IBzH (IBenzhydryl): Sterically-Flexible N-Aliphatic *N*-Heterocyclic Carbenes (NHC) for Iron-Catalyzed C(sp³)–C(sp²) Cross-Coupling of Unactivated Haloalkanes

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Electronic Supplementary Information

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List of Known Compounds/General Methods

All compounds reported in the manuscript are commercially available or have been previously described in literature unless indicated otherwise. All experiments involving iron were performed using standard Schlenk techniques under argon or nitrogen atmosphere unless stated otherwise. All solvents were purchased at the highest commercial grade and used as received or after purification by distillation from sodium/benzophenone under nitrogen. All solvents were deoxygenated prior to use. All other chemicals were purchased at the highest commercial grade and used as received. Reaction glassware was oven-dried at 140 °C for at least 24 h or flame-dried prior to use, allowed to cool under vacuum and purged with argon (three cycles). All products were identified using ^{1}H NMR analysis and comparison with authentic samples. All yields refer to yields determined by ^{1}H NMR using an internal standard unless stated otherwise. GC and/or GC/MS analysis was used for volatile products. ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ on Bruker spectrometers at 400 (^{1}H NMR) and 100 MHz (^{13}C NMR). All shifts are reported in parts per million (ppm) relative to residual $CHCl_3$ peak (7.27 and 77.2 ppm, ^{1}H NMR and ^{13}C NMR, respectively). All coupling constants (J) are reported in hertz (Hz). Abbreviations are: s, singlet; d, doublet; t, triplet; q, quartet; brs, broad singlet; dd, doublet of doublets; ddd. GC-MS chromatography was performed using Agilent HP5890/2 GC system using helium as the carrier gas at a flow rate of 1 mL/min and an initial oven temperature of 50 °C. The injector temperature was 250 °C. The detector temperature was 250 °C. For runs with the initial oven temperature of 50 °C, temperature was increased with a 10 °C/min ramp after 50 °C hold for 3 min to a final temperature of 250 °C, then hold at 250 °C for 15 min (splitless mode of injection, total run time of 35.0 min). All flash chromatography was performed using silica gel, 60 Å, 300 mesh. TLC analysis was carried out on aluminum plates coated with silica gel 60 F254, 0.2 mm thickness. The plates were visualized using a 254 nm ultraviolet lamp or aqueous potassium permanganate solutions. ^{1}H NMR and ^{13}C NMR data are given for all products in the Supplementary Experimental for characterization purposes. All products have been previously reported, unless stated otherwise.

Experimental Procedures and Characterization Data

IPr, IMes, ICy, I*t*Bu salts were purchased from Sigma Aldrich, AmBeed or Strem Chemicals. Other imidazolium salts, silver and selenium complexes were prepared by procedures reported in the literature.[1-4] **IPr*·HCl**,[1] **IBzH·HCl**,[2] **IBn·HCl**,[5] **[Se(IBzH)]**,[6] **2a**,[7] **2b**,[7] **2c**,[7] **2d**,[7] **2e**,[7] **2f**,[8] **2g**,[9] **2h**,[10] **2i**,[11] **2j**,[11] **2k**,[11] **2l**,[12] **2m**,[12] **2n**,[12] **2o**,[12] **2p**,[13] **2q**,[14] **2r**,[15] **2s**,[15] **2t**,[15] **2u**,[16] **2v**,[16] **2x**,[16] **2y**,[17] **2z**,[18] **2aa**,[19] **2ab**,[19] **2ac**,[19] **2ad**,[20] **2ae**,[21] **2af**,[22] **2ag**,[23] **2ah**[24] are known compounds. Spectroscopic data match those reported in the literature.

General Procedure for the Synthesis of IBzH·HCl. A mixture of (trimethylsilyl)imidazole (4.208 g, 30 mmol, 1.0 equiv.) and chlorodiphenylmethane (12.16 g, 60 mmol, 2.0 equiv.) in acetonitrile (60 ml) was refluxed for 24 h. After the removal of the solvents, the resulting solid was filtered, washed with diethyl ether (3 x 9 ml) and dried under vacuum. Yield: 90% (11.79 g).

General Procedure for the Synthesis of [Ag(IBzH)Cl]. A mixture of IBzH·HCl (131 mg, 0.3 mmol, 1.0 equiv.) and $AgNO_3$ (51 mg, 0.3 mmol, 1.0 equiv.), in dry dichloromethane (15 ml) was stirred for 2 min and then K_2CO_3 (691 mg, 5 mmol, 20 equiv.) was added. The reaction was stirred overnight in RT. The mixture was filtered and the solvent was concentrated. The product was obtained by precipitation with cold ether as white solid. Yield: 77% (125 mg).

