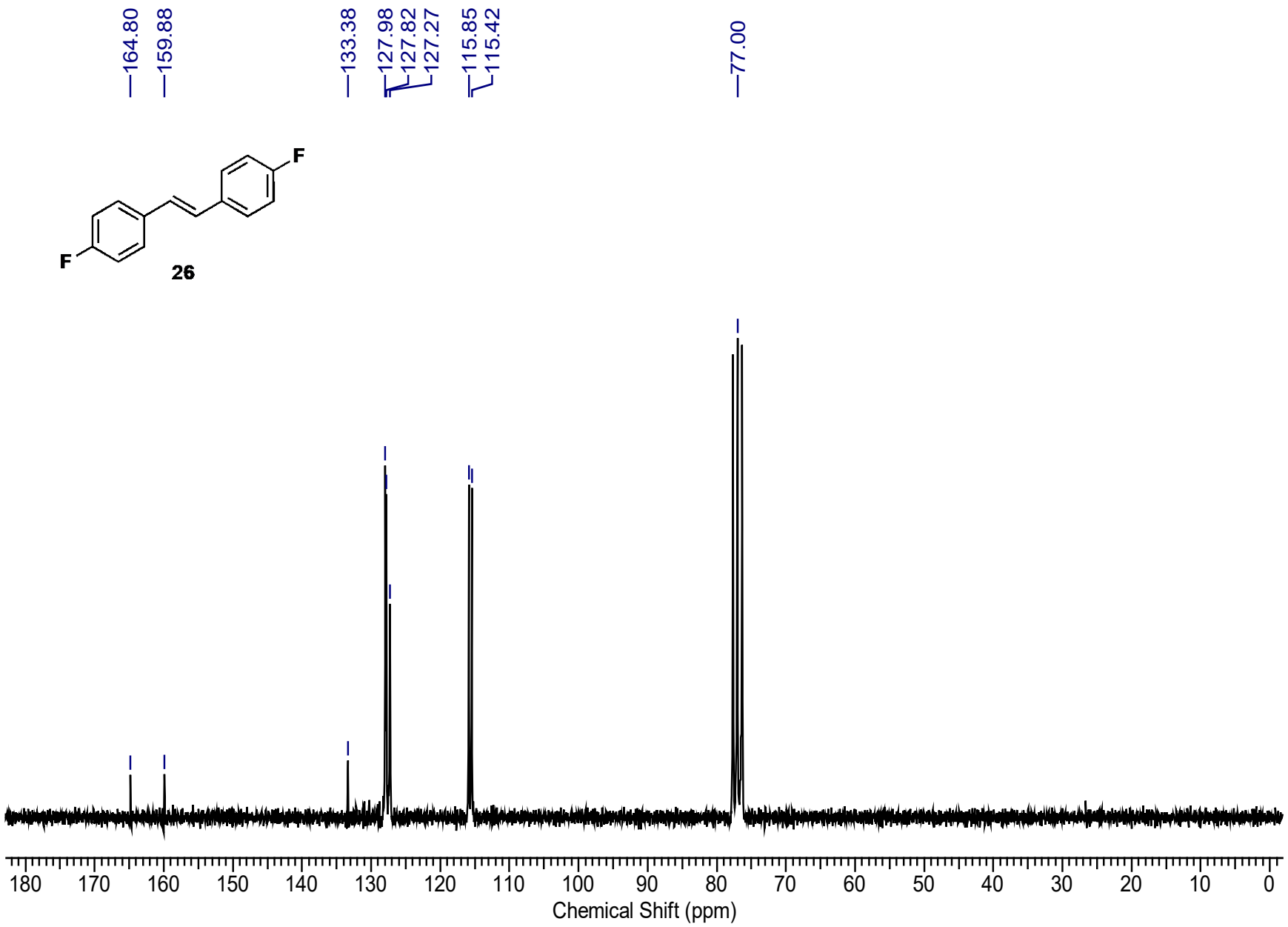

8.95
8.59
8.57
8.10
8.08
7.82
7.81
7.78
7.62
7.60
7.44
7.43
7.41
7.27
7.21
7.17
N
24
1.00 1.02 1.01 3.13 2.11 3.16 1.05 1.09
9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)
8.96
8.95
8.59
8.57
8.10
8.08
7.83
7.82
7.81
7.78
7.62
7.60
7.45
7.44
7.43
7.41
7.27
7.21
7.17
1.00 1.02 1.01 3.13 2.11 3.16 1.05 1.09
9.0 8.5 8.0 7.5
Chemical Shift (ppm)

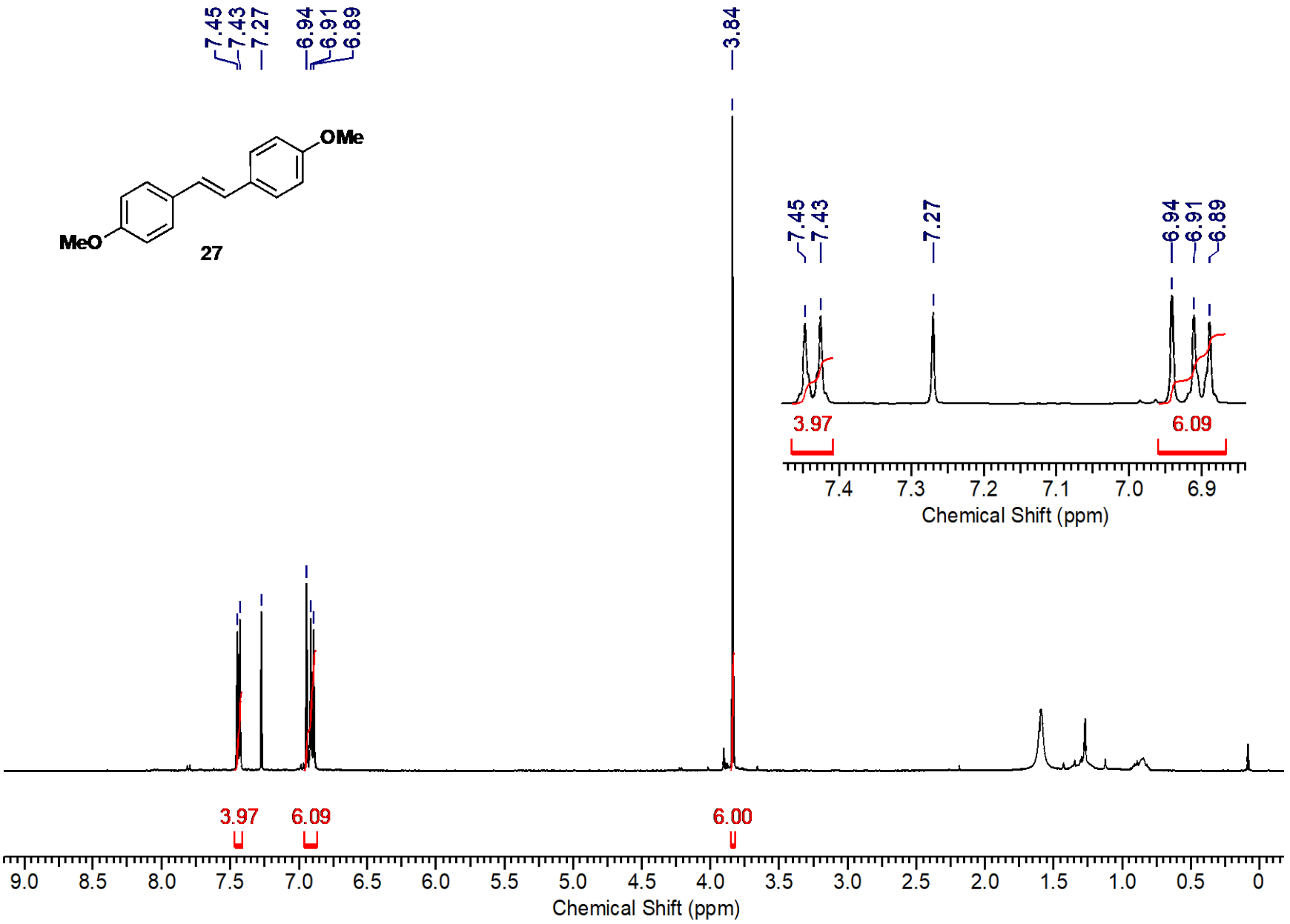

150.24
137.14
135.36
132.86
132.22
129.28
129.16
128.80
128.12
126.73
124.17
123.88
120.92
77.32
77.00
76.68
N
24
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

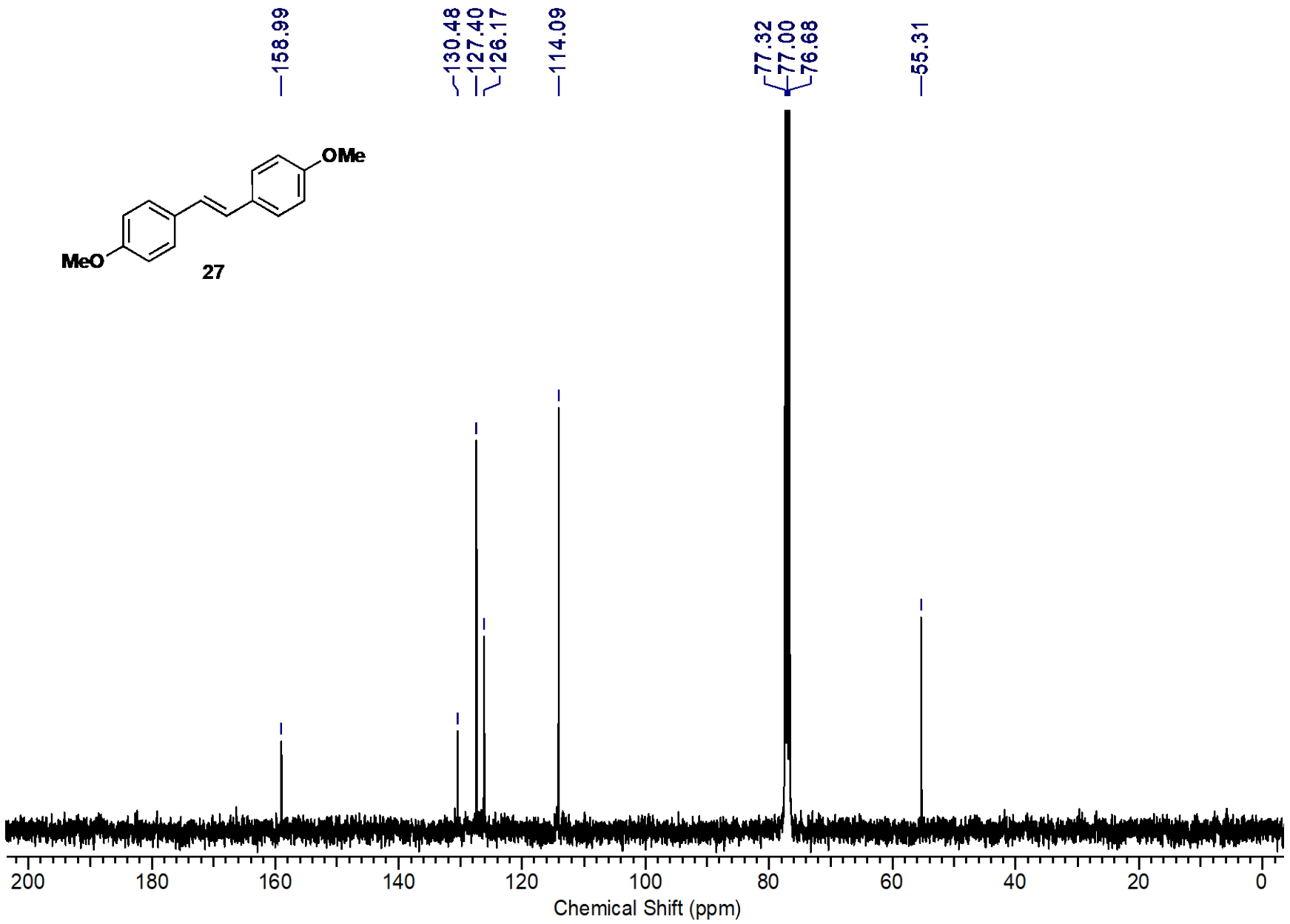

8.44
7.70
7.66
7.52
7.50
7.47
7.27
7.23
7.21
7.19
2.40
2.38
Me
N
Me
25
1.00
1.90
2.90
2.57
3.03
2.99
Chemical Shift (ppm)

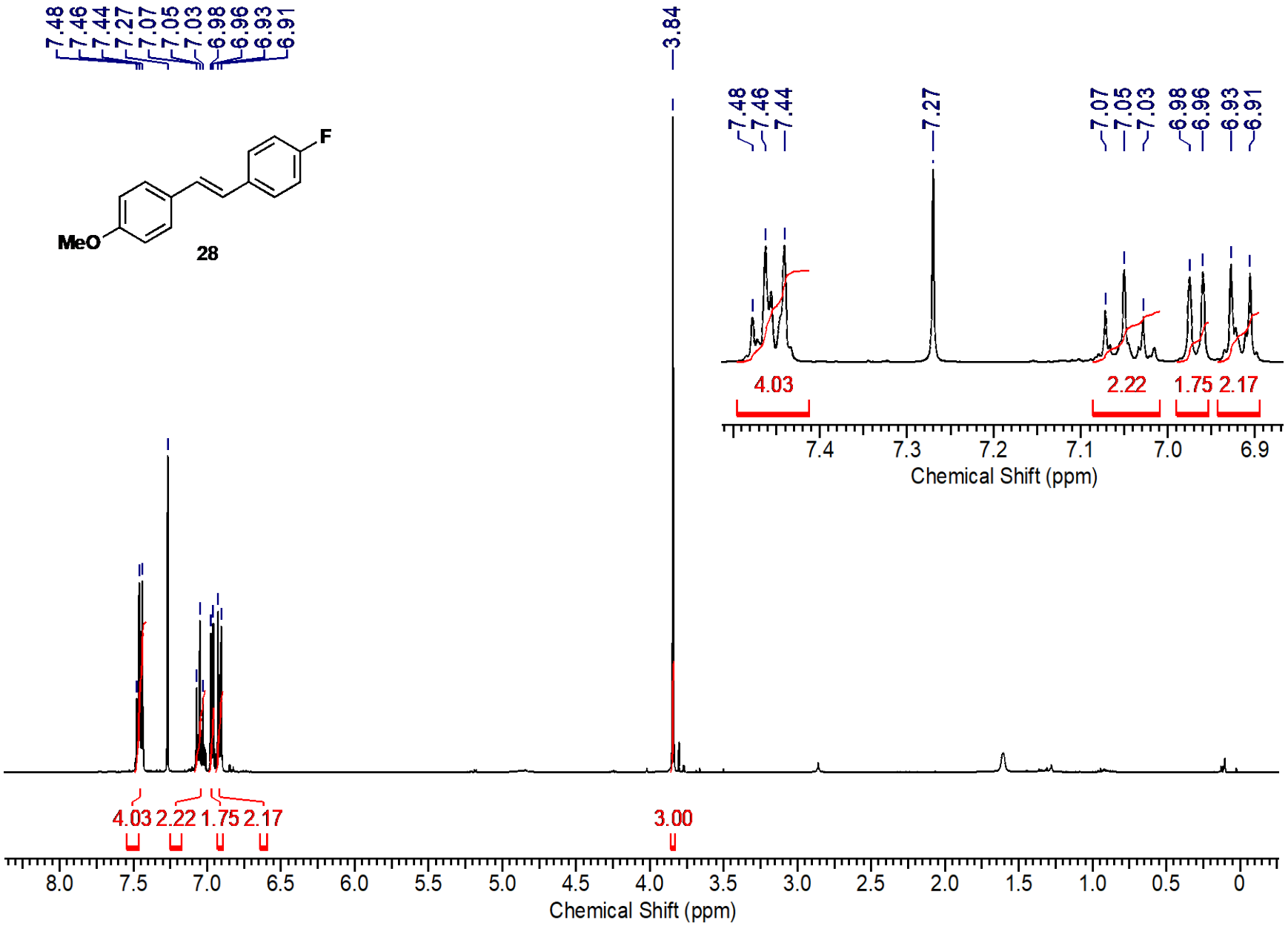

139.25
133.17
132.37
129.54
127.41
121.74
77.32
77.00
76.68
21.39
18.25
N
Me
Me
25
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

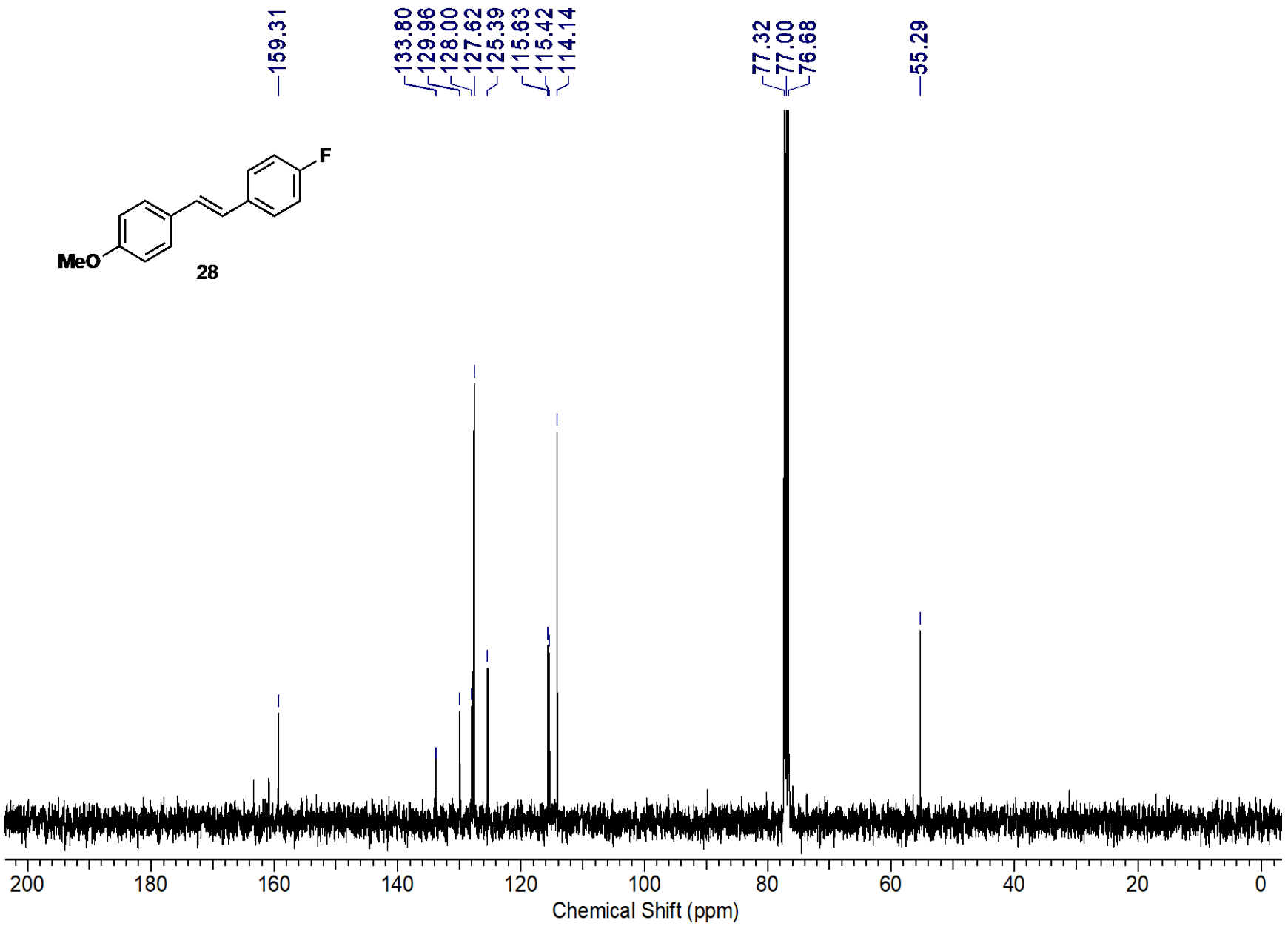

7.51
7.48
7.47
7.44
7.27
7.11
7.06
7.02
6.99
F
F
26
3.92
3.96
2.00
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

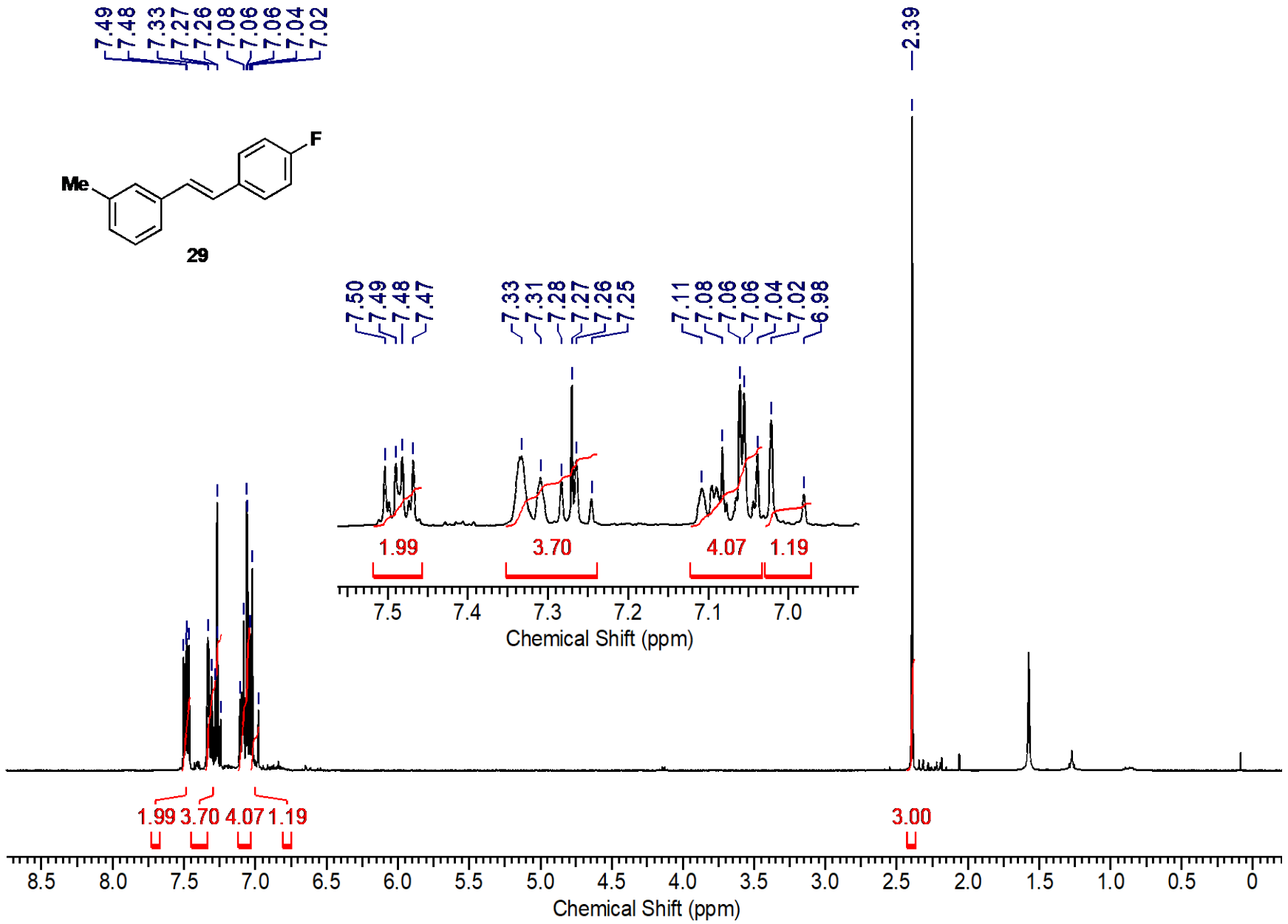

164.80
159.88
133.38
127.98
127.82
127.27
115.85
115.42
77.00
F
F
26
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