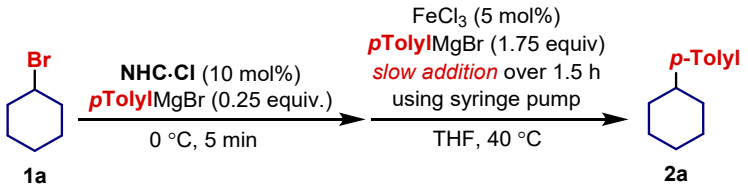
General Procedure for the Synthesis of [Se(IBzH)]. An oven-dried flask equipped with a stir bar was charged with IBzH·HCl (112 mg, 0.26 mmol, 1.0 equiv.) and selenium (62.4 mg, 0.79 mmol, 3.0 equiv.), placed under a positive pressure of argon and subjected to three evacuation/backfilling cycles under high vacuum. THF (2.6mL, 0.10 M) and NaHMDS (1.0 M in THF, 0.32 mL, 0.32 mmol, 1.2 equiv.) were added at -78 °C, the resulting mixture was stirred for 30 min at -78 °C and then at room temperature for 16 h. The reaction mixture was diluted with CH_2Cl_2 and filtered. The solution was collected and concentrated. The product was obtained by trituration from diethyl ether as a pale yellow solid. Yield: 81% (101 mg).

General Procedure for Iron-Catalyzed C(sp^3)–C(sp^2) Cross-Coupling. NHC·HCl (neat, typically, 10 mol%) was placed in Schlenk flask and dried under vacuum. Then a small portion of Grignard reagent solution (typically, 0.25 equiv.) was added at 0 °C and allowed to stir for 5 min. After indicated time 0.1 M THF solution of $FeCl_3$ (typically, 5 mol%) was added followed by the addition of alkyl bromide (typically, 0.25 mmol). Grignard reagent solution (typically,1.75 equiv.) was then added slowly using syringe pump over period of 90 min at 40 °C. The reaction mixture was stirred at that temperature for 10 min after completion of the addition of Grignard reagent. After the indicated time, the reaction mixture was cooled to room temperature, diluted with HCl (1.0 *N*, 1.0 mL) and Et_2O (1 x 2 mL), the organic layer was extracted with HCl (1.0 *N*, 2 x 5 mL), the reaction mixture was filtered through a pad of Florisil®, and dried in vacuo. The sample was analyzed by ^{1}H NMR ($CDCl_3$, 400 MHz) to obtain conversion, yield and selectivity using internal standard and comparison with authentic samples. Analytical sample was purified by chromatography on silica gel (EtOAc/hexanes).

General Procedure for Iron-Catalyzed C(sp^3)–C(sp^3) Cross-Coupling. NHC·HCl (neat, typically, 6 mol%) and iron (III) acetylacetonate (neat, typically, 2.5 mol%) were placed in Schlenk flask and dried under vacuum. Then dry THF (0.089M) was added and heated to 55 °C. A 0.5 M solution of alkylmagnesium bromide (30 mol%) was added to the mixture and stirred for 30 min at 55 °C, and then cooled to room temperature. Then alkyl bromide (typically, 0.25 mmol) was added. Grignard reagent solution (typically,1.50 mmol) was then added slowly using syringe pump over period of 17.5 hour (flow rate 0.16 ml/h). The reaction was stirred of 8 hours at room temperature after the addition of Grignard reagent solution. After the indicated time, hydrolyzed with saturated aqueous NH_4Cl solution (5 mL). The aqueous phase was extracted with DCM (3 × 5 mL) and the combined organic phases were dried over $MgSO_4$ and dried in vacuo. The sample was analyzed by ^{1}H NMR ($CDCl_3$, 400 MHz) to obtain conversion, yield and selectivity using internal standard and comparison with authentic samples. Analytical sample was purified by chromatography on silica gel (EtOAc/hexanes).

Additional Optimization Studies

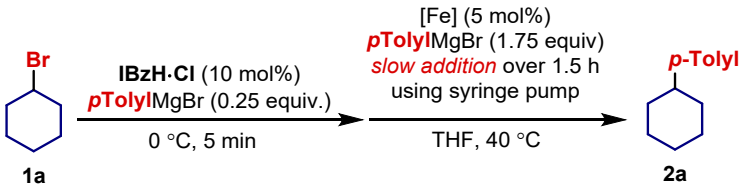
Table 1 Optimization of Fe–NHC Catalyzed C(sp³)–C(sp²) Cross-Coupling[a]



Entry	Catalyst	[Fe] mol%	Ligand	Yield **2a** (%)[b]
1	$FeCl_3$	5 mol%	IBzH·HCl	98
2[c]	$FeCl_3$	5 mol%	IBzH·HCl	25
3[d,e]	$FeCl_3$	5 mol%	IBzH·HCl	44
4[d]	$FeCl_3$	5 mol%	IBzH·HCl	97
5	$FeCl_3$	5 mol%	IPr·HCl	98
6[d]	$FeCl_3$	5 mol%	IPr·HCl	88
7	$FeCl_3$	5 mol%	SIPr·HCl	87
8	$FeCl_3$	5 mol%	IPr*·HCl	16
9	$FeCl_3$	5 mol%	IMes·HCl	88
10	$FeCl_3$	5 mol%	ICy·HCl	93
11[d]	$FeCl_3$	5 mol%	ICy·HCl	53
12	$FeCl_3$	5 mol%	I*t*Bu·HCl	85
13	$FeCl_3$	5 mol%	IBn·HCl	56
14	$FeCl_3$	5 mol%	-	10

[a]Conditions: bromocyclohexane **1a** (0.25 mmol), [Fe] (5 mol%) NHC·HCl (10 mol%), THF (0.45 M), p-TolMgBr (2.0 equiv, 1.0 M, THF), ArMgBr added over the period of 1.5 h by syringe pump, 40 °C, 10 min. [b]Determined by ^{1}H NMR. [c]p-TolylMgBr added by one shot. [d]Without initial activation. [e]RT.