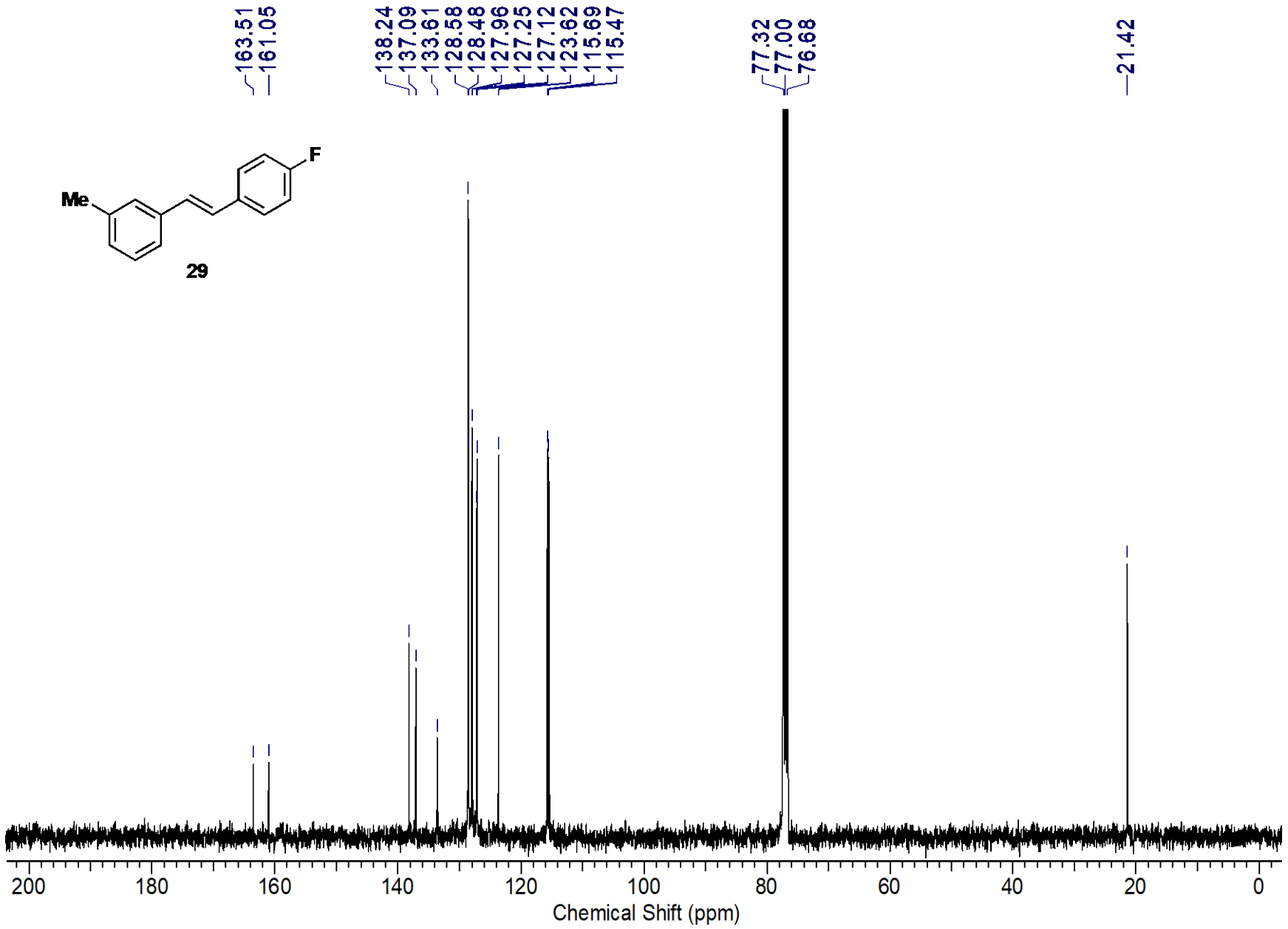

7.45
7.43
7.27
6.94
6.91
6.89
3.84
OMe
MeO
27
3.97
6.09
6.00
Chemical Shift (ppm)

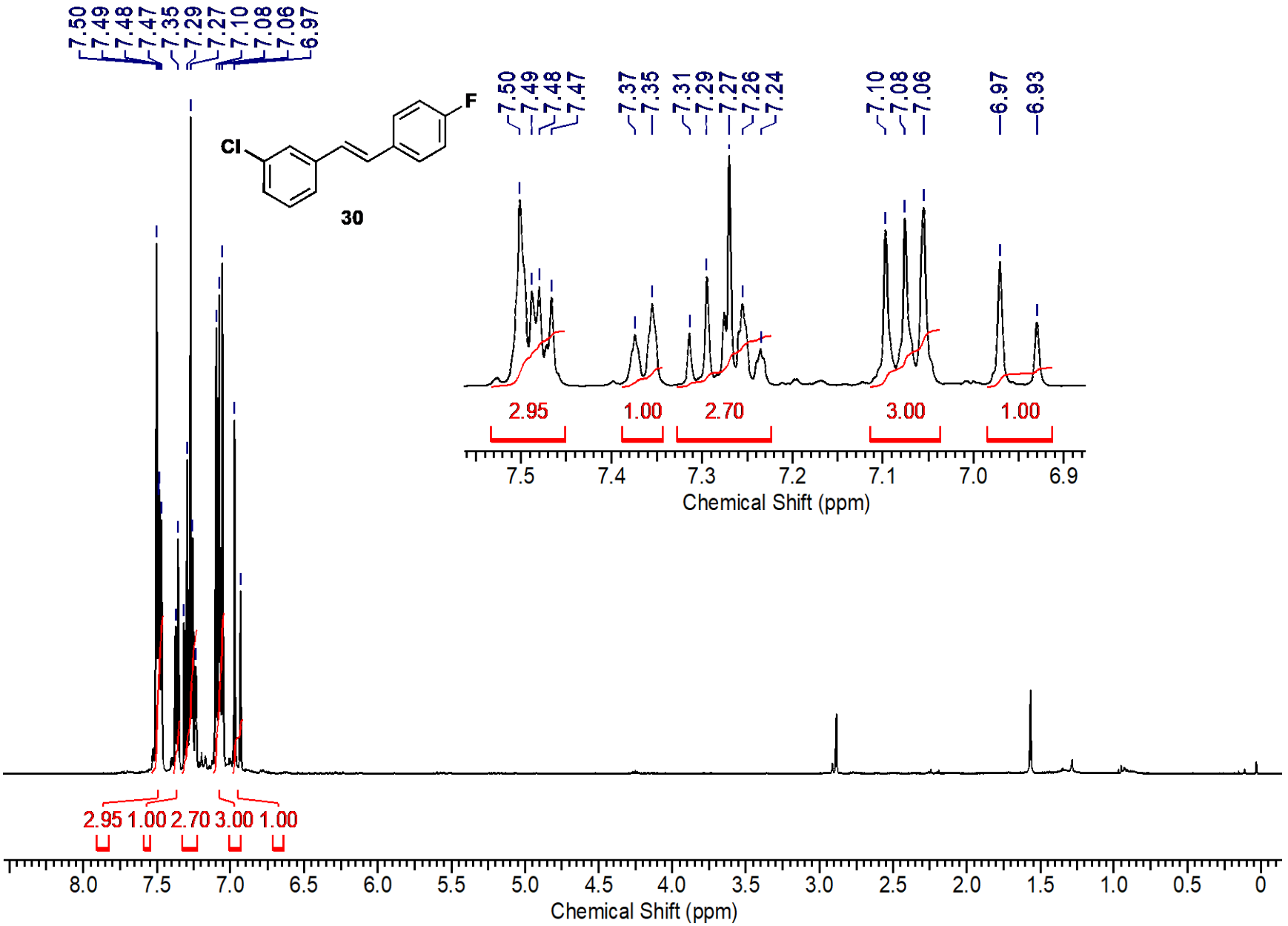

158.99
130.48
127.40
126.17
114.09
77.32
77.00
76.68
55.31
OMe
MeO
27
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

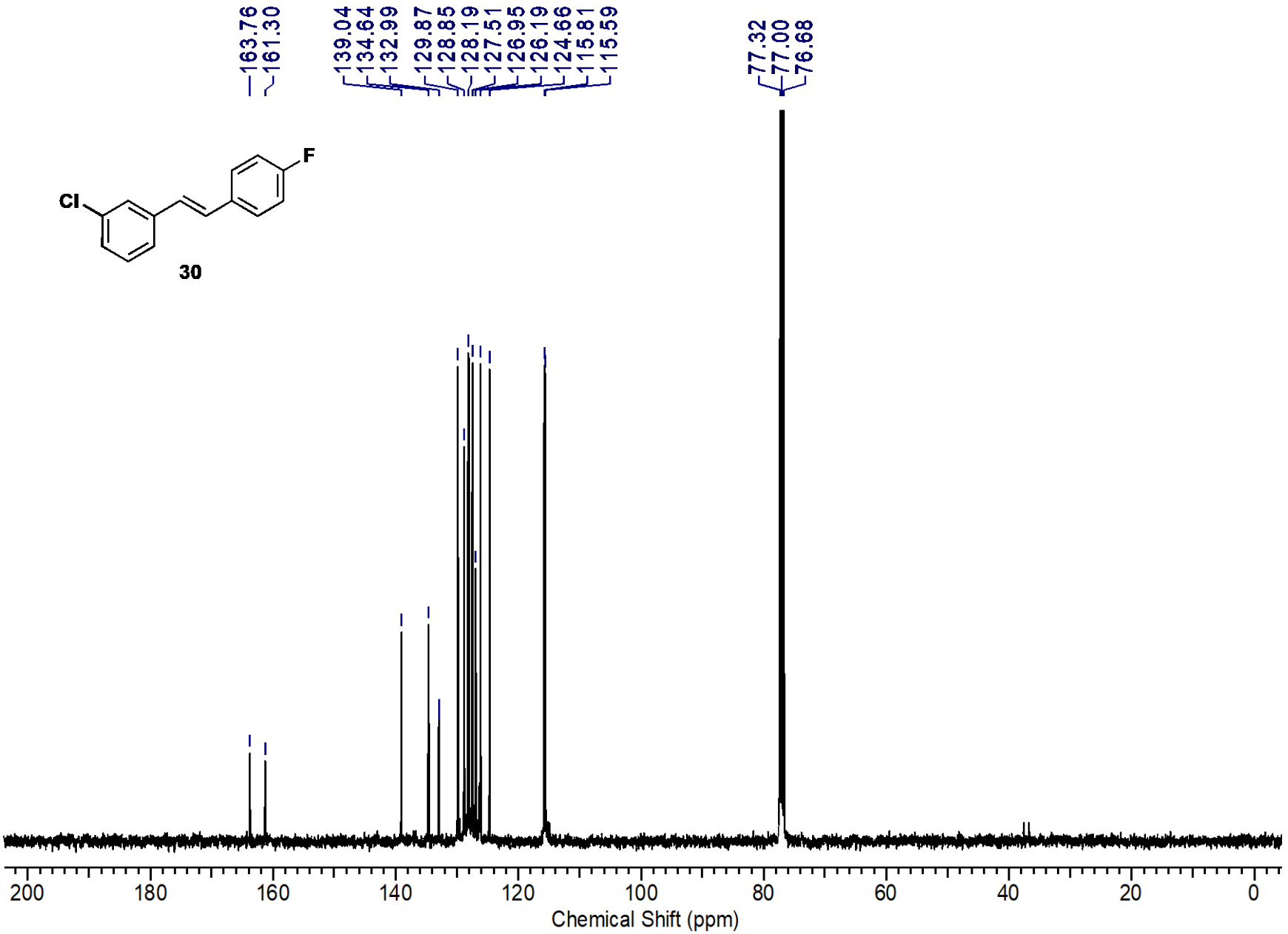

7.48
7.46
7.44
7.27
7.07
7.05
7.03
6.98
6.96
6.93
6.91
3.84
F
MeO
28
4.03
2.22
1.75
2.17
3.00
Chemical Shift (ppm)

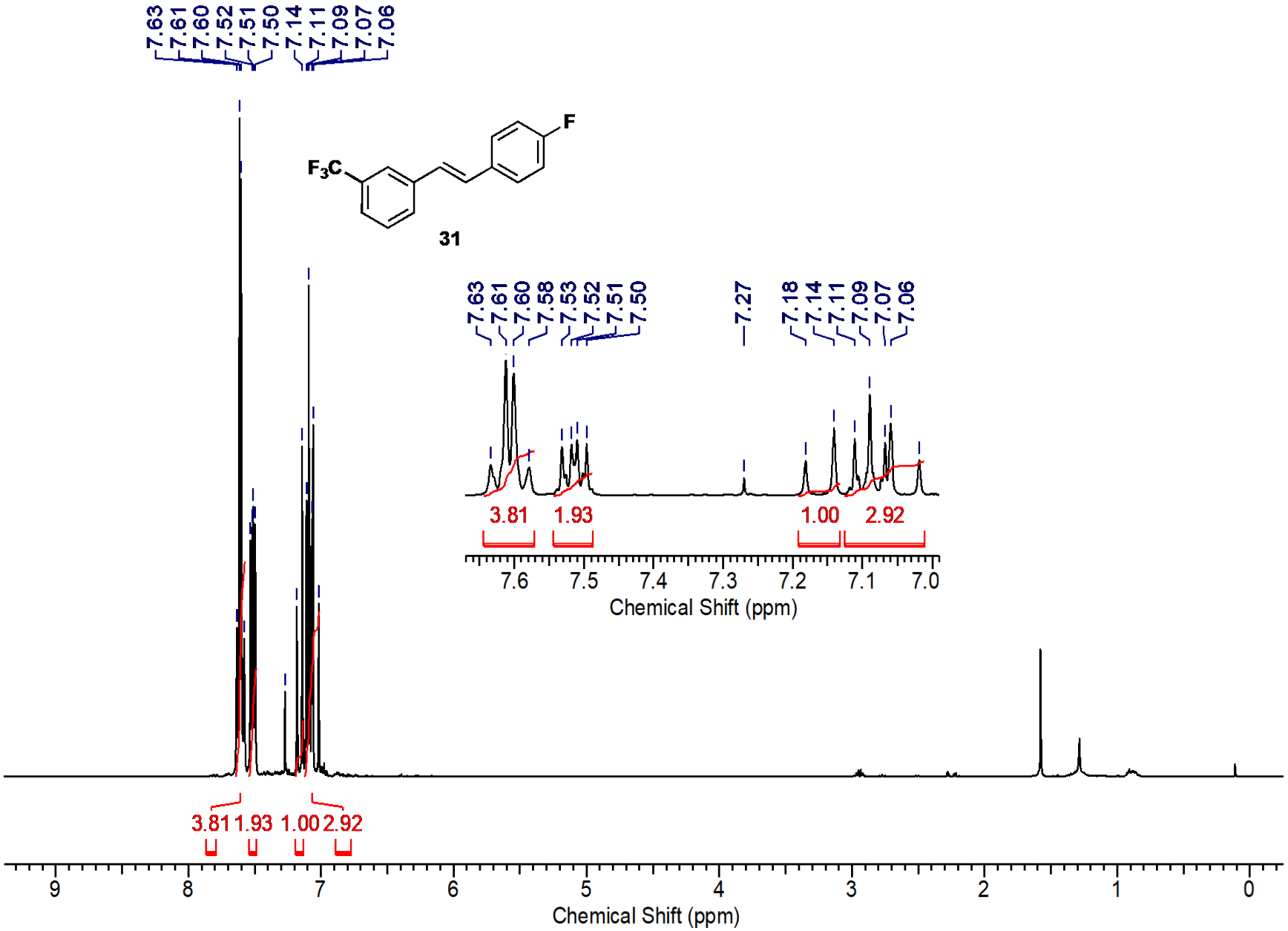

159.31
133.80
129.96
128.00
127.62
125.39
115.63
115.42
114.14
77.32
77.00
76.68
55.29
F
MeO
28
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

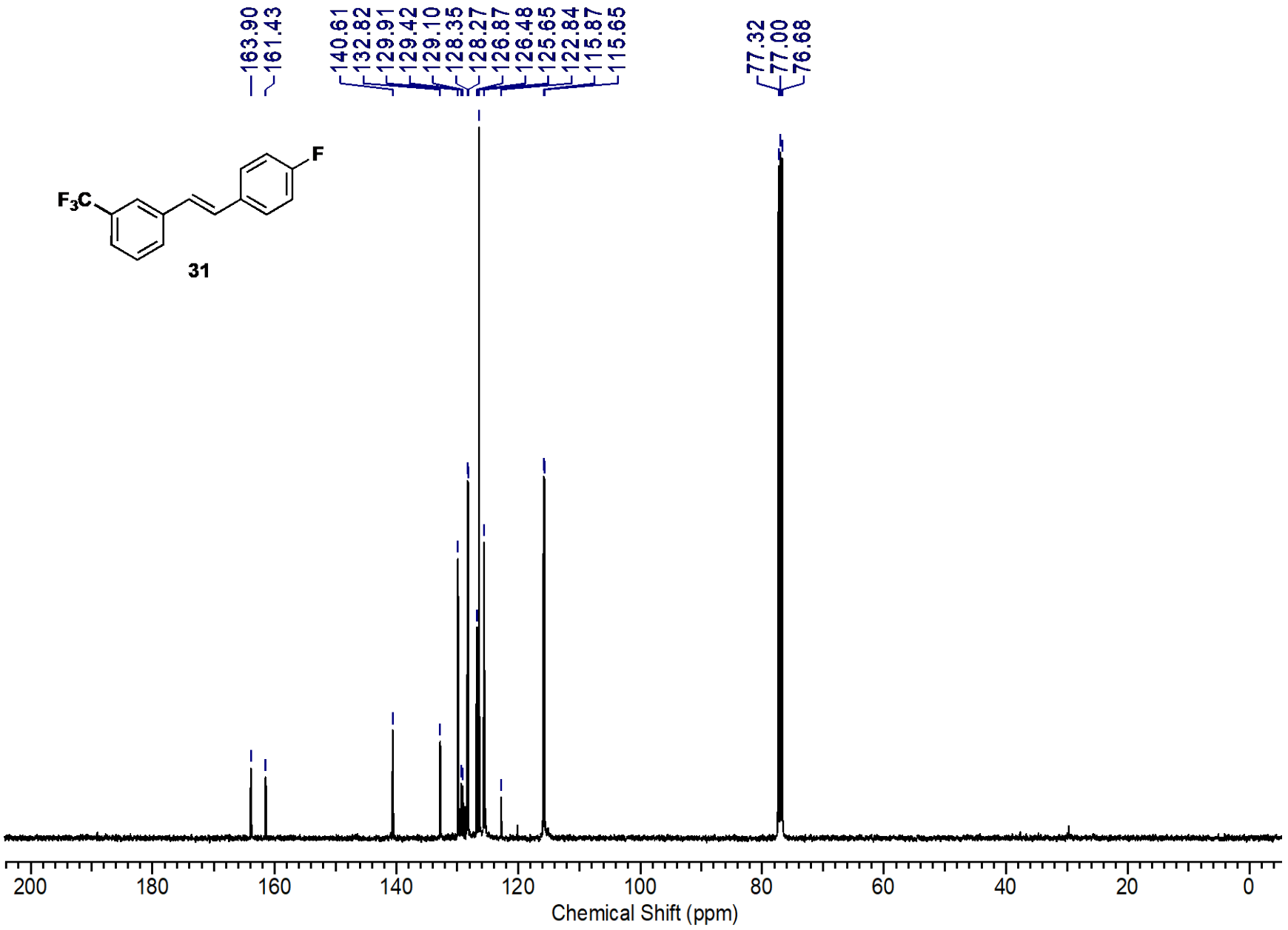

7.49
7.48
7.33
7.27
7.26
7.08
7.06
7.06
7.04
7.02
2.39
F
Me
29
7.50
7.49
7.48
7.47
7.33
7.31
7.28
7.27
7.26
7.25
7.11
7.08
7.06
7.06
7.04
7.02
6.98
1.99
3.70
4.07
1.19
7.5
7.4
7.3
7.2
7.1
7.0
Chemical Shift (ppm)
1.99 3.70 4.07 1.19
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

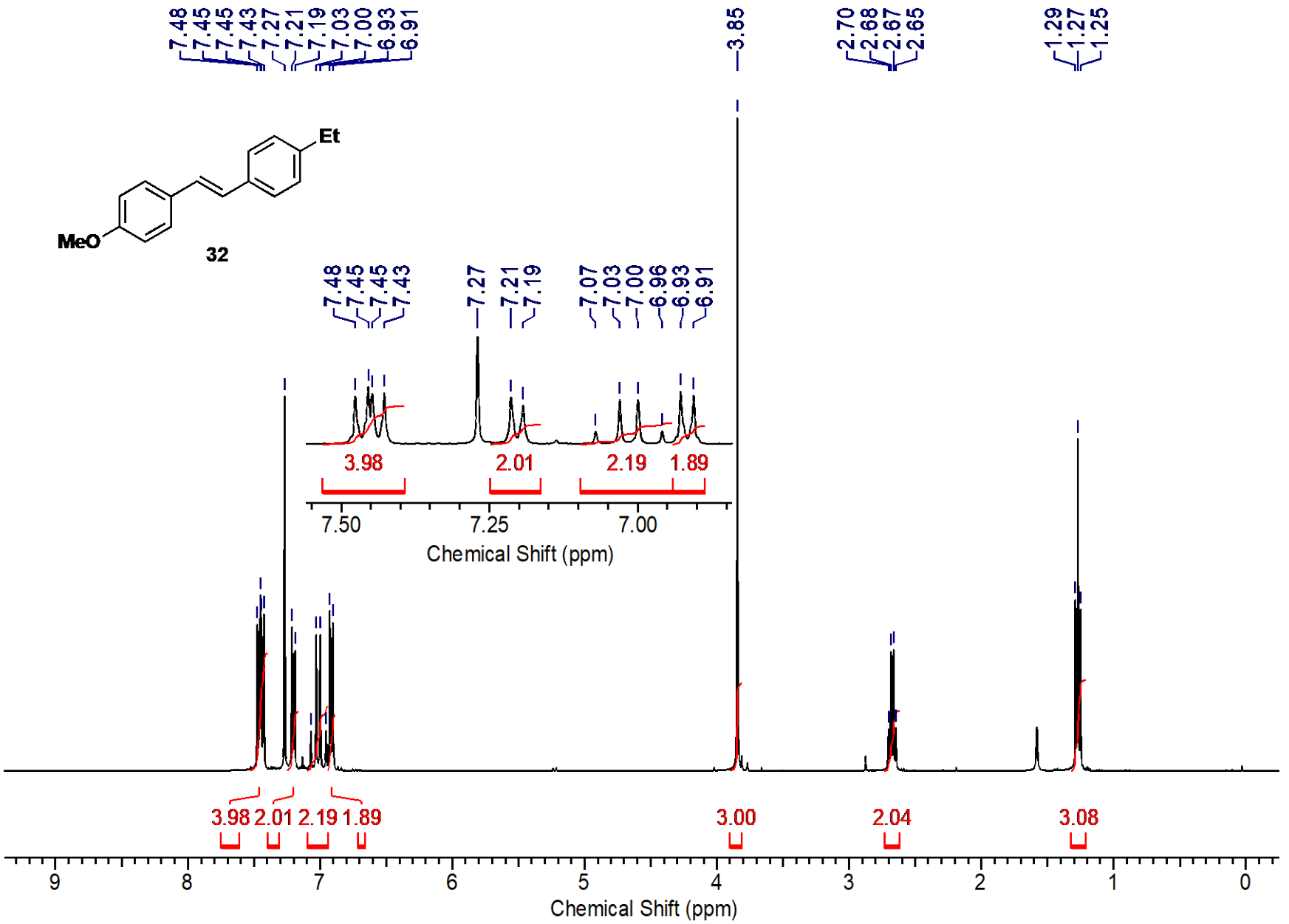

163.51
161.05
138.24
137.09
133.61
128.58
128.48
127.96
127.25
127.12
123.62
115.69
115.47
77.32
77.00
76.68
21.42
F
Me
29
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

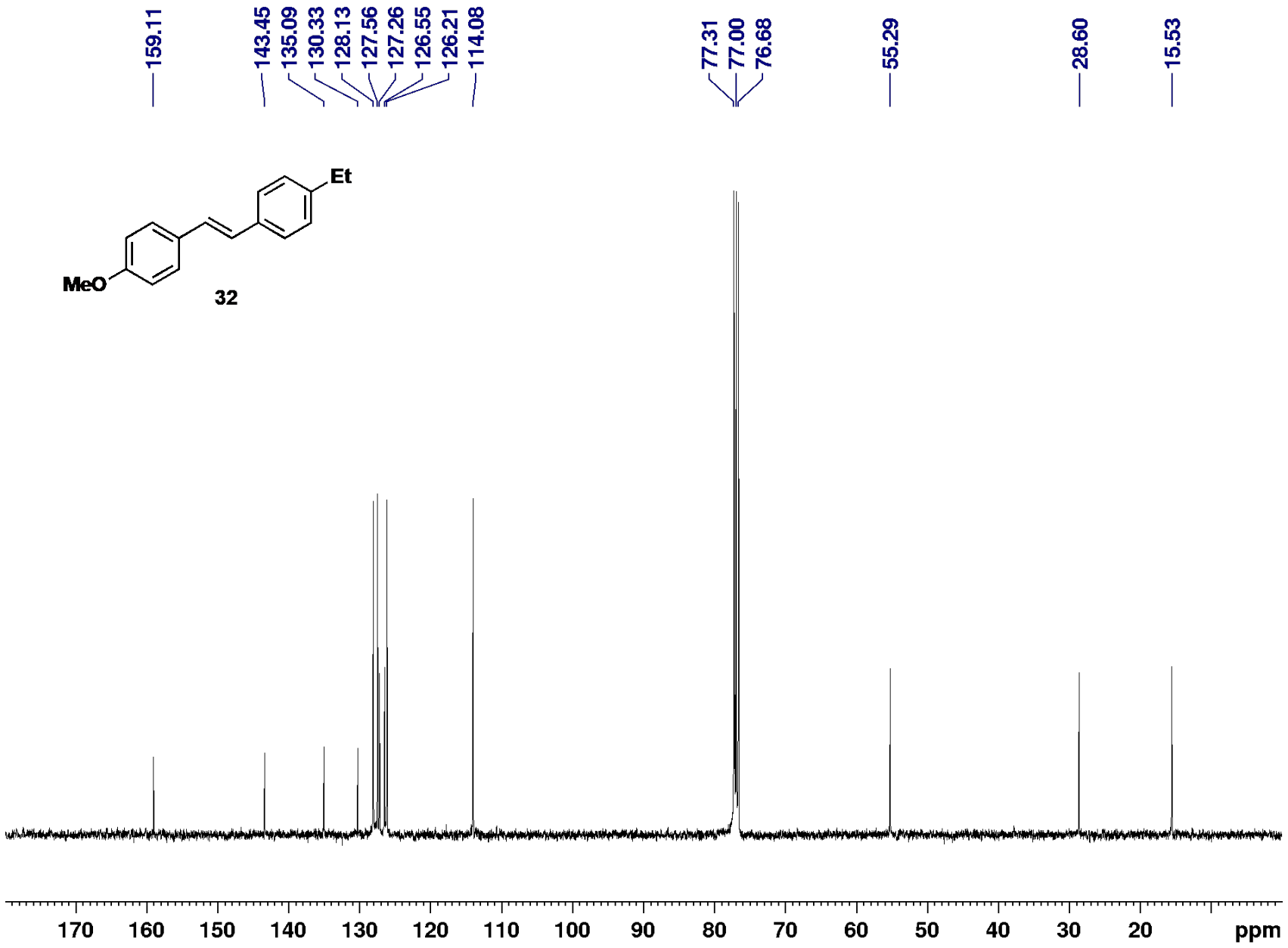

7.50
7.49
7.48
7.47
7.35
7.29
7.27
7.10
7.08
7.06
6.97
Cl
F
30
7.50
7.49
7.48
7.47
7.37
7.35
7.31
7.29
7.27
7.26
7.24
7.10
7.08
7.06
6.97
6.93
2.95
1.00
2.70
3.00
1.00
7.5
7.4
7.3
7.2
7.1
7.0
6.9
Chemical Shift (ppm)
2.95 1.00 2.70 3.00 1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

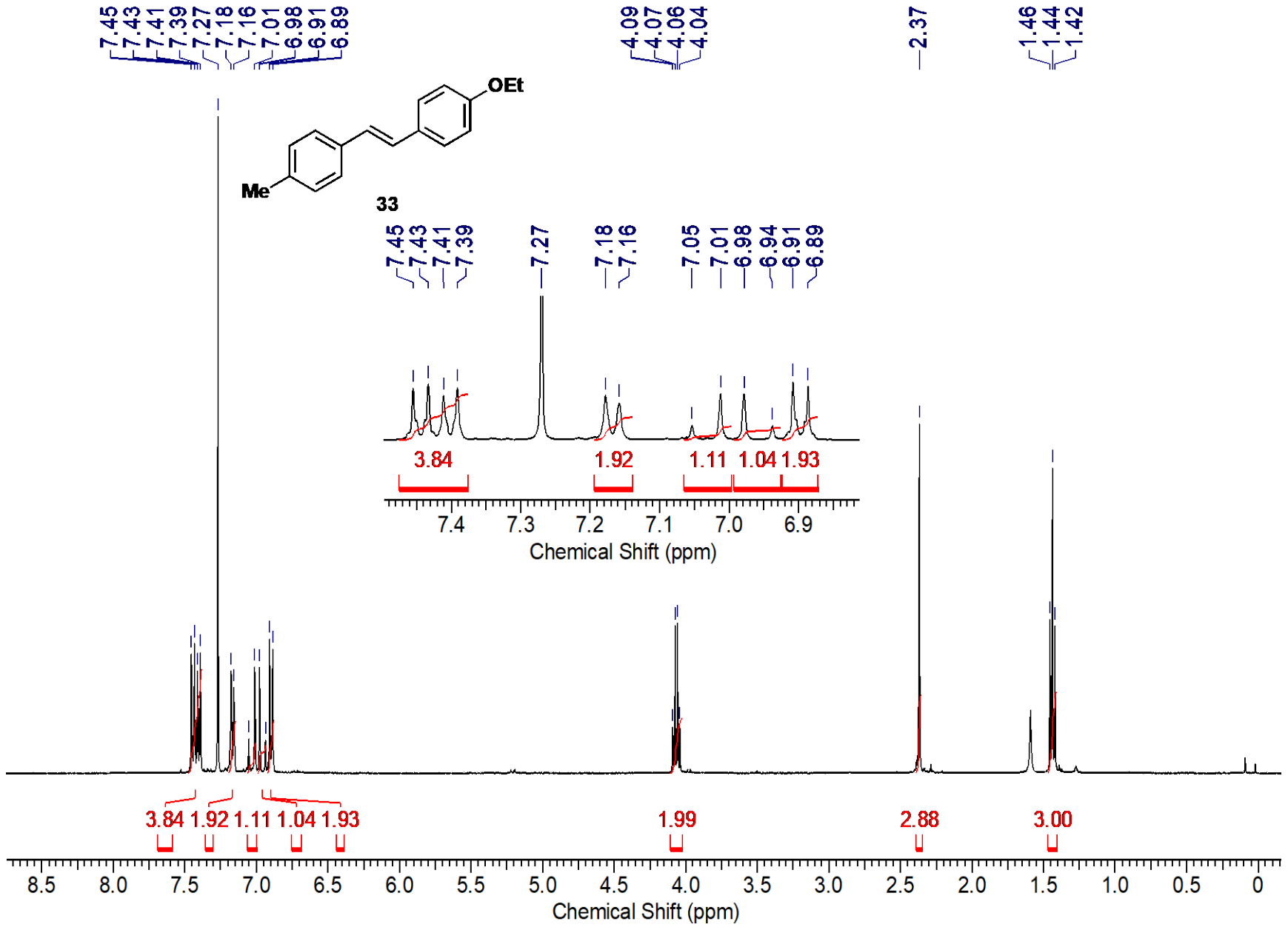

163.76
161.30
139.04
134.64
132.99
129.87
128.85
128.19
127.51
126.95
126.19
124.66
115.81
115.59
77.32
77.00
76.68
Cl
F
30
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

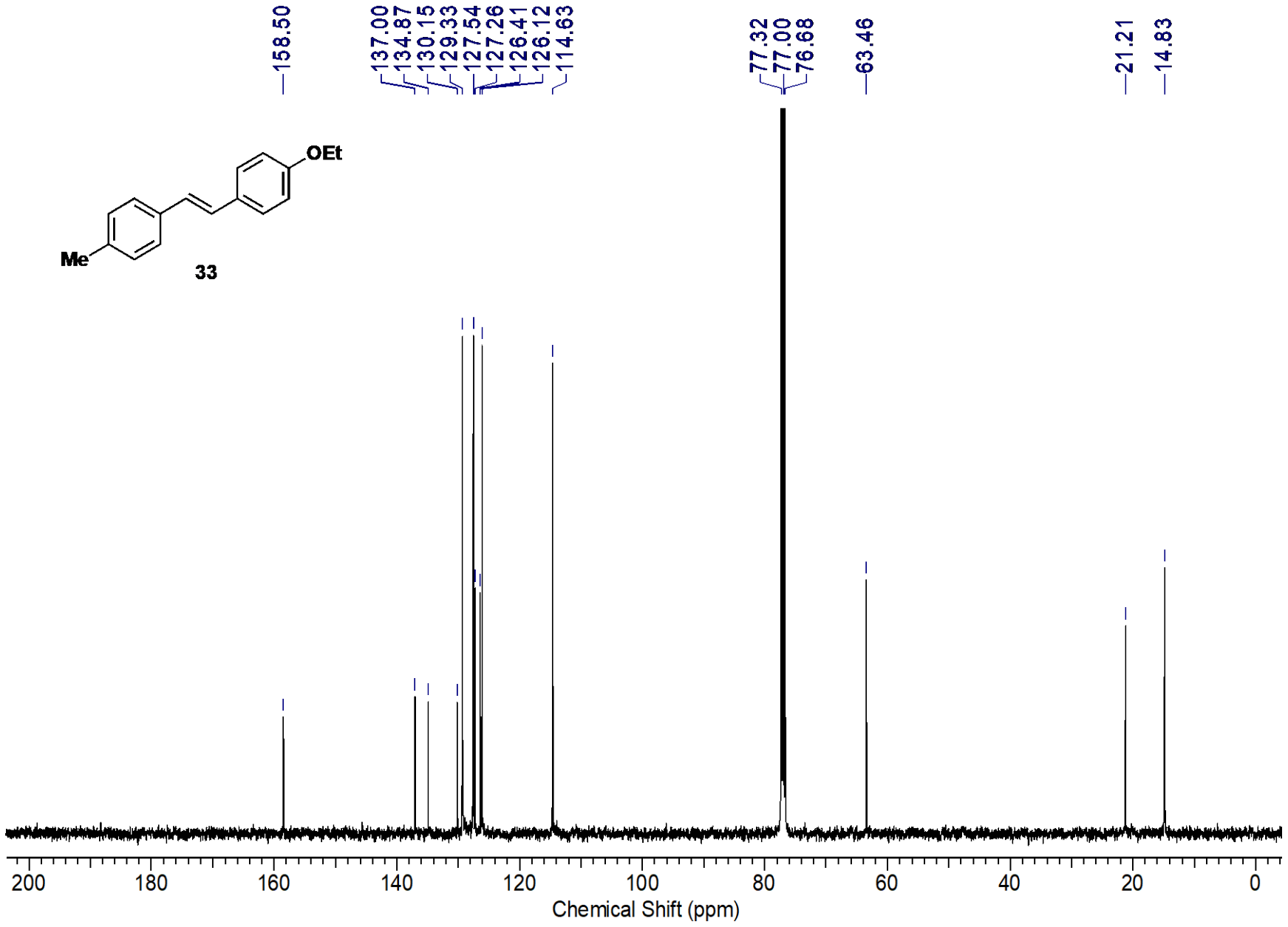

7.63
7.61
7.60
7.52
7.51
7.50
7.14
7.11
7.09
7.07
7.06
F
F3C
31
7.63
7.61
7.60
7.58
7.53
7.52
7.51
7.50
7.27
7.18
7.14
7.11
7.09
7.07
7.06
3.81
1.93
1.00
2.92
7.6
7.5
7.4
7.3
7.2
7.1
7.0
Chemical Shift (ppm)
3.81
1.93
1.00
2.92
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

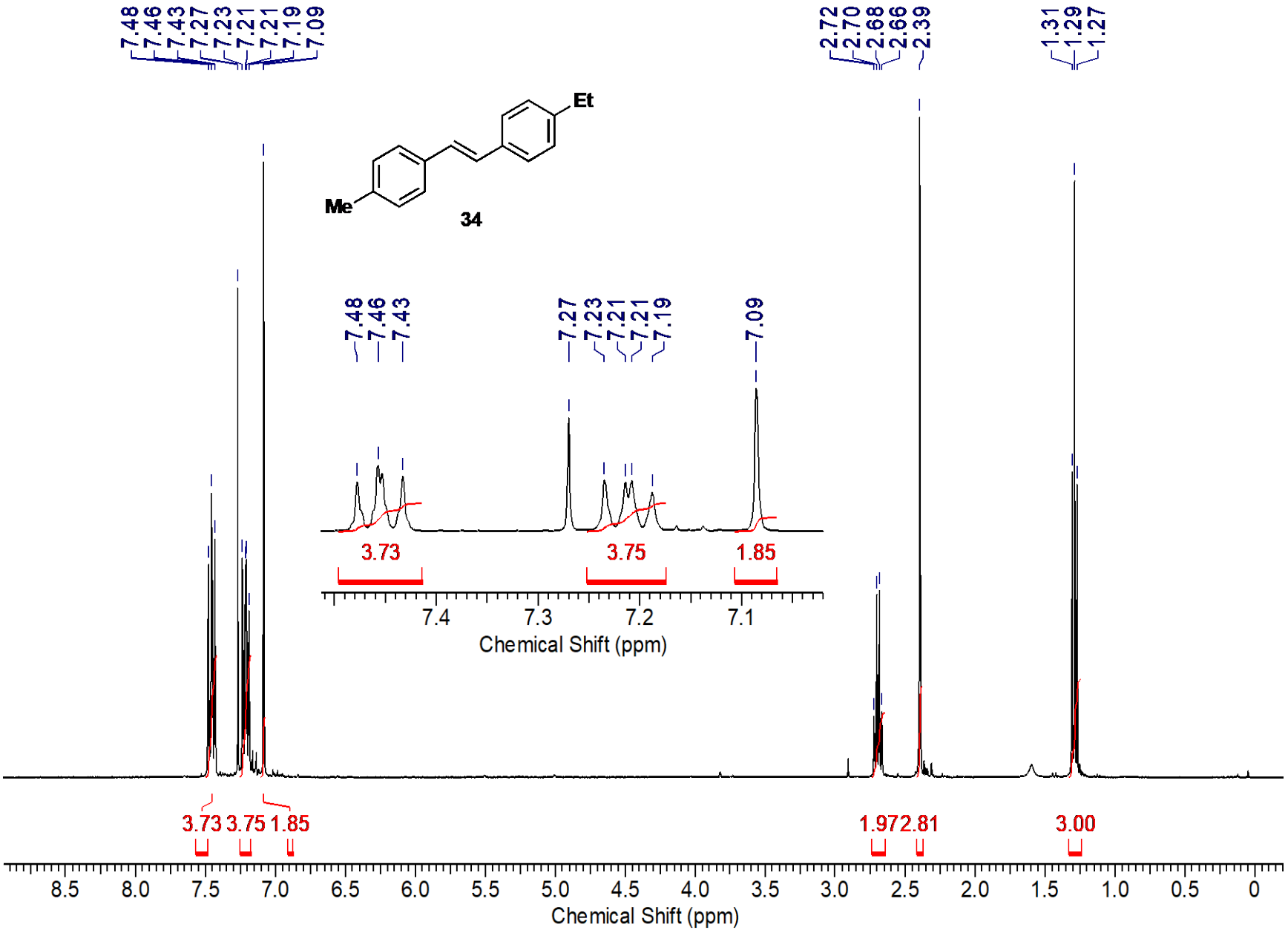

163.90
161.43
140.61
132.82
129.91
129.42
129.10
128.35
128.27
126.87
126.48
125.65
122.84
115.87
115.65
77.32
77.00
76.68
F
F3C
31
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

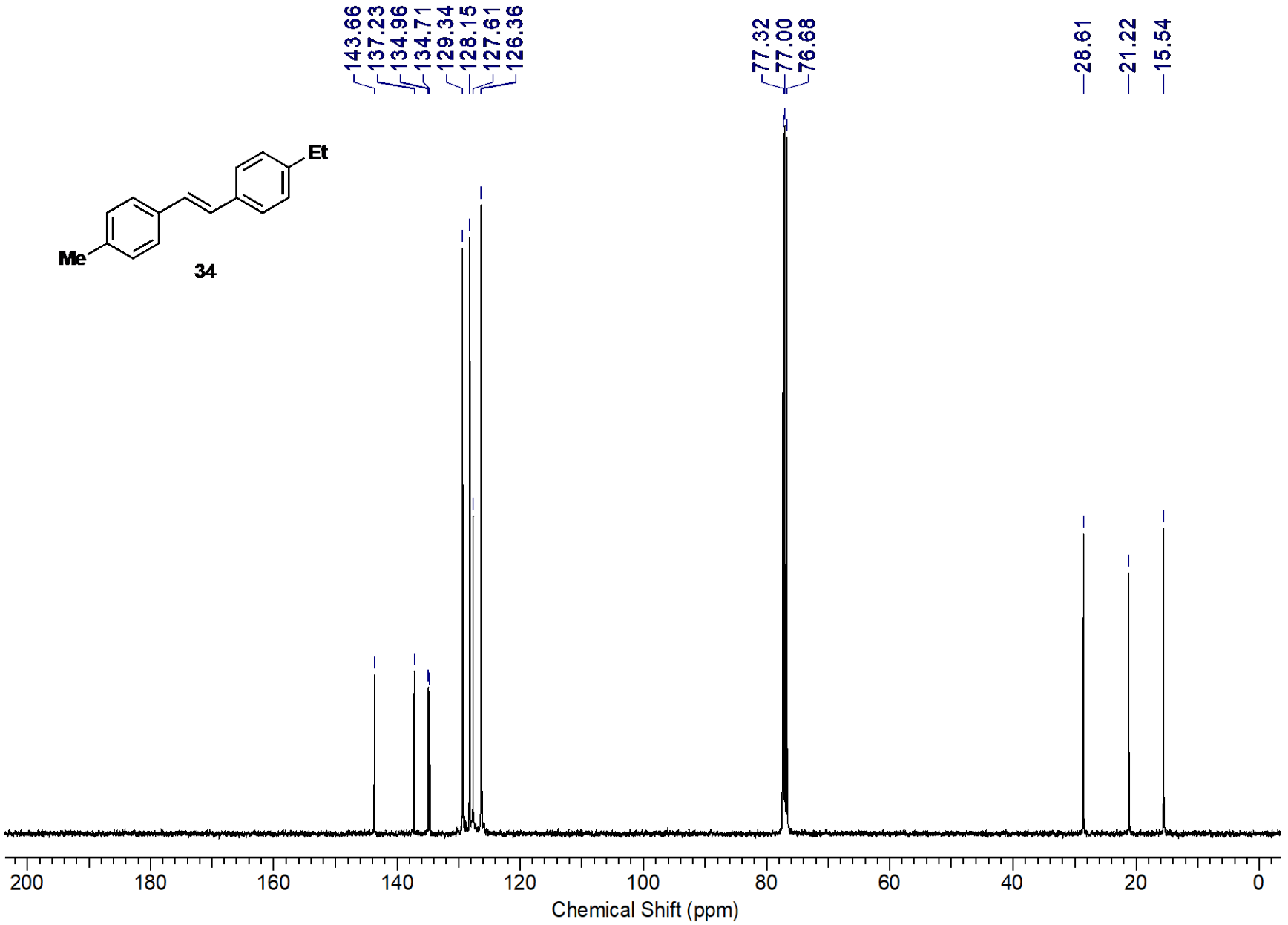

7.48
7.45
7.45
7.43
7.27
7.21
7.19
7.03
7.00
6.93
6.91
3.85
2.70
2.68
2.67
2.65
1.29
1.27
1.25
Et
MeO
32
3.98
2.01
2.19
1.89
7.50
7.25
7.00
Chemical Shift (ppm)
3.98
2.01
2.19
1.89
3.00
2.04
3.08
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

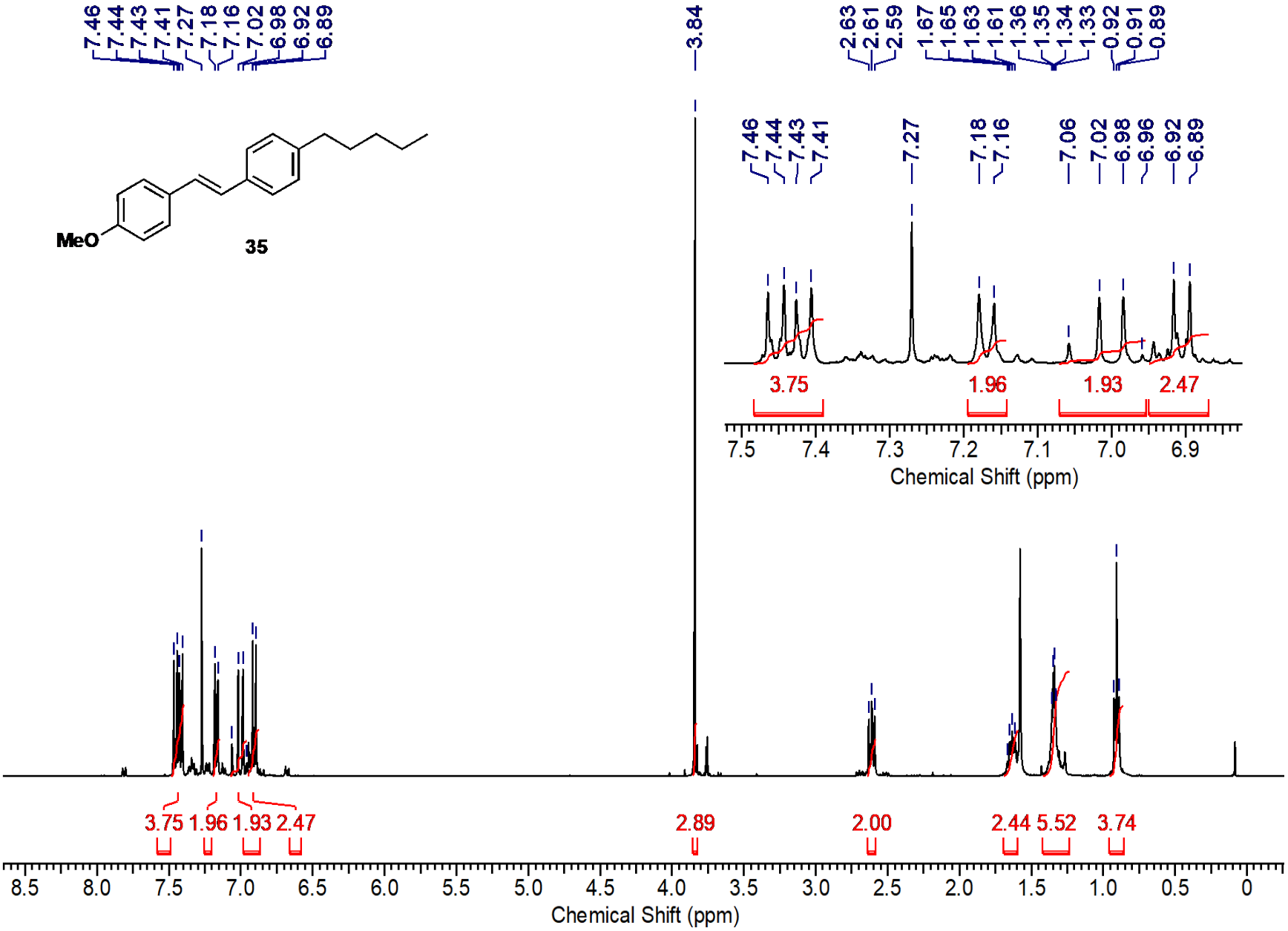

159.11
143.45
135.09
130.33
128.13
127.56
127.26
126.55
126.21
114.08
77.31
77.00
76.68
55.29
28.60
15.53
Et
MeO
32
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

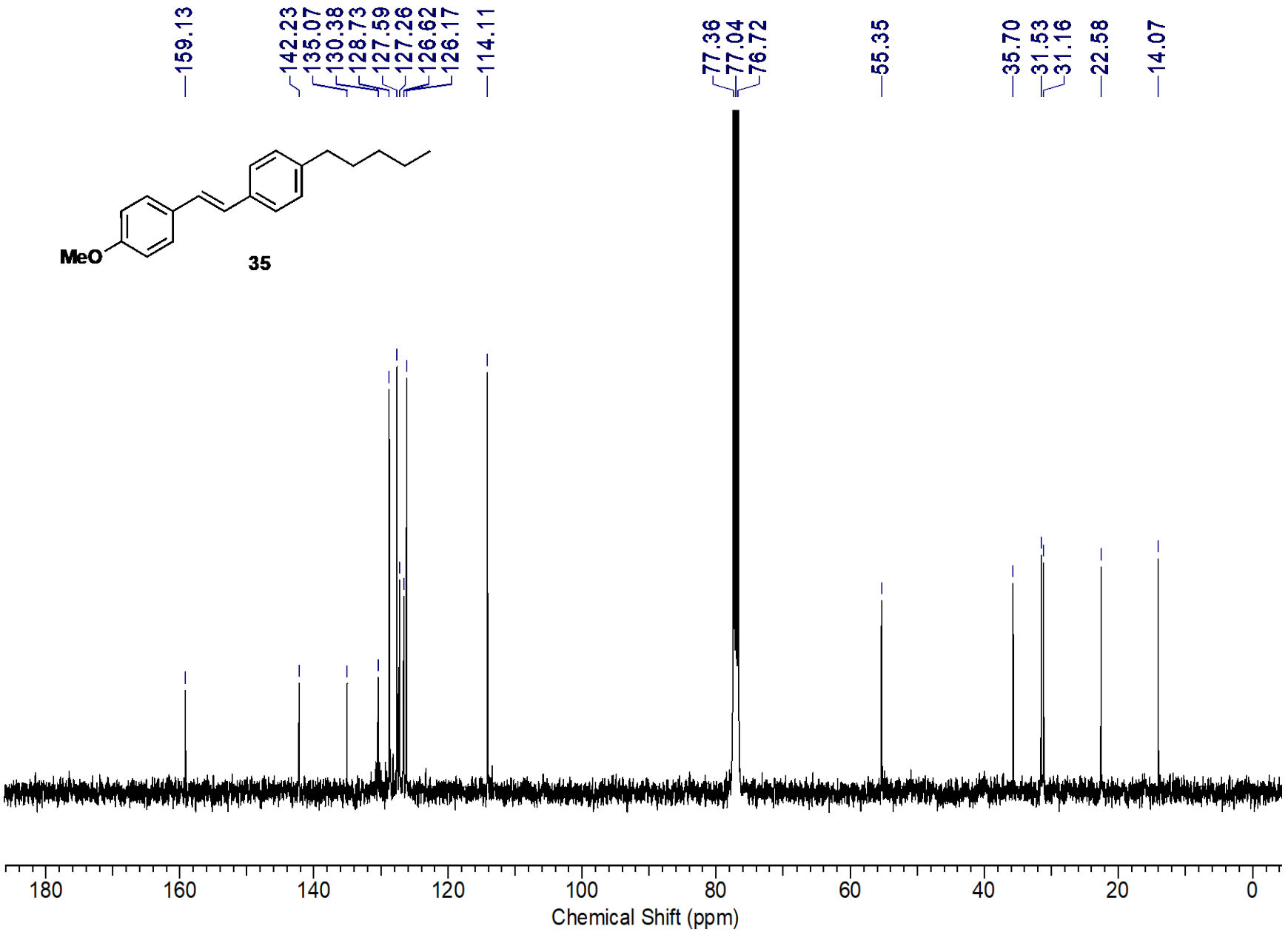

7.45
7.43
7.41
7.39
7.27
7.18
7.16
7.01
6.98
6.91
6.89
4.09
4.07
4.06
4.04
2.37
1.46
1.44
1.42
OEt
Me
33
7.45
7.43
7.41
7.39
7.27
7.18
7.16
7.05
7.01
6.98
6.94
6.91
6.89
3.84
1.92
1.11
1.04
1.93
7.4
7.3
7.2
7.1
7.0
6.9
Chemical Shift (ppm)
3.84
1.92
1.11
1.04
1.93
1.99
2.88
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

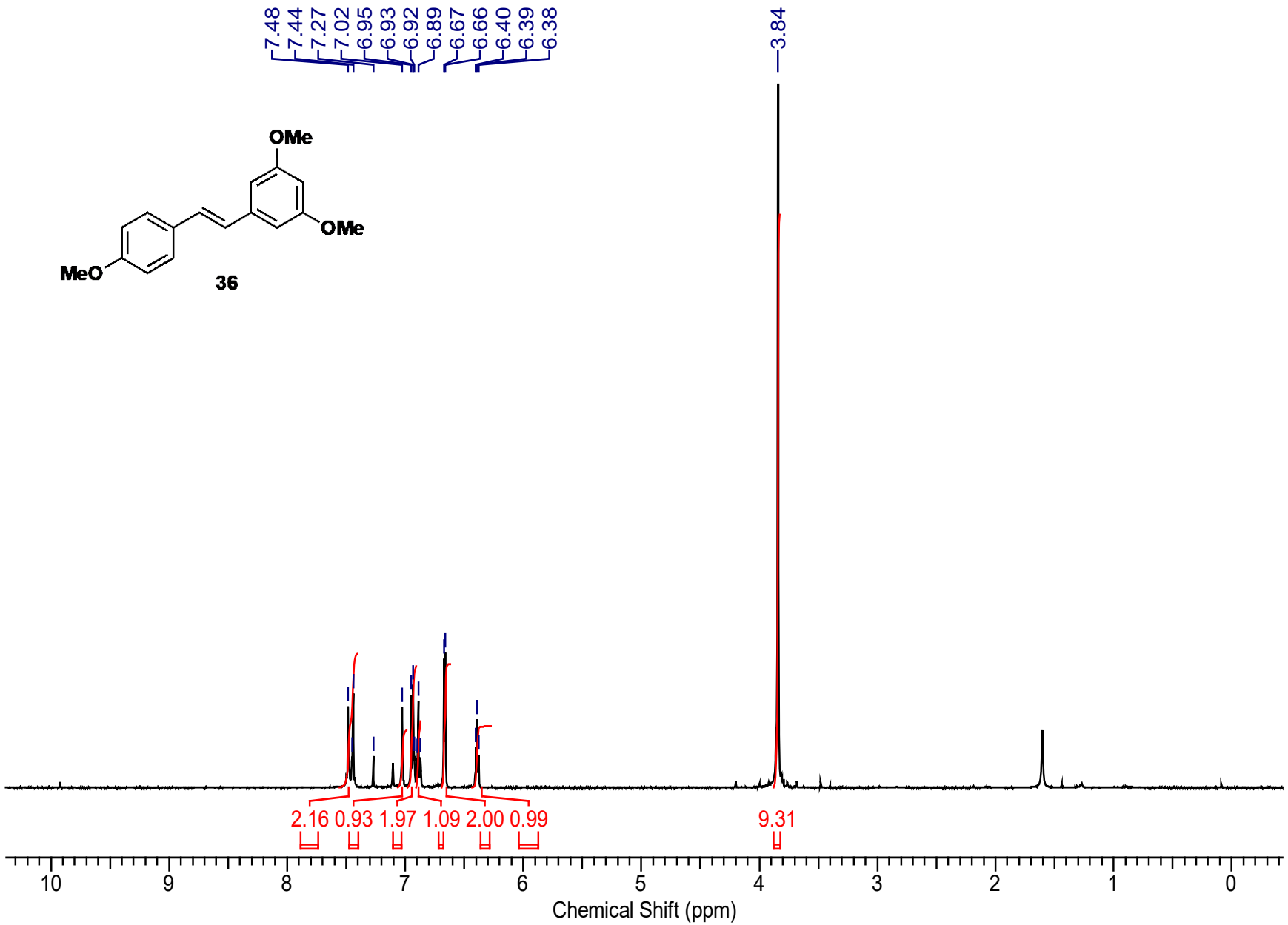

158.50
137.00
134.87
130.15
129.33
127.54
127.26
126.41
126.12
114.63
77.32
77.00
76.68
63.46
21.21
14.83
OEt
Me
33
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

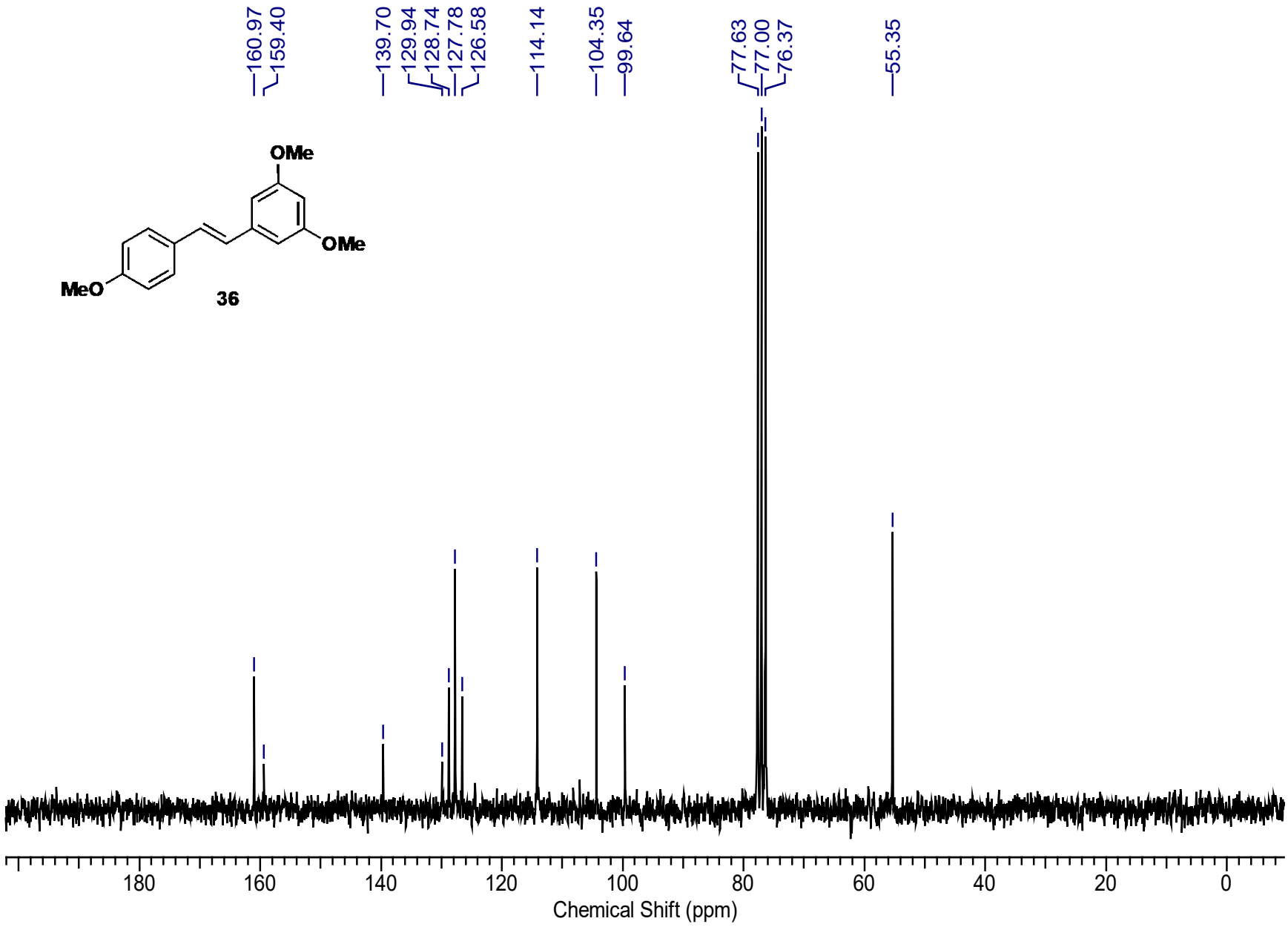

7.48
7.46
7.43
7.27
7.23
7.21
7.21
7.19
7.09
2.72
2.70
2.68
2.66
2.39
1.31
1.29
1.27
Et
Me
34
3.73
3.75
1.85
7.4
7.3
7.2
7.1
Chemical Shift (ppm)
3.73
3.75
1.85
1.97
2.81
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

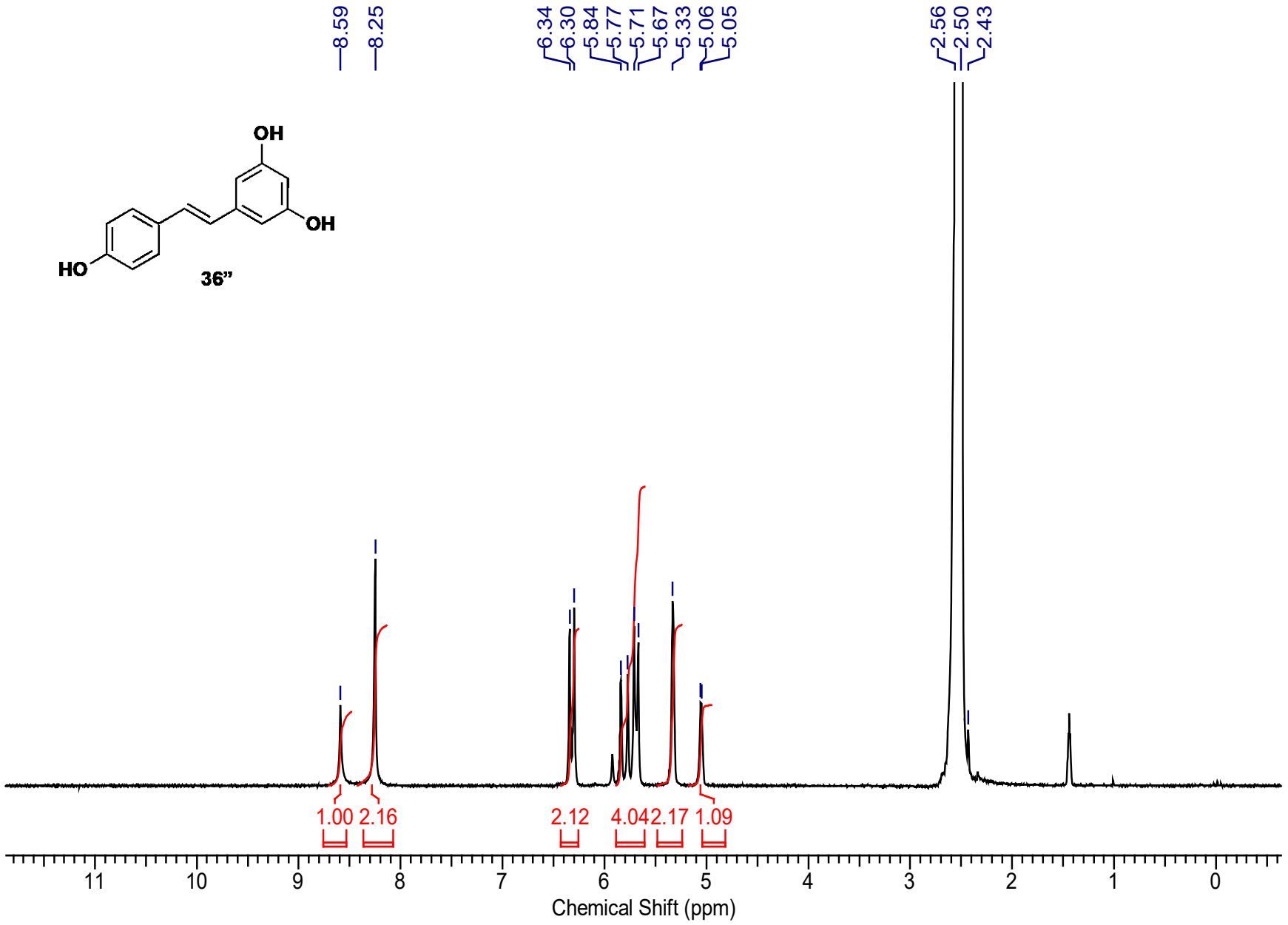

143.66
137.23
134.96
134.71
129.34
128.15
127.61
126.36
77.32
77.00
76.68
28.61
21.22
15.54
Et
Me
34
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

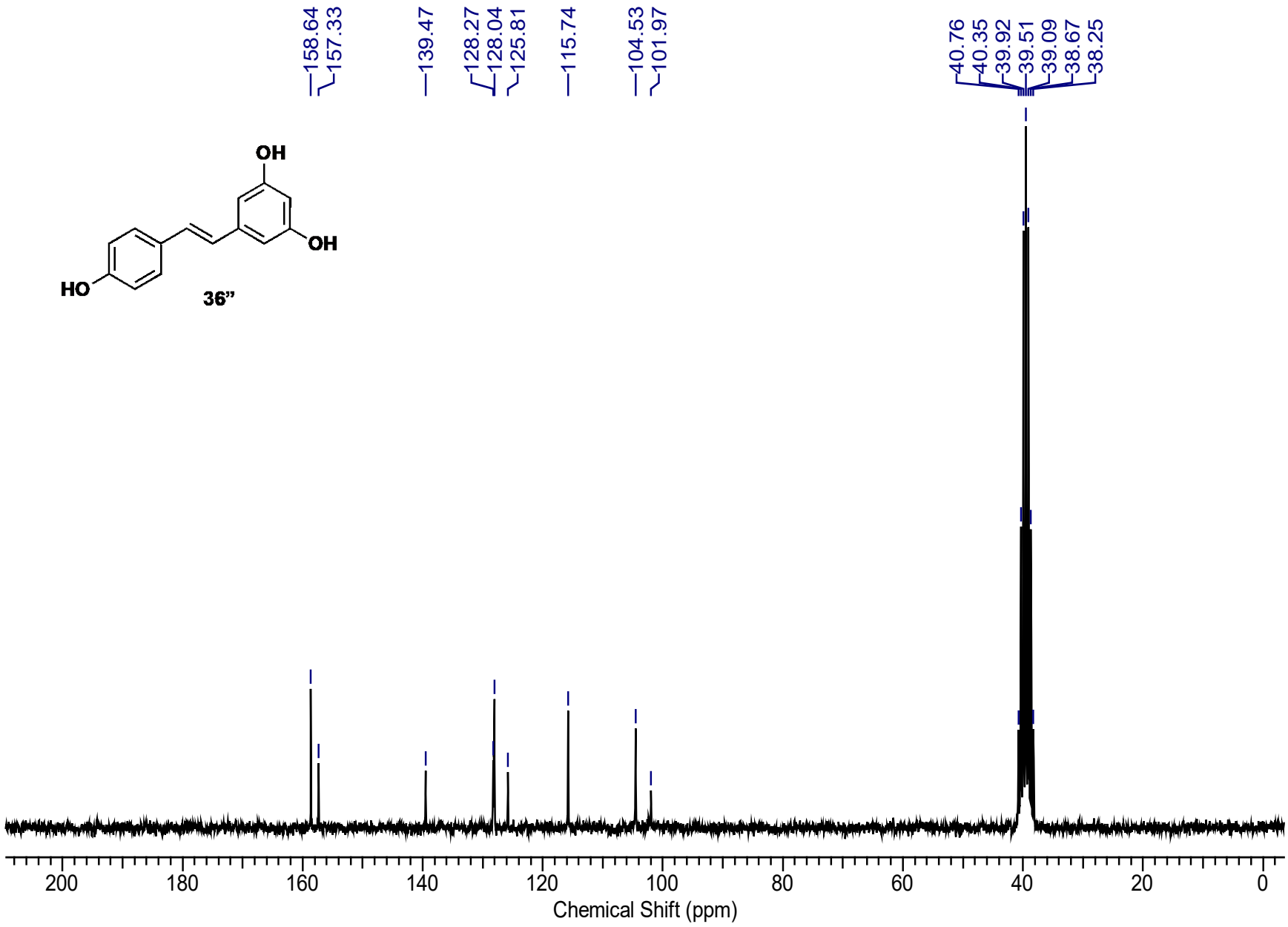

7.46
7.44
7.43
7.41
7.27
7.18
7.16
7.02
6.98
6.92
6.89
3.84
2.63
2.61
2.59
1.67
1.65
1.63
1.61
1.36
1.35
1.34
1.33
0.92
0.91
0.89
MeO
35
3.75
1.96
1.93
2.47
Chemical Shift (ppm)
2.89
2.00
2.44
5.52
3.74
Chemical Shift (ppm)

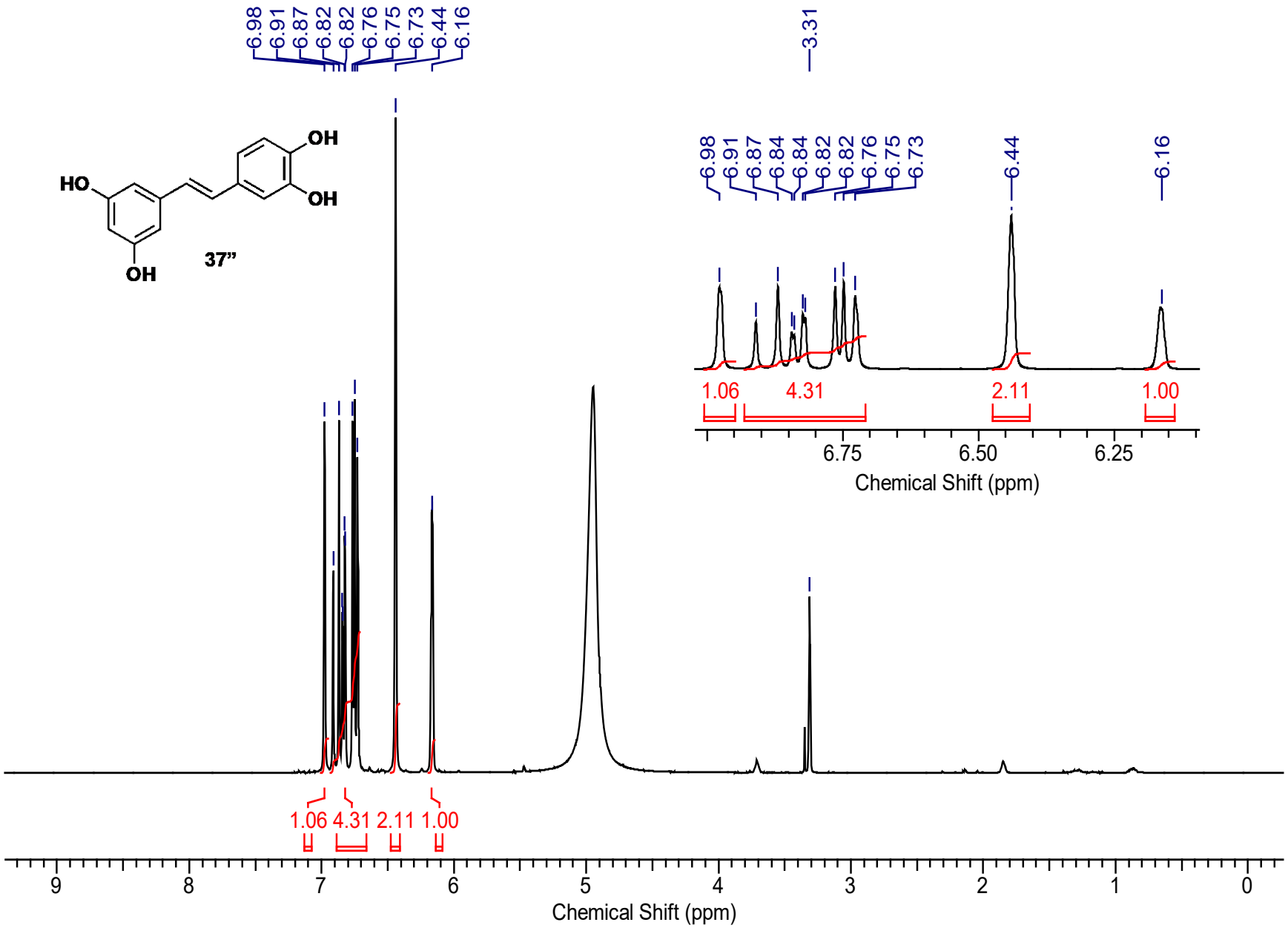

159.13
142.23
135.07
130.38
128.73
127.59
127.26
126.62
126.17
114.11
77.36
77.04
76.72
55.35
35.70
31.53
31.16
22.58
14.07
MeO
35
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

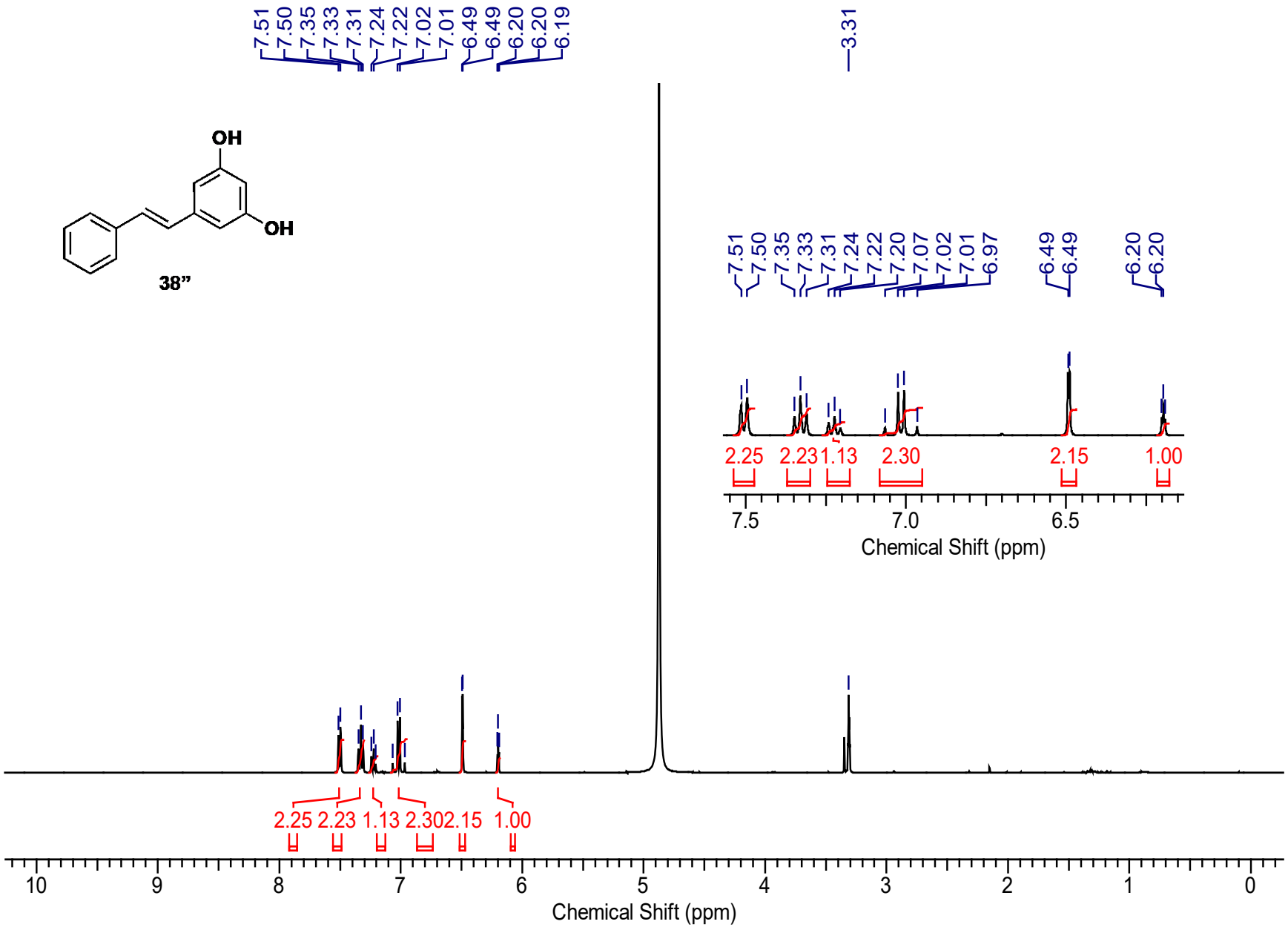

7.48
7.44
7.27
7.02
6.95
6.93
6.92
6.89
6.67
6.66
6.40
6.39
6.38
3.84
OMe
OMe
MeO
36
2.16 0.93 1.97 1.09 2.00 0.99
9.31
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

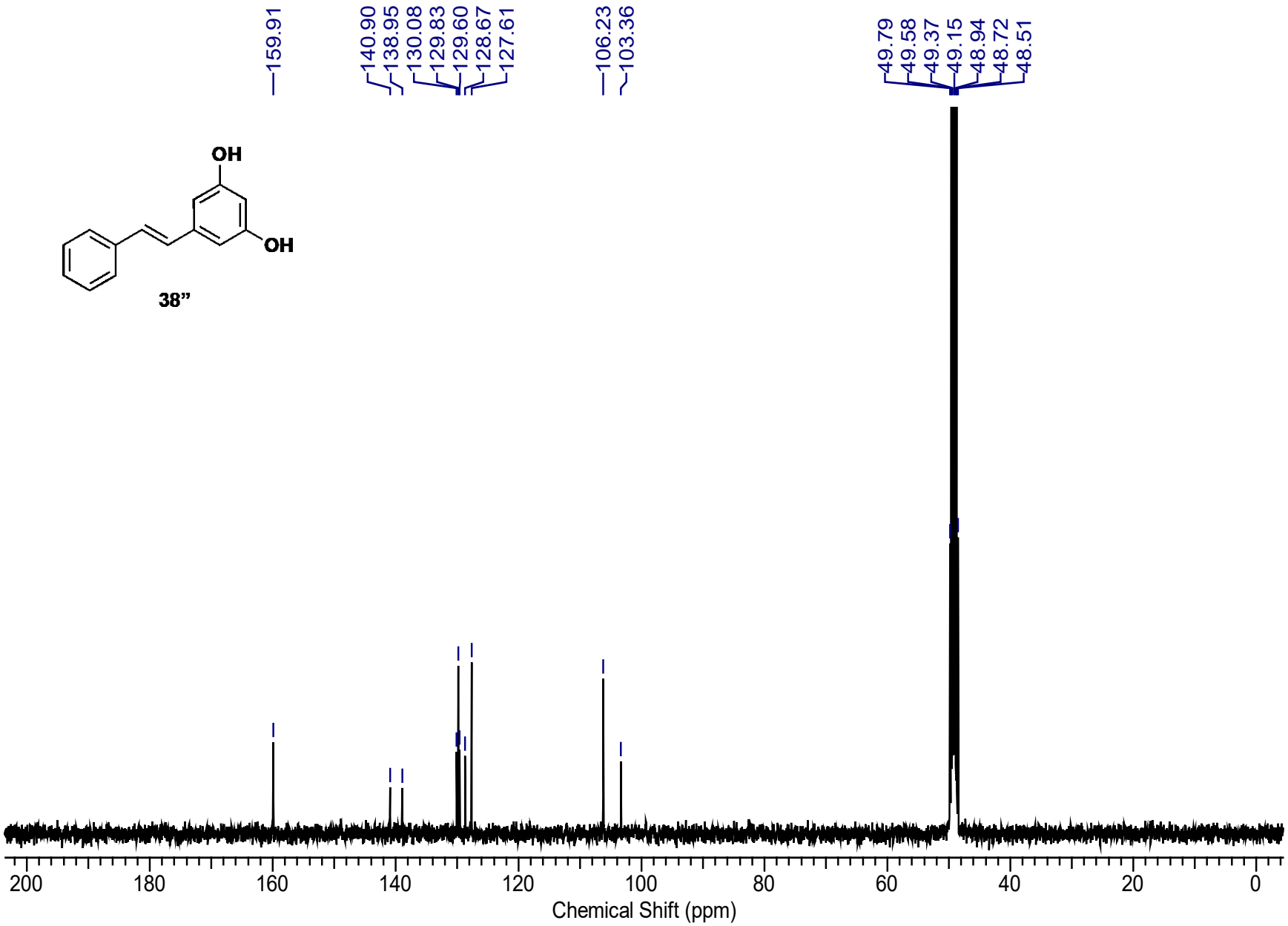

160.97
159.40
139.70
129.94
128.74
127.78
126.58
114.14
104.35
99.64
77.63
77.00
76.37
55.35
OMe
OMe
MeO
36
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

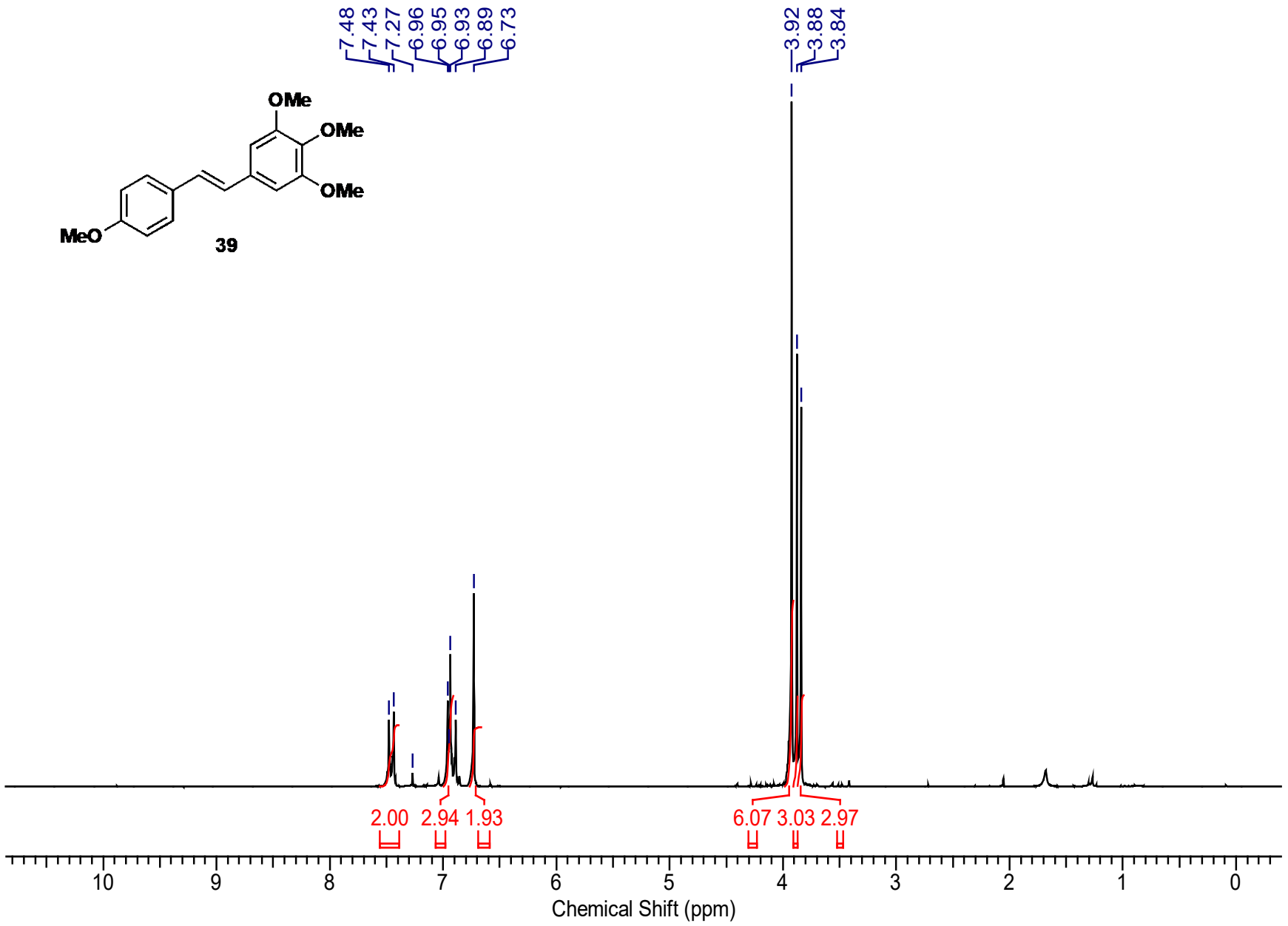

8.59
8.25
6.34
6.30
5.84
5.77
5.71
5.67
5.33
5.06
5.05
2.56
2.50
2.43
OH
OH
HO
36”
1.00
2.16
2.12
4.04
2.17
1.09
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

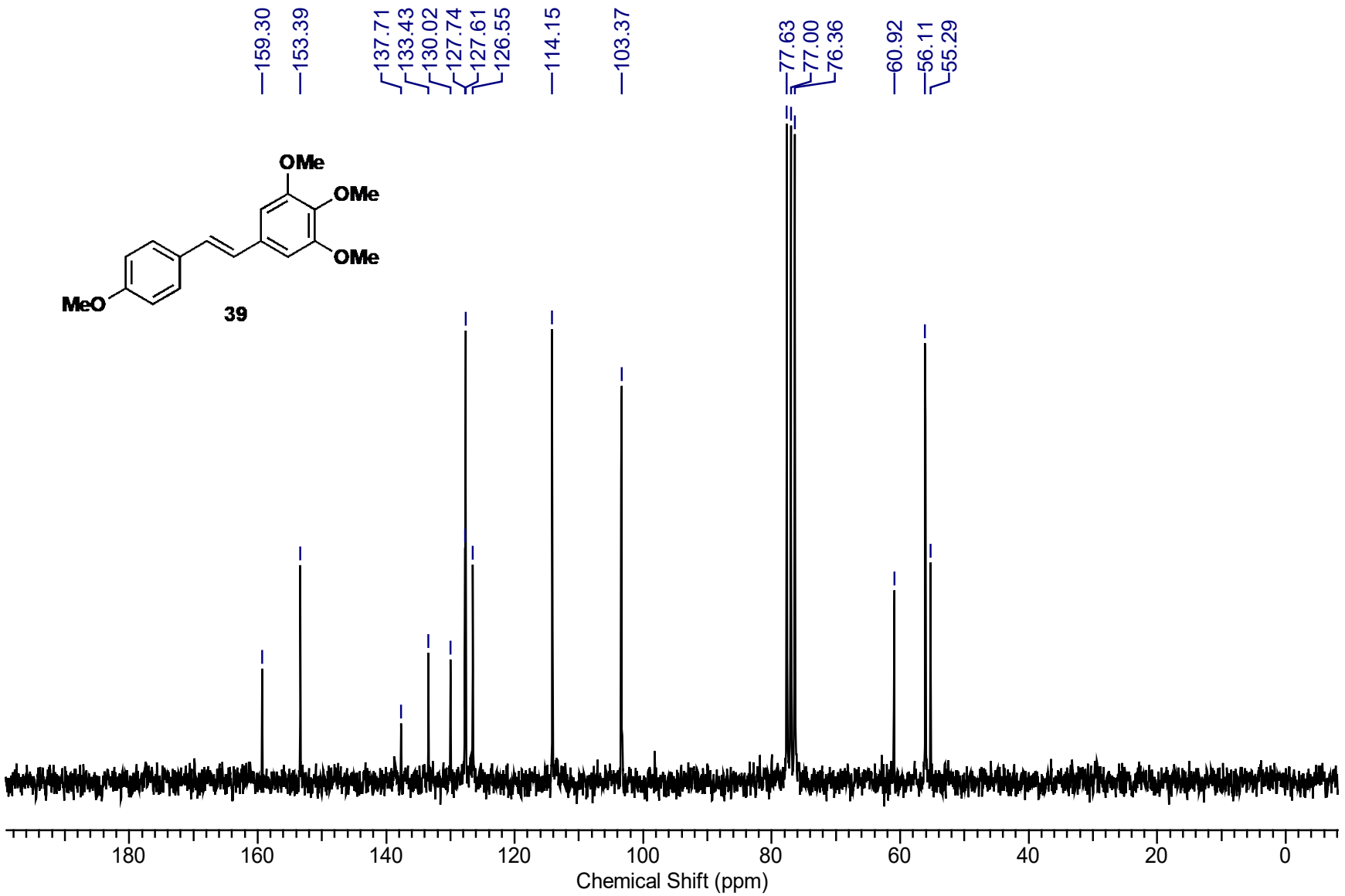

158.64
157.33
139.47
128.27
128.04
125.81
115.74
104.53
101.97
40.76
40.35
39.92
39.51
39.09
38.67
38.25
OH
OH
HO
36”
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)


6.98
6.91
6.87
6.82
6.82
6.76
6.75
6.73
6.44
6.16
3.31
HO
OH
OH
OH
37”
1.06
4.31
2.11
1.00
Chemical Shift (ppm)
Chemical Shift (ppm)


7.51
7.50
7.35
7.33
7.31
7.24
7.22
7.02
7.01
6.49
6.49
6.20
6.20
6.19
3.31
OH
OH
38”
7.51
7.50
7.35
7.33
7.31
7.24
7.22
7.20
7.07
7.02
7.01
6.97
6.49
6.49
6.20
6.20
2.25
2.23
1.13
2.30
2.15
1.00
7.5
7.0
6.5
Chemical Shift (ppm)
2.25
2.23
1.13
2.30
2.15
1.00
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


159.91
140.90
138.95
130.08
129.83
129.60
128.67
127.61
106.23
103.36
49.79
49.58
49.37
49.15
48.94
48.72
48.51
OH
OH
38”
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)


7.48
7.43
7.27
6.96
6.95
6.93
6.89
6.73
3.92
3.88
3.84
OMe
OMe
OMe
MeO
39
2.00
2.94
1.93
6.07
3.03
2.97
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


159.30
153.39
137.71
133.43
130.02
127.74
127.61
126.55
114.15
103.37
77.63
77.00
76.36
60.92
56.11
55.29
OMe
OMe
OMe
MeO
39
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

9. PBE/TZVP optimized geometries for all the compounds and transition states

Diphenylacetylene

C	-1.809439	0.772982	-0.395728
C	-1.197654	0.680749	0.659315
C	-2.529793	0.864420	-1.617085
C	-2.485851	2.041894	-2.398746
C	-3.311379	-0.225307	-2.067133
C	-3.203623	2.122378	-3.591551
H	-1.884613	2.886960	-2.060106
C	-4.027616	-0.132344	-3.260336
H	-3.351830	-1.136508	-1.469700
C	-3.978002	1.038610	-4.027516
H	-3.161024	3.037665	-4.185697
H	-4.631151	-0.979653	-3.592979
H	-4.539593	1.106572	-4.961244
C	-0.487947	0.562369	1.886180
C	-0.055985	-0.703810	2.345026
C	-0.206496	1.704680	2.669554
C	0.632426	-0.816984	3.553361
H	-0.266510	-1.590649	1.744637
C	0.479713	1.578249	3.877232
H	-0.536166	2.685999	2.321870
C	0.900854	0.320133	4.324486
H	0.960721	-1.800931	3.894693
H	0.686045	2.469223	4.474343
H	1.438649	0.226846	5.269295

Z-stilbene

C	-3.599103	0.579378	0.201898
C	-2.897335	0.174976	1.287769
C	-5.045962	0.790024	0.033218
C	-6.015037	0.003685	0.690523
C	-5.493332	1.768011	-0.878994
C	-7.376206	0.213341	0.469488
H	-5.694206	-0.785102	1.372476
C	-6.856981	1.986225	-1.091634
H	-4.757262	2.368454	-1.419965
C	-7.805569	1.211770	-0.414978
H	-8.108948	-0.411743	0.984567
H	-7.179282	2.757608	-1.794453
H	-8.871802	1.374415	-0.584775
C	-3.342004	-0.040902	2.674638
C	-2.728809	-1.052382	3.442224
C	-4.312010	0.770824	3.298766
C	-3.104507	-1.278210	4.768955
H	-1.954812	-1.673762	2.984157

C	-4.678057	0.553807	4.627300
H	-4.773825	1.583969	2.736594
C	-4.084312	-0.477930	5.366740
H	-2.624986	-2.076357	5.339679
H	-5.426509	1.198239	5.093542
H	-4.374882	-0.647151	6.405556
H	-1.829780	-0.011635	1.125481
H	-3.012340	0.766140	-0.704461

E-stilbene

C	-3.633500	0.858631	0.319454
C	-2.917205	-0.219398	0.719955
C	-5.088313	0.944388	0.192978
C	-5.968386	-0.087261	0.592120
C	-5.653402	2.117563	-0.354435
C	-7.346991	0.050007	0.439784
H	-5.572299	-1.004581	1.032246
C	-7.034807	2.253607	-0.507601
H	-4.990874	2.929611	-0.665170
C	-7.889860	1.219543	-0.111966
H	-8.007489	-0.759739	0.757411
H	-7.444731	3.170430	-0.936634
H	-8.970517	1.322342	-0.228049
H	-3.100844	1.774289	0.040771
C	-1.462235	-0.305049	0.846204
C	-0.596868	0.798255	0.666570
C	-0.881618	-1.552551	1.165509
C	0.783644	0.652280	0.791856
H	-1.007164	1.782559	0.432323
C	0.501715	-1.697753	1.290278
H	-1.533179	-2.417700	1.313751
C	1.342767	-0.595757	1.102710
H	1.432200	1.519514	0.650197
H	0.924141	-2.674400	1.535726
H	2.424636	-0.704527	1.200716
H	-3.447552	-1.144859	0.969627

Complex A

C	-3.991885	0.134585	1.722830
C	-2.852507	-0.433449	1.127304
C	-1.922250	-1.117624	1.923990
C	-2.125064	-1.230574	3.301066
C	-3.257458	-0.661648	3.891308
C	-4.192256	0.016093	3.100373
P	-2.515828	-0.249442	-0.675261
Ni	-0.436098	-0.726029	-1.133219
Cl	-1.048842	-2.886945	-1.168564
C	-3.116253	1.462127	-1.082191

C	-2.333039	2.585057	-0.406405
C	-0.913546	2.734380	-0.951560
P	0.234025	1.300186	-0.674740
C	0.656409	1.314797	1.120968
C	1.351264	0.212496	1.649420
C	1.666120	0.167026	3.008236
C	1.275017	1.209951	3.855171
C	0.584301	2.307784	3.334024
C	0.278419	2.365747	1.970746
C	1.724191	1.921299	-1.567936
C	2.859177	2.372648	-0.883791
C	3.947138	2.882363	-1.601651
C	3.902929	2.944164	-2.997465
C	2.766524	2.492926	-3.680751
C	1.681231	1.978860	-2.969762
C	-3.768656	-1.259080	-1.577650
C	-4.692665	-2.070503	-0.907592
C	-5.640841	-2.795102	-1.637752
C	-5.666463	-2.715839	-3.033478
C	-4.738216	-1.909328	-3.703252
C	-3.789797	-1.184020	-2.979313
H	-0.415535	3.625305	-0.540911
H	-2.323224	2.437322	0.684656
H	-3.069348	1.555773	-2.178268
Cl	1.674060	-1.276025	-1.652159
H	-1.039103	-1.558612	1.459610
H	-4.730958	0.667944	1.122081
H	-1.390156	-1.755563	3.913974
H	-5.079511	0.459322	3.556596
H	-3.413510	-0.745114	4.968712
H	-4.673722	-2.144195	0.180767
H	-3.056090	-0.574101	-3.512146
H	-6.358772	-3.426630	-1.110671
H	-4.749296	-1.848163	-4.793266
H	-6.406094	-3.284536	-3.600440
H	1.641437	-0.608885	0.990598
H	-0.252932	3.236715	1.586446
H	2.206984	-0.692657	3.408504
H	0.279103	3.126251	3.988781
H	1.508764	1.167099	4.920736
H	2.901604	2.325679	0.205646
H	0.808730	1.603078	-3.510298
H	4.831852	3.230183	-1.064465
H	2.729130	2.533907	-4.771073
H	4.753977	3.340668	-3.554726
H	-4.179655	1.501067	-0.805603
H	-2.865096	3.532579	-0.583542
H	-0.939635	2.869110	-2.044461

Complex B

C	-3.214220	-0.132446	2.080288
C	-2.548246	-0.841692	1.069183
C	-1.869555	-2.029944	1.392324
C	-1.862376	-2.500202	2.706237
C	-2.515891	-1.782246	3.714335
C	-3.192319	-0.600904	3.398182
P	-2.483601	-0.255248	-0.681537
Ni	-0.447683	-0.388393	-1.500460
O	1.264628	-0.404610	-2.283321
C	2.260908	-1.142249	-1.620943
C	-3.290355	1.423667	-0.682568
C	-2.479216	2.570130	-0.074185
C	-1.213527	2.916126	-0.858999
P	0.088355	1.587136	-0.803748
C	0.575103	1.523260	0.976152
C	0.761940	0.270376	1.578095
C	1.094790	0.179570	2.931930
C	1.246566	1.342584	3.692304
C	1.069818	2.596938	3.095517
C	0.734760	2.690415	1.742404
C	1.498563	2.371150	-1.690114
C	2.750384	2.534921	-1.082685
C	3.799708	3.128904	-1.791822
C	3.605133	3.560778	-3.106816
C	2.355506	3.393604	-3.716413
C	1.306951	2.797118	-3.014473
C	-3.783485	-1.219875	-1.573858
C	-3.813333	-1.150637	-2.975390
C	-4.819641	-1.806344	-3.687249
C	-5.795034	-2.544702	-3.005262
C	-5.762790	-2.619365	-1.609437
C	-4.760347	-1.956460	-0.891691
H	-0.757086	3.840046	-0.475344
H	-2.221458	2.354619	0.974853
H	-3.500034	1.631081	-1.744111
H	-1.347285	-2.580592	0.606459
H	-3.756775	0.786860	1.857852
H	-1.333153	-3.424704	2.946039
H	-3.707890	-0.037243	4.178281
H	-2.498747	-2.144142	4.744361
H	-3.038084	-0.597827	-3.511256
H	-4.740741	-2.020143	0.197927
H	-4.836916	-1.749761	-4.777525
H	-6.519005	-3.196069	-1.072861
H	-6.577375	-3.063499	-3.562869
H	0.627109	-0.635449	0.983255
H	0.601518	3.675882	1.291722
H	1.224426	-0.801442	3.392613
H	1.189236	3.507169	3.686381

H	1.501125	1.274261	4.751857
H	2.911746	2.201824	-0.056185
H	0.343446	2.652228	-3.508661
H	4.772343	3.253850	-1.311209
H	2.198356	3.724617	-4.745075
H	4.424790	4.026095	-3.657958
H	-4.266995	1.320834	-0.186653
H	-3.122430	3.463881	-0.052657
H	-1.447121	3.087232	-1.921419
H	3.146012	-1.212774	-2.283406
H	2.605958	-0.657435	-0.681356
H	1.945726	-2.175363	-1.370642
Cl	-0.752684	-2.585301	-1.979233

Catalyst 1

C	3.941499	2.955379	-2.965742
C	3.562110	3.529912	-1.746621
C	2.464832	3.024042	-1.044048
C	1.746921	1.930746	-1.553852
C	2.133684	1.353810	-2.771175
C	3.224767	1.869069	-3.478434
P	0.242419	1.293079	-0.682761
C	0.681971	1.316649	1.112930
C	1.291254	0.169372	1.649104
C	1.631378	0.117566	3.001560
C	1.349964	1.204587	3.837354
C	0.738608	2.346453	3.311297
C	0.407294	2.406435	1.953315
C	-0.913549	2.734356	-0.938179
C	-2.314153	2.594992	-0.332015
C	-3.195335	1.534385	-1.002879
P	-2.611607	-0.209330	-0.704691
C	-3.912983	-1.194343	-1.571354
C	-4.928459	-1.884980	-0.895951
C	-5.889069	-2.603161	-1.617748
C	-5.841534	-2.634771	-3.014877
C	-4.823113	-1.952680	-3.692329
C	-3.857665	-1.243746	-2.974356
Ni	-0.485402	-0.621388	-1.214290
C	-2.903164	-0.476589	1.100568
C	-2.006105	-1.310832	1.786862
C	-2.153706	-1.532120	3.158075
C	-3.195811	-0.915553	3.857790
C	-4.094471	-0.083207	3.180798
C	-3.950309	0.136780	1.807875
H	-0.410719	3.637606	-0.559881
H	-2.248400	2.399272	0.750190
H	-3.201986	1.670712	-2.095712
H	0.980303	-0.773616	-1.385058

H	-1.184925	-1.778418	1.238224
H	-4.660992	0.789315	1.296697
H	-1.445465	-2.176360	3.682675
H	-4.909842	0.399927	3.723075
H	-3.307879	-1.081179	4.931314
H	-4.974117	-1.867019	0.194477
H	-3.048006	-0.738061	-3.506627
H	-6.676341	-3.139106	-1.083340
H	-4.774669	-1.982033	-4.782858
H	-6.592548	-3.194566	-3.575973
H	1.481557	-0.689121	1.000438
H	-0.068361	3.308161	1.565089
H	2.104301	-0.779175	3.406935
H	0.514807	3.196966	3.958389
H	1.604399	1.160064	4.898202
H	2.182248	3.474790	-0.089704
H	1.582378	0.491069	-3.153779
H	4.124078	4.372493	-1.338570
H	3.519464	1.415313	-4.426864
H	4.799064	3.352459	-3.512666
H	-4.237032	1.623890	-0.662398
H	-2.819164	3.568676	-0.433944
H	-0.979362	2.849096	-2.031890
Cl	-0.707577	-2.767257	-1.769230

Int-1

C	0.958400	-3.895578	-5.980162
C	-0.413576	-3.610850	-5.981188
C	-0.940400	-2.687399	-5.081293
C	-0.098191	-2.029573	-4.153498
C	1.280619	-2.323845	-4.160138
C	1.799780	-3.246397	-5.068882
C	-0.675739	-1.096338	-3.228164
C	-1.614557	-0.309641	-2.882559
C	-2.902932	0.302216	-3.061828
C	-3.994662	-0.503053	-3.464224
C	-5.261552	0.055114	-3.636935
C	-5.469989	1.421690	-3.413888
C	-4.395434	2.228837	-3.020491
C	-3.127258	1.677115	-2.839622
Ni	-0.244590	-0.323559	-1.387429
P	-0.778671	1.219046	0.128004
C	-0.684640	3.012188	-0.368800
C	-1.136741	4.003279	0.520101
C	-1.070660	5.352792	0.167111
C	-0.542964	5.730628	-1.073556
C	-0.077649	4.751785	-1.955803
C	-0.149654	3.399872	-1.602787
C	-2.557265	1.083226	0.680517

C	-3.011102	-0.273178	1.241051
C	-3.055843	-1.427153	0.230696
P	-1.352479	-1.991404	-0.257296
C	-1.621446	-3.486623	-1.300688
C	-2.873421	-3.854165	-1.812948
C	-2.987412	-4.968104	-2.653065
C	-1.856181	-5.718676	-2.983859
C	-0.604109	-5.352588	-2.475983
C	-0.484895	-4.238976	-1.644966
C	-0.729949	-2.713880	1.329613
C	0.393121	-2.166880	1.962956
C	0.819062	-2.672038	3.197042
C	0.130993	-3.729246	3.798854
C	-0.985641	-4.288133	3.161798
C	-1.414692	-3.784336	1.931895
C	0.212164	1.265819	1.689649
C	1.611534	1.300362	1.562549
C	2.420975	1.335965	2.699850
C	1.843591	1.330260	3.975069
C	0.452201	1.301082	4.106075
C	-0.362480	1.272692	2.969306
H	-2.752347	1.875488	1.417805
H	-2.393398	-0.564659	2.105520
H	-3.578507	-1.114850	-0.686855
H	0.385227	0.824855	-2.023718
H	0.939877	-1.358094	1.479936
H	-2.281930	-4.230797	1.439448
H	1.691546	-2.233901	3.686054
H	-1.522532	-5.118592	3.625024
H	0.463316	-4.122636	4.761843
H	-3.768110	-3.282184	-1.563261
H	0.497261	-3.933423	-1.276030
H	-3.966138	-5.246105	-3.049989
H	0.285748	-5.924444	-2.746211
H	-1.947553	-6.583564	-3.644031
H	2.065772	1.266982	0.570804
H	-1.445017	1.253784	3.098926
H	3.507217	1.358991	2.589577
H	-0.006182	1.299560	5.097237
H	2.477096	1.348168	4.864109
H	-1.530405	3.730626	1.501532
H	0.213782	2.635377	-2.295435
H	-1.427804	6.112066	0.865787
H	0.341970	5.036364	-2.922705
H	-0.490202	6.786165	-1.347774
H	-3.603156	-2.279418	0.659590
H	-4.030489	-0.132604	1.633665
H	-3.146001	1.335629	-0.215371
H	-6.093014	-0.583135	-3.943170
H	-3.836984	-1.570627	-3.629105

H	-2.294747	2.309037	-2.528742
H	-4.548044	3.296455	-2.848294
H	-6.463271	1.854694	-3.545914
H	-2.011827	-2.480416	-5.071894
H	1.918420	-1.838290	-3.420017
H	-1.077705	-4.119138	-6.683697
H	2.869417	-3.468015	-5.061073
H	1.367185	-4.624212	-6.683337
Cl	1.957774	-1.062729	-0.973066

TS1

C	-1.902421	-4.017561	-2.296576
C	-2.784607	-3.353106	-1.428098
C	-4.135223	-3.736062	-1.394555
C	-4.594713	-4.769470	-2.217428
C	-3.711845	-5.428613	-3.078801
C	-2.363537	-5.053430	-3.112255
P	-2.099547	-1.959103	-0.419965
C	-3.611842	-1.003394	0.103281
C	-3.271544	0.219261	0.966455
C	-2.634035	1.381886	0.197483
P	-0.883195	1.098396	-0.379486
C	0.147167	1.231170	1.159137
C	-0.356587	1.733624	2.368966
C	0.459230	1.787004	3.504751
C	1.785005	1.348640	3.441914
C	2.294381	0.850919	2.236554
C	1.478505	0.782322	1.105627
Ni	-0.460856	-0.748376	-1.325835
Cl	1.146703	-2.396460	-1.342388
C	-1.623672	-2.761420	1.184686
C	-0.472709	-2.317452	1.850473
C	-0.135590	-2.840740	3.102776
C	-0.936614	-3.825567	3.689597
C	-2.079220	-4.283762	3.021519
C	-2.423184	-3.753374	1.774840
C	-0.543585	2.696248	-1.258850
C	-0.676545	3.927242	-0.595863
C	-0.445629	5.122092	-1.283088
C	-0.087019	5.098282	-2.636840
C	0.047775	3.874632	-3.300169
C	-0.177774	2.678431	-2.611231
C	-1.662178	-0.546351	-3.656105
C	-0.533102	-0.861351	-4.030791
C	0.733111	-1.193625	-4.575660
C	1.647647	-0.178881	-4.938425
C	2.884301	-0.510370	-5.489450
C	3.232466	-1.852973	-5.687972
C	2.332241	-2.864906	-5.332075

C	1.095069	-2.544302	-4.776302
C	-3.044810	-0.208755	-3.549461
C	-3.456824	1.124309	-3.327206
C	-4.812473	1.437673	-3.235321
C	-5.781625	0.434112	-3.361334
C	-5.383335	-0.886633	-3.599093
C	-4.030097	-1.209852	-3.698118
H	-2.655850	2.304875	0.795742
H	-2.634071	-0.081894	1.814479
H	-4.139102	-0.697368	-0.813726
H	0.628198	0.210484	-1.650789
H	0.159823	-1.566287	1.376167
H	-3.315250	-4.121550	1.262715
H	0.759781	-2.481936	3.615401
H	-2.703974	-5.057993	3.472042
H	-0.671085	-4.239343	4.664702
H	-4.846290	-3.223568	-0.745531
H	-0.854066	-3.709454	-2.326522
H	-5.648724	-5.053420	-2.189514
H	-1.670474	-5.562889	-3.785620
H	-4.073903	-6.231170	-3.724759
H	1.862046	0.350669	0.178422
H	-1.387047	2.081901	2.446963
H	3.326560	0.499282	2.180229
H	0.052122	2.172454	4.441813
H	2.418264	1.389065	4.330352
H	-0.941677	3.961790	0.463199
H	-0.075248	1.716041	-3.116517
H	-0.542610	6.075064	-0.758931
H	0.327998	3.849537	-4.355258
H	0.091069	6.033626	-3.171108
H	-4.273708	-1.677374	0.665865
H	-4.208780	0.589713	1.410689
H	-3.207432	1.589304	-0.718616
H	-6.132172	-1.674093	-3.706435
H	-3.720409	-2.238824	-3.879755
H	-2.703183	1.906206	-3.226145
H	-5.115043	2.472046	-3.060739
H	-6.841594	0.681820	-3.280503
H	0.397196	-3.330639	-4.488074
H	1.377322	0.867686	-4.788228
H	2.600154	-3.912750	-5.482198
H	3.580523	0.283154	-5.768372
H	4.201474	-2.108862	-6.120880

Int-2

C	6.980605	6.312291	-4.501452
C	6.242220	5.736078	-5.544583
C	5.794048	6.548399	-6.599909

C	6.093684	7.912987	-6.616048
C	6.833678	8.482061	-5.574100
C	7.273423	7.679109	-4.517101
P	5.769070	3.947642	-5.555684
Ni	3.689088	3.461373	-5.204281
C	3.654189	4.813837	-3.801171
C	3.409597	6.115304	-4.066341
C	3.166312	7.219279	-3.124356
C	3.470734	8.537060	-3.531262
C	3.260125	9.626216	-2.683125
C	2.723485	9.430125	-1.404838
C	2.394457	8.131600	-0.992779
C	2.608050	7.042823	-1.839492
C	6.443511	3.448472	-7.229500
C	6.403657	1.946074	-7.512407
C	5.003613	1.418655	-7.836737
P	3.760668	1.578258	-6.460256
C	2.229782	1.046384	-7.350611
C	1.669433	-0.227975	-7.194683
C	0.528690	-0.586304	-7.922245
C	-0.052184	0.322016	-8.812093
C	0.506884	1.596355	-8.970125
C	1.637273	1.960571	-8.236378
C	4.136272	0.193379	-5.294922
C	5.151296	-0.748538	-5.517746
C	5.435114	-1.718977	-4.550201
C	4.706305	-1.760298	-3.357899
C	3.682667	-0.830970	-3.136428
C	3.402975	0.143532	-4.095690
C	6.954282	3.097878	-4.420188
C	6.462503	2.183093	-3.480146
C	7.343259	1.460848	-2.670914
C	8.721733	1.653854	-2.791339
C	9.220346	2.568746	-3.727952
C	8.342203	3.287589	-4.541588
C	3.934297	4.242536	-2.471205
C	3.214719	3.148901	-1.945397
C	3.565885	2.580146	-0.719834
C	4.651246	3.079489	0.009731
C	5.371646	4.169249	-0.494145
C	5.017821	4.742903	-1.714574
H	5.034320	0.367292	-8.159504
H	6.847740	1.392062	-6.669672
H	5.876324	4.000829	-7.994104
H	5.386712	2.034121	-3.381962
H	8.744333	3.996461	-5.268876
H	6.945918	0.749162	-1.944687
H	10.296960	2.722236	-3.825830
H	9.411612	1.090932	-2.159106
H	5.194750	6.125462	-7.409310

H	7.332871	5.695058	-3.674074
H	5.739807	8.533630	-7.441740
H	7.848236	8.116207	-3.698003
H	7.062032	9.549578	-5.583244
H	2.615816	0.878971	-3.917900
H	5.733101	-0.736708	-6.439916
H	3.108781	-0.856159	-2.207958
H	6.232696	-2.442278	-4.731167
H	4.934963	-2.514447	-2.602280
H	2.117993	-0.944710	-6.504105
H	2.051447	2.966412	-8.342292
H	0.095392	-1.580285	-7.791746
H	0.053939	2.312464	-9.659009
H	-0.941324	0.040248	-9.379901
H	7.478397	3.819346	-7.259759
H	7.049629	1.745964	-8.381830
H	4.573272	1.990608	-8.673893
H	2.992318	1.733628	-0.334709
H	2.369850	2.759047	-2.514236
H	5.580412	5.592372	-2.104903
H	6.220039	4.570809	0.065293
H	4.933747	2.623463	0.960996
H	3.896802	8.695747	-4.525374
H	2.333357	6.040339	-1.509441
H	3.514240	10.633587	-3.021486
H	1.957290	7.968131	-0.004692
H	2.553438	10.279787	-0.740222
H	3.402856	6.426491	-5.117250
Cl	1.436765	3.263630	-4.966758

TS2

C	-0.016620	0.583488	-5.998941
C	-0.760729	-0.449847	-5.382485
C	-1.542916	-1.279595	-6.216127
C	-1.555803	-1.093436	-7.599284
C	-0.798063	-0.074066	-8.193572
C	-0.029668	0.768208	-7.381458
C	-0.700011	-0.538993	-3.919116
C	-1.138483	-1.447002	-3.010499
C	-1.574380	-2.822540	-3.215247
C	-2.661787	-3.361861	-2.496147
C	-3.043105	-4.692293	-2.665304
C	-2.334038	-5.527897	-3.536483
C	-1.237458	-5.016367	-4.241194
C	-0.859167	-3.684529	-4.079149
Ni	-1.122723	-0.376819	-1.385008
Cl	-3.358563	0.031873	-1.592534
P	0.479312	-1.516615	-0.499753
C	0.065977	-3.311479	-0.298552

C	0.810630	-4.336418	-0.897204
C	0.446536	-5.672944	-0.703031
C	-0.653735	-5.995760	0.095491
C	-1.403269	-4.975042	0.690724
C	-1.054896	-3.639746	0.483783
C	2.159429	-1.489507	-1.273070
C	3.316312	-1.177022	-0.541292
C	4.554971	-1.086979	-1.184059
C	4.656196	-1.317742	-2.558887
C	3.510482	-1.645513	-3.291761
C	2.270588	-1.724631	-2.655473
C	0.758371	-1.080031	1.300658
C	1.033141	0.383791	1.663358
C	-0.179755	1.311783	1.524880
P	-0.655813	1.514424	-0.262114
C	-1.962462	2.813856	-0.275539
C	-2.944959	2.866883	0.723962
C	-3.986297	3.795844	0.636606
C	-4.063477	4.669103	-0.453025
C	-3.093025	4.609432	-1.459412
C	-2.050648	3.684586	-1.373490
C	0.823402	2.415229	-0.932077
C	1.197611	3.662243	-0.400423
C	2.333725	4.318020	-0.879476
C	3.109583	3.737286	-1.891715
C	2.744976	2.497127	-2.421359
C	1.605503	1.842547	-1.942883
H	3.997608	4.252525	-2.263410
H	2.615515	5.287024	-0.462396
H	0.597169	4.130367	0.382803
H	-3.146507	5.285493	-2.315537
H	-1.298860	3.645787	-2.165037
H	3.346702	2.031219	-3.204335
H	1.334238	0.866757	-2.345427
H	5.443894	-0.831927	-0.603861
H	5.623993	-1.241385	-3.058437
H	-2.148957	-2.070601	-5.773482
H	-2.170695	-1.746454	-8.223036
H	-0.814089	0.067532	-9.275991
H	0.556970	1.576036	-7.825064
H	0.577691	1.252557	-5.369616
H	-0.256409	0.378059	-3.496611
H	3.269592	-0.994642	0.532176
H	-4.879229	5.391819	-0.520502
H	0.037805	2.302310	1.950244
H	-4.743332	3.833284	1.422802
H	1.357809	0.404564	2.715653
H	-2.911110	2.183200	1.574267
H	-1.045748	0.893561	2.059781
H	-0.152936	-1.420675	1.815503

H	1.676444	-4.098286	-1.516477
H	-3.196876	-2.708831	-1.804857
H	0.000517	-3.295082	-4.628530
H	-0.667613	-5.662943	-4.912642
H	-2.624435	-6.573972	-3.654645
H	-3.885733	-5.089406	-2.094674
H	-0.933236	-7.040262	0.247145
H	-2.272097	-5.218011	1.305750
H	-1.671817	-2.851371	0.922390
H	1.028353	-6.463799	-1.180727
H	1.376699	-1.946415	-3.238256
H	3.578896	-1.832317	-4.365460
H	1.876069	0.784653	1.078361
H	1.572447	-1.731150	1.653267

Int-3

C	-3.453530	-1.739705	-5.152362
C	-3.856917	-0.645422	-4.360312
C	-5.221163	-0.528193	-4.022315
C	-6.156497	-1.452678	-4.491111
C	-5.745188	-2.524575	-5.291970
C	-4.389833	-2.665987	-5.613154
C	-2.894277	0.376682	-3.930976
C	-2.597982	1.488135	-4.669428
C	-3.216375	2.025765	-5.893095
C	-4.119869	1.345364	-6.741474
C	-4.646732	1.967550	-7.875346
C	-4.298728	3.285232	-8.198638
C	-3.402836	3.975686	-7.373413
C	-2.869554	3.352613	-6.244913
Ni	-2.381925	0.716287	-2.092443
Cl	-0.288354	1.734725	-2.368484
P	-3.006529	1.973193	-0.323369
C	-3.185335	3.675574	-1.027796
C	-2.671170	4.816382	-0.395463
C	-2.821528	6.073926	-0.990367
C	-3.481937	6.201190	-2.216743
C	-3.998277	5.064247	-2.849365
C	-3.850246	3.807511	-2.259536
C	-2.054870	2.190186	1.238154
C	-0.673677	2.437622	1.138788
C	0.099337	2.580199	2.291798
C	-0.490676	2.457561	3.554859
C	-1.861262	2.203516	3.658745
C	-2.644066	2.075242	2.506674
C	-4.757362	1.585936	0.180231
C	-4.998966	0.150881	0.663934
C	-4.856676	-0.935740	-0.408880
P	-3.149439	-1.058553	-1.131759

C	-3.097308	-2.681099	-2.009954
C	-1.848517	-3.105592	-2.493595
C	-1.722129	-4.345841	-3.118097
C	-2.842306	-5.172481	-3.267860
C	-4.086797	-4.748770	-2.794846
C	-4.218102	-3.506021	-2.167031
O	-0.102628	-0.973344	-4.555272
C	0.374460	-0.054398	-5.544830
C	-2.067615	-1.430077	0.332048
C	-0.776072	-0.889673	0.398795
C	0.054657	-1.187709	1.482872
C	-0.399507	-2.023227	2.506701
C	-1.685380	-2.573062	2.438790
C	-2.516070	-2.284081	1.353512
H	-0.972676	-2.460545	-2.391703
H	-4.967026	-5.382362	-2.920821
H	-2.745293	-6.142632	-3.759393
H	-0.748108	-4.665840	-3.493564
H	-5.201154	-3.188358	-1.819729
H	-5.536619	-0.747627	-1.253500
H	-5.128968	-1.911952	0.017742
H	-6.027816	0.096911	1.052800
H	-4.339343	-0.084556	1.513531
H	-3.511726	-2.730903	1.312132
H	-2.044669	-3.229665	3.233866
H	0.246331	-2.247673	3.357970
H	1.054226	-0.751648	1.531978
H	-0.430210	-0.214712	-0.389136
H	-0.209217	2.501629	0.151824
H	-3.713050	1.889388	2.614737
H	-2.329394	2.107894	4.640656
H	0.116888	2.559095	4.456372
H	1.170032	2.775558	2.202927
H	-5.070786	2.314868	0.942512
H	-1.818061	2.148042	-4.279410
H	-4.231292	2.922253	-2.774961
H	-4.509053	5.152257	-3.810280
H	-3.592716	7.183674	-2.679913
H	-2.418644	6.957309	-0.490467
H	-2.151912	4.729118	0.560175
H	-5.338117	1.414729	-8.515689
H	-4.717656	3.765735	-9.085088
H	-3.117397	5.003018	-7.611078
H	-2.170482	3.898773	-5.606123
H	-5.545322	0.324082	-3.420275
H	-2.394899	-1.847036	-5.397155
H	-4.058738	-3.509679	-6.222512
H	-6.475122	-3.251199	-5.654313
H	-5.359670	1.790838	-0.718981
H	-7.211314	-1.334618	-4.232544

H	-4.407528	0.319395	-6.519307
H	1.101237	-0.593416	-6.168137
H	0.868835	0.819001	-5.086251
H	-0.442869	0.312361	-6.191060
H	-0.747997	-0.478107	-4.002426

TS3

C	-3.921362	-1.463912	-5.478693
C	-3.899505	-0.456426	-4.487699
C	-5.100629	-0.230859	-3.778174
C	-6.266114	-0.945722	-4.054922
C	-6.269287	-1.931059	-5.051204
C	-5.086260	-2.181074	-5.758855
C	-2.667932	0.275362	-4.173700
C	-2.363945	1.505240	-4.679322
C	-3.125948	2.451689	-5.510218
C	-4.367909	2.190787	-6.133179
C	-5.033122	3.185897	-6.851900
C	-4.482205	4.467814	-6.979458
C	-3.246168	4.741499	-6.383200
C	-2.581287	3.746727	-5.667962
Ni	-1.945726	0.429829	-2.028007
Cl	-0.251097	1.956111	-2.072584
P	-3.053586	1.773698	-0.737552
C	-3.474118	3.334925	-1.631150
C	-2.590515	4.425589	-1.578394
C	-2.900605	5.612123	-2.244808
C	-4.084640	5.718450	-2.982439
C	-4.958411	4.631288	-3.051710
C	-4.653720	3.443050	-2.383948
C	-2.272754	2.336630	0.841373
C	-1.102239	1.722690	1.300857
C	-0.564318	2.076684	2.541981
C	-1.188248	3.054825	3.322335
C	-2.352063	3.681533	2.858801
C	-2.896518	3.323417	1.623295
C	-4.707058	1.181547	-0.122257
C	-4.626519	-0.133682	0.653450
C	-4.364518	-1.344229	-0.246839
P	-2.692632	-1.370459	-1.046463
C	-2.725088	-2.960190	-1.993908
C	-1.573810	-3.762764	-2.058146
C	-1.599030	-4.975991	-2.746819
C	-2.769027	-5.397736	-3.390026
C	-3.911232	-4.595157	-3.341447
C	-3.890463	-3.378445	-2.653253
O	-0.626228	-1.116167	-3.152413
C	0.664091	-0.783525	-3.658673
C	-1.497774	-1.712299	0.328508

C	-0.132190	-1.458919	0.108539
C	0.801437	-1.693363	1.119708
C	0.379968	-2.161773	2.369448
C	-0.976928	-2.409995	2.595381
C	-1.913688	-2.195384	1.578458
H	-0.655168	-3.441922	-1.568804
H	-4.825261	-4.903292	-3.852484
H	-2.786595	-6.346519	-3.930440
H	-0.698912	-5.593237	-2.783310
H	-4.787926	-2.759952	-2.657684
H	-5.092184	-1.358555	-1.072107
H	-4.488649	-2.288264	0.303001
H	-5.588995	-0.292794	1.163122
H	-3.866807	-0.062468	1.448994
H	-2.964778	-2.406086	1.778575
H	-1.313948	-2.773400	3.568264
H	1.107394	-2.330480	3.165965
H	1.859384	-1.495597	0.935620
H	0.185592	-1.060450	-0.856378
H	-0.614972	0.972314	0.679685
H	-3.800829	3.823304	1.268547
H	-2.838409	4.451916	3.460590
H	-0.768970	3.332946	4.291355
H	0.344678	1.586631	2.896705
H	-5.108048	1.986271	0.510697
H	-1.401501	1.929971	-4.372799
H	-5.349143	2.607432	-2.463868
H	-5.874355	4.697094	-3.641460
H	-4.319045	6.643484	-3.512433
H	-2.209133	6.455758	-2.193285
H	-1.660094	4.343572	-1.016014
H	-5.995166	2.959546	-7.318475
H	-5.012036	5.244330	-7.535415
H	-2.805014	5.737653	-6.466143
H	-1.626986	3.973469	-5.184021
H	-5.107277	0.545087	-3.012603
H	-3.002495	-1.682372	-6.028127
H	-5.068170	-2.956373	-6.529015
H	-7.175903	-2.500330	-5.265568
H	-5.386119	1.071528	-0.979444
H	-7.177591	-0.733408	-3.489931
H	-4.819242	1.203709	-6.042924
H	1.101702	-1.661010	-4.165835
H	1.331596	-0.485820	-2.833814
H	0.616282	0.058343	-4.368338
H	-1.427779	-0.625314	-3.727041

Int-4

C	-0.353650	-5.315715	-4.440780

C	-1.604946	-4.702260	-4.322919
C	-1.708323	-3.371363	-3.911973
C	-0.560833	-2.618662	-3.590272
C	0.697023	-3.249900	-3.733904
C	0.799411	-4.575720	-4.151028
C	-0.569745	-1.185080	-3.267201
C	-1.720555	-0.220821	-2.843599
C	-3.105276	-0.471977	-2.432988
C	-3.587443	-1.680765	-1.888390
C	-4.918194	-1.817393	-1.495917
C	-5.812607	-0.745996	-1.622066
C	-5.353873	0.465275	-2.151480
C	-4.022838	0.598475	-2.550854
Ni	-0.244600	-0.323600	-1.387400
P	-0.825165	1.504594	-0.261195
C	-1.368048	2.903751	-1.364742
C	-2.545440	3.630539	-1.127382
C	-2.912866	4.680540	-1.976198
C	-2.107442	5.023650	-3.064914
C	-0.927036	4.310537	-3.302436
C	-0.566354	3.255250	-2.462301
C	-2.292257	1.286118	0.859859
C	-2.178819	0.157817	1.891721
C	-2.321479	-1.253091	1.309123
P	-0.836592	-1.773991	0.305983
C	-1.146558	-3.557947	-0.061239
C	-2.360289	-4.207844	0.208701
C	-2.512475	-5.565987	-0.092203
C	-1.454493	-6.283109	-0.656902
C	-0.242027	-5.638148	-0.925499
C	-0.089257	-4.282532	-0.636143
C	0.396445	-1.912238	1.693909
C	1.318292	-0.882494	1.921860
C	2.153673	-0.913294	3.043246
C	2.086633	-1.984117	3.939494
C	1.175220	-3.022725	3.711676
C	0.331801	-2.986230	2.597493
C	0.476642	2.322369	0.769501
C	1.785963	2.352854	0.259334
C	2.812594	2.952521	0.992548
C	2.546107	3.511316	2.247424
C	1.246459	3.474080	2.762837
C	0.212581	2.886490	2.027057
H	-2.488194	2.241399	1.367657
H	-1.240104	0.244030	2.462748
H	-3.208451	-1.304477	0.660745
H	0.309767	0.814062	-2.104658
H	1.397494	-0.065077	1.208904
H	-0.376203	-3.801064	2.432274
H	2.863309	-0.099402	3.208506

H	1.118796	-3.865226	4.404262
H	2.742343	-2.012898	4.812307
H	-3.195060	-3.668546	0.658633
H	0.851191	-3.774739	-0.861962
H	-3.461915	-6.062245	0.120110
H	0.582873	-6.189336	-1.379896
H	-1.575029	-7.342591	-0.892188
H	2.007833	1.866450	-0.692846
H	-0.793629	2.873105	2.448184
H	3.826701	2.970036	0.587995
H	1.032367	3.904769	3.743154
H	3.350901	3.969721	2.825526
H	-3.197191	3.388977	-0.288461
H	0.348558	2.694219	-2.673108
H	-3.837067	5.228771	-1.782373
H	-0.289566	4.567489	-4.150665
H	-2.397312	5.841849	-3.727080
H	-2.447466	-1.983067	2.122031
H	-2.990051	0.300823	2.622534
H	-3.143406	1.096691	0.186886
H	-5.260250	-2.767612	-1.078781
H	-2.906545	-2.520060	-1.759344
H	-3.674220	1.551081	-2.956302
H	-6.035567	1.312332	-2.254259
H	-6.852709	-0.854855	-1.309015
H	-2.690528	-2.901308	-3.878482
H	1.594389	-2.677605	-3.488186
H	-2.512291	-5.259914	-4.566269
H	1.784613	-5.038981	-4.243410
H	-0.277193	-6.356968	-4.760554
Cl	2.055629	-0.899989	-1.323302
H	-1.582379	0.776198	-3.270007
H	0.212870	-0.636107	-3.797252

TS4

C	-1.922281	-4.595934	-0.630556
C	-2.701102	-3.423534	-0.644807
C	-3.992240	-3.463870	-1.191900
C	-4.502172	-4.661932	-1.703852
C	-3.729351	-5.826091	-1.677703
C	-2.436635	-5.789150	-1.139508
P	-1.937460	-1.858028	-0.035354
C	-3.377075	-0.831474	0.548376
C	-2.906693	0.470605	1.214375
C	-2.424884	1.542105	0.229184
P	-0.785407	1.199602	-0.596463
C	0.483392	1.713434	0.660727
C	0.269927	2.790751	1.535593
C	1.258275	3.157113	2.454126

C	2.469495	2.457178	2.503118
C	2.690536	1.389701	1.626910
C	1.700945	1.017186	0.712500
Ni	-0.454715	-0.786566	-1.298053
Cl	1.113914	-2.467472	-1.236806
C	-1.244505	-2.377841	1.605770
C	-0.006848	-1.878128	2.029081
C	0.478246	-2.178700	3.306283
C	-0.268951	-2.989949	4.165445
C	-1.504321	-3.499376	3.744276
C	-1.992428	-3.192667	2.471563
C	-0.675480	2.571830	-1.851935
C	-1.623827	3.605487	-1.926754
C	-1.489854	4.620588	-2.880948
C	-0.406124	4.622433	-3.762665
C	0.547259	3.600290	-3.688880
C	0.409139	2.581556	-2.744963
C	-1.769776	-0.469671	-3.520637
C	-0.598087	-1.077518	-3.897583
C	-0.300750	-2.435719	-4.364749
C	0.718474	-2.597042	-5.326012
C	1.059705	-3.861521	-5.811343
C	0.406803	-4.999401	-5.323724
C	-0.579740	-4.856726	-4.339103
C	-0.923955	-3.593635	-3.861674
C	-3.178781	-0.886362	-3.593602
C	-4.140258	-0.050005	-2.983483
C	-5.504990	-0.330494	-3.049089
C	-5.954396	-1.449071	-3.760461
C	-5.021247	-2.263482	-4.412710
C	-3.655980	-1.989353	-4.331751
H	-2.366440	2.517359	0.732845
H	-2.130256	0.259392	1.967746
H	-4.016935	-0.605686	-0.317493
H	0.636798	0.108302	-1.752975
H	0.577201	-1.264196	1.344216
H	-2.955621	-3.596188	2.151153
H	1.443232	-1.779970	3.626882
H	-2.090254	-4.136952	4.409704
H	0.108886	-3.228464	5.161784
H	-4.608285	-2.565032	-1.236884
H	-0.906000	-4.563670	-0.234181
H	-5.506649	-4.678401	-2.131190
H	-1.823720	-6.692821	-1.123118
H	-4.129899	-6.759612	-2.078309
H	1.861951	0.172314	0.037125
H	-0.660584	3.360361	1.506784
H	3.632430	0.838215	1.658624
H	1.080705	3.994358	3.132054
H	3.239091	2.745307	3.221973

H	-2.476476	3.638863	-1.248333
H	1.149751	1.778144	-2.705787
H	-2.238811	5.413676	-2.930121
H	1.397478	3.590445	-4.373822
H	-0.304789	5.414833	-4.506849
H	-3.965339	-1.435245	1.254134
H	-3.758327	0.894612	1.768981
H	-3.161060	1.649636	-0.581046
H	-5.360028	-3.126927	-4.989075
H	-2.953718	-2.635768	-4.855390
H	-3.800556	0.843068	-2.454281
H	-6.219350	0.330587	-2.553923
H	-7.020722	-1.675958	-3.816832
H	-1.661590	-3.501396	-3.066331
H	1.242766	-1.713407	-5.699735
H	-1.073620	-5.738733	-3.925193
H	1.843670	-3.959797	-6.565487
H	0.675416	-5.990445	-5.695525
H	-1.667142	0.597263	-3.301450
H	0.257234	-0.400083	-3.977293

Int-5

C	7.300680	6.194656	-4.735324
C	6.377142	5.614428	-5.616583
C	5.782282	6.412861	-6.610302
C	6.108311	7.765576	-6.720933
C	7.024775	8.340939	-5.832717
C	7.619035	7.553254	-4.842615
P	5.835011	3.845040	-5.532709
Ni	3.705250	3.540769	-5.246370
C	3.541177	4.808571	-3.630032
C	3.477236	6.274194	-4.059899
C	2.828007	7.163981	-3.017582
C	3.552048	8.179258	-2.373224
C	2.952113	8.989279	-1.401604
C	1.609719	8.795968	-1.058932
C	0.873630	7.789253	-1.697858
C	1.478892	6.982526	-2.665526
C	6.468089	3.282462	-7.206520
C	6.387013	1.773378	-7.440177
C	4.976653	1.287053	-7.776579
P	3.682770	1.646785	-6.485966
C	2.175781	1.141333	-7.435766
C	1.545109	-0.095376	-7.246530
C	0.436449	-0.445408	-8.026309
C	-0.043197	0.433853	-9.001502
C	0.586456	1.670138	-9.193844
C	1.684899	2.026183	-8.409356
C	3.877090	0.337766	-5.196817

C	4.834741	-0.684155	-5.265414
C	4.982997	-1.581708	-4.202634
C	4.173390	-1.471532	-3.068857
C	3.205086	-0.462647	-3.000591
C	3.062028	0.441211	-4.054025
C	7.030303	2.966620	-4.429388
C	6.534585	2.032191	-3.512870
C	7.410932	1.276845	-2.729647
C	8.791078	1.447813	-2.860322
C	9.295096	2.371801	-3.784688
C	8.420839	3.125392	-4.570383
C	4.390439	4.454655	-2.469318
C	4.045264	3.328275	-1.686555
C	4.806021	2.939813	-0.586543
C	5.942946	3.673557	-0.222072
C	6.287983	4.806370	-0.965267
C	5.519213	5.194657	-2.064692
H	4.960901	0.209828	-8.000649
H	6.791613	1.234665	-6.568226
H	5.902009	3.828885	-7.976597
H	5.458111	1.899371	-3.410930
H	8.829545	3.832679	-5.295085
H	7.008697	0.555576	-2.015703
H	10.373302	2.503958	-3.896734
H	9.477620	0.859478	-2.247709
H	5.038277	5.983847	-7.286544
H	7.767456	5.593345	-3.955072
H	5.636082	8.374150	-7.494599
H	8.334571	7.994899	-4.145986
H	7.273972	9.400844	-5.912910
H	2.318258	1.240204	-3.995541
H	5.480089	-0.787681	-6.138738
H	2.567918	-0.372171	-2.118395
H	5.739384	-2.367028	-4.262084
H	4.295870	-2.170330	-2.238843
H	1.914426	-0.790583	-6.489917
H	2.151960	3.005074	-8.541038
H	-0.050728	-1.410313	-7.869918
H	0.212131	2.364354	-9.949238
H	-0.907579	0.159285	-9.609755
H	7.511094	3.626231	-7.261667
H	7.044323	1.518742	-8.286836
H	4.613029	1.801111	-8.680284
H	4.516300	2.057032	-0.011254
H	3.164762	2.743974	-1.968508
H	5.796860	6.092284	-2.616184
H	7.161694	5.399238	-0.682823
H	6.546918	3.368707	0.635022
H	4.600730	8.339822	-2.639472
H	0.899757	6.198435	-3.162012

H	3.534712	9.773366	-0.912345
H	-0.177424	7.635203	-1.442062
H	1.137858	9.426068	-0.302005
H	4.472567	6.669220	-4.299398
Cl	1.436887	3.681177	-5.435870
H	2.523953	4.458635	-3.417726
H	2.889098	6.323333	-4.990307

TS5

C	1.705302	1.829165	-2.225058
C	0.895884	2.495119	-1.295357
C	1.317856	3.735391	-0.785937
C	2.530595	4.289280	-1.203622
C	3.331030	3.616026	-2.136303
C	2.916142	2.384302	-2.647620
P	-0.686472	1.702986	-0.743937
C	-1.955920	2.998444	-1.096202
C	-3.063451	3.166570	-0.247714
C	-4.054754	4.101370	-0.560692
C	-3.962951	4.862104	-1.731568
C	-2.869398	4.687337	-2.587508
C	-1.871255	3.761329	-2.272027
Ni	-1.074137	-0.315797	-1.576176
P	0.364608	-1.321521	-0.256613
C	0.408330	-0.638380	1.484104
C	0.616072	0.873427	1.626833
C	-0.546603	1.726537	1.110352
C	-1.272851	-1.759705	-2.991770
C	-2.537279	-2.504018	-3.083520
C	-2.620165	-3.716875	-2.360657
C	-3.785046	-4.479842	-2.342831
C	-4.901164	-4.078327	-3.088642
C	-4.824832	-2.903086	-3.844864
C	-3.667852	-2.120795	-3.835493
C	-0.844666	-0.550500	-3.779115
C	-1.686390	0.221074	-4.769747
C	-1.361001	0.188136	-6.134106
C	-2.043629	0.999160	-7.047994
C	-3.056920	1.856302	-6.606361
C	-3.387266	1.892327	-5.245886
C	-2.702055	1.087287	-4.335212
Cl	-3.289111	-0.273612	-0.819698
C	0.052270	-3.104189	0.141620
C	0.968992	-4.128592	-0.137792
C	0.659738	-5.456523	0.178295
C	-0.560353	-5.770657	0.784949
C	-1.479856	-4.751634	1.063419
C	-1.183124	-3.428051	0.732001
C	2.134994	-1.306395	-0.808289

C	3.197229	-0.898622	0.012992
C	4.498626	-0.821947	-0.495575
C	4.759927	-1.169280	-1.823386
C	3.710988	-1.597931	-2.645448
C	2.410454	-1.654641	-2.143339
H	4.278168	4.051776	-2.460516
H	2.854235	5.251076	-0.800829
H	0.699843	4.275825	-0.065320
H	-2.793819	5.270928	-3.507068
H	-1.024454	3.630900	-2.948550
H	3.533655	1.845539	-3.368936
H	1.399330	0.853645	-2.601877
H	5.310667	-0.487824	0.153537
H	5.775759	-1.106173	-2.218307
H	-2.945242	1.120653	-3.269430
H	-4.165076	2.570464	-4.887818
H	-3.577410	2.503196	-7.315736
H	-1.768392	0.974693	-8.104738
H	-0.553248	-0.461759	-6.481350
H	-0.506293	0.301154	-3.023487
H	3.024599	-0.629782	1.055578
H	-4.741518	5.587494	-1.976519
H	-0.435893	2.772130	1.433822
H	-4.905838	4.229728	0.111560
H	0.743272	1.090626	2.699394
H	-3.164916	2.564749	0.654991
H	-1.502695	1.348415	1.501761
H	-0.564390	-0.920435	1.915981
H	1.930750	-3.893874	-0.597191
H	-1.756811	-4.040405	-1.777550
H	-3.643365	-1.207626	-4.425161
H	-5.678714	-2.587381	-4.449203
H	-5.815918	-4.674681	-3.082426
H	-3.822345	-5.394451	-1.746172
H	-0.796529	-6.806495	1.036709
H	-2.439843	-4.991595	1.525097
H	-1.927127	-2.644887	0.901875
H	1.381317	-6.245441	-0.045125
H	1.600038	-1.971335	-2.802782
H	3.903549	-1.876538	-3.683547
H	1.553926	1.188399	1.141411
H	1.175335	-1.193318	2.044946
H	0.139133	-0.760211	-4.228740
H	-0.442407	-2.458834	-2.846259

Int-6

C	7.130379	6.176645	-4.309332
C	6.214977	5.779921	-5.296907
C	5.833249	6.700289	-6.289021

C	6.354311	7.995701	-6.286957
C	7.256790	8.389898	-5.292974
C	7.644761	7.477123	-4.306624
P	5.510415	4.062473	-5.359503
Ni	3.431468	3.562959	-4.898768
C	3.113982	5.125659	-3.579931
C	3.328549	6.561764	-4.024299
C	6.068452	3.640315	-7.101457
C	6.068184	2.153654	-7.451026
C	4.667159	1.577895	-7.634303
P	3.566643	1.652403	-6.131830
C	2.004296	1.076428	-6.942189
C	1.476523	-0.205510	-6.749318
C	0.311805	-0.592689	-7.423017
C	-0.324765	0.293545	-8.296936
C	0.205526	1.574807	-8.495948
C	1.360957	1.965678	-7.818054
C	4.105281	0.243874	-5.059191
C	5.108030	-0.660336	-5.440691
C	5.528297	-1.661178	-4.558256
C	4.945116	-1.775499	-3.293460
C	3.935227	-0.884667	-2.912142
C	3.524465	0.125016	-3.783696
C	6.687156	3.068333	-4.331324
C	6.192505	2.319393	-3.257311
C	7.048823	1.515938	-2.500452
C	8.408908	1.456010	-2.812240
C	8.913614	2.208994	-3.880441
C	8.058523	3.011548	-4.638249
C	3.794720	4.712269	-2.325313
C	3.296864	3.613599	-1.581228
C	3.934945	3.162875	-0.427209
C	5.093390	3.800730	0.039275
C	5.583230	4.907486	-0.659857
C	4.941898	5.360347	-1.816342
H	4.697326	0.537498	-7.990723
H	6.630354	1.587827	-6.691664
H	5.416121	4.200766	-7.788697
H	5.131065	2.365373	-3.013650
H	8.468158	3.594292	-5.465904
H	6.645441	0.934353	-1.669505
H	9.976843	2.169186	-4.126435
H	9.079208	0.824495	-2.225240
H	5.105183	6.420788	-7.052644
H	7.441685	5.470855	-3.538900
H	6.040660	8.703313	-7.056837
H	8.352044	7.774854	-3.529800
H	7.657977	9.405343	-5.288351
H	2.751188	0.833586	-3.479224
H	5.576793	-0.596181	-6.423413

H	3.474465	-0.967731	-1.925522
H	6.316472	-2.352479	-4.863719
H	5.277536	-2.555206	-2.605084
H	1.967481	-0.904031	-6.069001
H	1.757211	2.974885	-7.960833
H	-0.096352	-1.593106	-7.263385
H	-0.286621	2.272508	-9.176975
H	-1.233008	-0.010655	-8.821343
H	7.079799	4.057846	-7.204602
H	6.618049	2.026562	-8.397274
H	4.126525	2.154262	-8.401343
H	3.528726	2.303801	0.112466
H	2.403695	3.102429	-1.947473
H	5.345132	6.231877	-2.331434
H	6.475085	5.428107	-0.301850
H	5.600569	3.442759	0.937589
H	4.398022	6.808977	-4.085959
Cl	1.275085	2.866066	-4.419858
H	2.037438	4.938418	-3.486291
C	2.700285	6.994168	-5.333456
C	2.053851	6.110729	-6.210295
C	2.807694	8.343101	-5.720400
C	1.550566	6.551374	-7.441275
H	1.945602	5.058306	-5.931035
C	2.307136	8.789434	-6.944880
H	3.312998	9.048664	-5.054830
C	1.677332	7.891156	-7.817350
H	1.054617	5.840472	-8.107332
H	2.412901	9.840412	-7.223902
H	1.287681	8.235827	-8.777662
H	2.935654	7.224257	-3.226206

TS6

C	0.408419	4.189431	-4.482826
C	0.779202	3.063315	-5.237327
C	-0.171783	2.050508	-5.465302
C	-1.467870	2.169105	-4.962619
C	-1.831379	3.293730	-4.209450
C	-0.890536	4.301600	-3.973481
P	2.520855	2.739521	-5.747672
C	2.352382	2.187814	-7.513135
C	1.658695	2.974539	-8.448317
C	1.615830	2.592190	-9.791331
C	2.264503	1.422946	-10.210952
C	2.949977	0.635392	-9.281860
C	2.992853	1.015478	-7.936121
Ni	3.947795	1.519265	-4.637117
P	5.936189	2.124240	-5.237304
C	5.890879	3.947217	-5.640923

C	4.726843	4.384089	-6.560336
C	3.303134	4.429474	-5.962858
Cl	3.569996	-0.697123	-4.708137
C	6.483688	1.313479	-6.815499
C	6.363109	-0.083482	-6.911655
C	6.718656	-0.743492	-8.089833
C	7.181314	-0.015042	-9.192257
C	7.300431	1.374988	-9.103543
C	6.956807	2.038580	-7.920703
C	7.374036	1.903798	-4.094541
C	7.239004	0.925182	-3.097661
C	8.273111	0.700508	-2.184792
C	9.442547	1.465824	-2.254172
C	9.580006	2.444898	-3.245719
C	8.552609	2.661042	-4.169277
C	2.696959	2.257530	-1.927566
C	2.077111	0.971800	-1.627367
C	2.735814	-0.065965	-0.934458
C	2.069578	-1.248719	-0.622464
C	0.730301	-1.429761	-0.995797
C	0.067599	-0.415979	-1.696510
C	0.733951	0.768810	-2.008454
C	3.971732	2.644749	-1.651535
C	4.509568	3.993063	-1.840009
C	3.690067	5.112636	-2.111657
C	4.239828	6.383160	-2.273360
C	5.623497	6.576937	-2.161244
C	6.449841	5.481407	-1.886914
C	5.899971	4.208234	-1.724628
H	2.659275	5.040564	-6.612909
H	4.719212	3.774140	-7.477675
H	5.820009	4.451771	-4.664392
H	5.951328	-0.647662	-6.071365
H	7.060886	3.123218	-7.877572
H	6.616776	-1.828945	-8.154152
H	7.659322	1.951169	-9.959169
H	7.443267	-0.529000	-10.119483
H	8.678046	3.422925	-4.941659
H	6.308890	0.352179	-3.040706
H	10.492703	3.041903	-3.301138
H	8.161242	-0.064315	-1.413471
H	10.247496	1.299969	-1.535296
H	3.526706	0.404588	-7.205850
H	1.148969	3.887541	-8.131273
H	3.459152	-0.276254	-9.602035
H	1.077917	3.209706	-10.513883
H	2.234064	1.129539	-11.262414
H	0.108179	1.162375	-6.036883
H	1.125068	4.990661	-4.291955
H	-2.195663	1.377202	-5.152235

H	-1.167193	5.183386	-3.391855
H	-2.843492	3.382394	-3.810149
H	6.843799	4.260117	-6.092181
H	4.960798	5.409495	-6.888204
H	3.328132	4.904553	-4.970029
H	2.593775	-2.035302	-0.075125
H	3.775745	0.057554	-0.625261
H	0.214621	1.556141	-2.560748
H	-0.974696	-0.547273	-1.995794
H	0.208290	-2.353487	-0.737934
H	4.162517	2.845537	-4.152416
H	2.606713	4.991674	-2.171846
H	6.554165	3.357416	-1.520486
H	3.583350	7.233439	-2.470556
H	7.529158	5.620144	-1.794840
H	6.049438	7.575672	-2.274927
H	4.678747	1.917821	-1.240949
H	2.016429	2.985752	-2.379814

TS6'

C	0.228793	4.345118	-5.765963
C	0.859121	3.148068	-6.120945
C	0.144629	1.945714	-6.095712
C	-1.205187	1.910863	-5.715137
C	-1.828510	3.123108	-5.375647
C	-1.121606	4.326552	-5.397135
C	-1.972954	0.606654	-5.695616
C	-2.791059	0.361938	-4.425557
Ni	-1.877695	0.503017	-1.905122
O	-0.676259	-1.013159	-3.111091
C	0.629135	-0.801871	-3.665905
C	-3.980993	-0.445904	-4.533505
C	-4.134883	-1.475450	-5.507069
C	-5.312405	-2.216308	-5.611020
C	-6.399158	-1.976009	-4.758670
C	-6.275936	-0.967064	-3.787003
C	-5.100352	-0.231956	-3.678346
Cl	-0.356570	2.093750	-2.268529
P	-2.982634	1.861067	-0.608240
C	-4.627022	1.273506	0.037708
C	-4.550854	-0.073753	0.760324
C	-4.330275	-1.264766	-0.178907
P	-2.664583	-1.316250	-0.992380
C	-1.463820	-1.654699	0.380627
C	-0.107228	-1.349464	0.173529
C	0.834222	-1.586304	1.177202
C	0.427863	-2.113605	2.407590
C	-0.919893	-2.419164	2.620678
C	-1.862619	-2.198921	1.610643

C	-3.417889	3.419064	-1.503874
C	-2.575385	4.539314	-1.414605
C	-2.857799	5.692511	-2.148961
C	-3.974862	5.738941	-2.990150
C	-4.814362	4.625301	-3.087539
C	-4.536668	3.470610	-2.350488
C	-2.135674	2.421012	0.935798
C	-0.883181	1.888073	1.263051
C	-0.258003	2.244472	2.461423
C	-0.877722	3.145887	3.332127
C	-2.124319	3.692605	3.001894
C	-2.754540	3.331487	1.808799
C	-2.705218	-2.922522	-1.913500
C	-1.555831	-3.729575	-1.966744
C	-1.579320	-4.945707	-2.649765
C	-2.746950	-5.367976	-3.298578
C	-3.886100	-4.561260	-3.261399
C	-3.867370	-3.341351	-2.577482
H	-0.639128	-3.409453	-1.471882
H	-4.798659	-4.868265	-3.776102
H	-2.763961	-6.319811	-3.833633
H	-0.681010	-5.566170	-2.676487
H	-4.764255	-2.722647	-2.587070
H	-5.063369	-1.237170	-1.000161
H	-4.479817	-2.218211	0.347974
H	-5.504248	-0.233480	1.286884
H	-3.773565	-0.043182	1.541912
H	-2.906382	-2.454950	1.797861
H	-1.243975	-2.831513	3.578293
H	1.159893	-2.285761	3.199109
H	1.884403	-1.343950	1.002156
H	0.202314	-0.911201	-0.777220
H	-0.404481	1.195448	0.571316
H	-3.723409	3.770565	1.559514
H	-2.607836	4.402961	3.675578
H	-0.390879	3.426067	4.268544
H	0.714504	1.816342	2.713158
H	-5.007892	2.055470	0.710309
H	-5.205541	2.614777	-2.450668
H	-5.689269	4.649702	-3.740294
H	-4.189394	6.639479	-3.568867
H	-2.195618	6.557232	-2.069719
H	-1.693364	4.506386	-0.774673
H	-5.021991	0.553913	-2.924462
H	-3.305062	-1.702869	-6.180220
H	-5.381932	-3.003426	-6.366886
H	-7.318178	-2.558403	-4.845665
H	-5.325494	1.208525	-0.809530
H	-7.110168	-0.752821	-3.112938
H	1.365667	-1.180239	-2.943055

H	0.820643	0.265556	-3.850126
H	0.734211	-1.370807	-4.604328
H	-1.417477	-0.627231	-3.713639
H	0.647153	1.012406	-6.363947
H	-2.875788	3.123406	-5.064463
H	1.912681	3.147801	-6.410870
H	-1.624316	5.252478	-5.108773
H	0.785623	5.284950	-5.774950
H	-1.265808	-0.213100	-5.919408
H	-2.666834	0.610421	-6.563786
H	-2.947651	1.279286	-3.838929

Pdt'

C	-2.226434	0.308867	-0.020486
H	-1.923540	0.868004	-0.920232
H	-3.325945	0.249317	-0.028440
C	-1.778107	1.120240	1.225140
H	-2.186370	2.139534	1.135752
H	-0.680440	1.206940	1.215166
C	-1.638327	-1.080898	-0.058007
C	-2.362861	-2.187427	0.412536
C	-0.326322	-1.289640	-0.515418
C	-1.796401	-3.466123	0.427018
H	-3.383044	-2.042010	0.777353
C	0.245545	-2.565413	-0.502899
H	0.253915	-0.440385	-0.887669
C	-0.488677	-3.659935	-0.030214
H	-2.378236	-4.313418	0.797260
H	1.265574	-2.707190	-0.867753
H	-0.044161	-4.657655	-0.020894
C	-2.229439	0.498944	2.524586
C	-3.539793	0.693100	2.992506
C	-1.372600	-0.329285	3.266607
C	-3.981982	0.079347	4.168484
H	-4.220369	1.336354	2.427346
C	-1.808658	-0.945289	4.444162
H	-0.353048	-0.497028	2.910551
C	-3.115999	-0.743038	4.899639
H	-5.003591	0.245714	4.517913
H	-1.126273	-1.586251	5.007450
H	-3.458135	-1.220591	5.820304