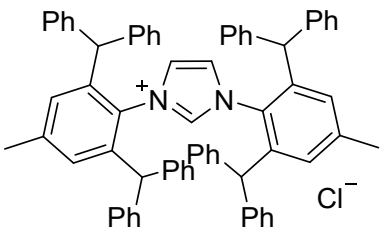
Table 2 Optimization of Fe–NHC Catalyzed Cross-Coupling: Screening of Iron Source[a]



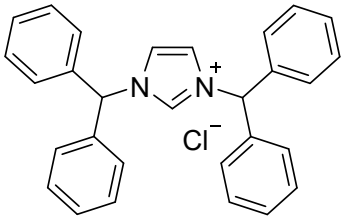
Entry	Catalyst	[Fe] mol%	Yield **2a** (%)[b]
1	$FeCl_3$	5 mol%	98
2	$Fe(acac)_3$	5 mol%	81
3	$FeBr_3$	5 mol%	96
4	$FeF_3{\cdot}3H_2O$	5 mol%	0
5	-	-	0

[a]Conditions: bromocyclohexane **1a** (0.25 mmol), [Fe] (5 mol%) IBzH·HCl (10 mol%), THF (0.45 M), p-TolMgBr (2.0 equiv, 1.0 M, THF), ArMgBr added over the period of 1.5 h by syringe pump, 40 °C, 10 min. [b]Determined by ^{1}H NMR.

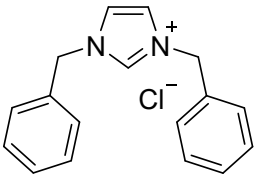
Characterization Data of Ligands and Complexes



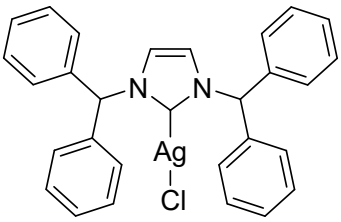
IPr*·HCl Yield 79%, (0.804 g). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 12.02 (s, 1H), 7.30 – 7.12 (m, 24H), 6.79 (d, *J* = 6.1 Hz, 12H), 5.55 (s, 2H), 5.21 (s, 4H), 2.21 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 142.65, 141.89, 140.71, 131.04, 130.18, 130.03, 129.40, 128.91, 128.82, 127.23, 127.14, 123.80, 51.57, 22.09.



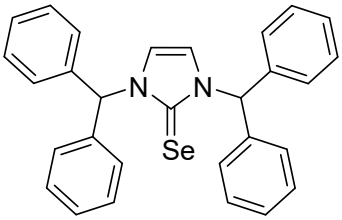
IBzH·HCl Yield 65%, (7.835 g). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.41 (s, 1H), 7.54 (s, 2H), 7.40 – 7.37 (m, 12H), 7.26 – 7.24 (m, 8H), 7.15 (d, *J* = 1.5 Hz, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 138.80, 136.46, 129.53, 128.35, 121.39, 67.22.



IBn·HCl Yield 50%, (1.757 g). Pale yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.99 (s, 1H), 7.48 – 7.46 (m, 4H), 7.44 (s, 2H), 7.33 – 7.32 (m, 6H), 5.55 (s, 4H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 137.25, 133.12, 129.39, 129.37, 128.95, 122.13, 53.26.

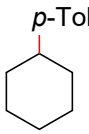


[Ag(IBzH)Cl] Yield 77%, (0.125 g). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.37 – 7.36 (m, 12H), 7.11 (d, *J* = 5.4 Hz, 8H), 6.89 (s, 4H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 138.54, 129.23, 128.86, 128.36, 120.94, 69.63. Anal. calcd for $C_{29}H_{25}AgClN_2$ (544.85): C, 63.93; H, 4.63; N, 5.14. Found: C, 63.95; H, 4.60; N, 5.15.



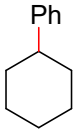
[Se(IBzH)] Yield 81%, (1.01 g). Pale yellow solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.66 (s, 2H), 7.38 – 7.32 (m, 12H), 7.18 – 7.16 (m, 8H), 6.73 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 138.71, 128.94, 128.75, 128.26, 118.30, 66.06. **^{77}Se NMR (95 MHz, CDCl3)** δ 22.83.

Characterization Data of Cross-Coupling Products



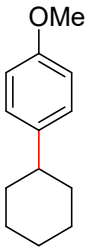
2a

1-Cyclohexyl-4-methylbenzene (**2a**). Yield 98% (42.70 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.10 (s, 4H), 2.49 – 2.42 (m, 1H), 2.31 (s, 3H),1.87 – 1.81 (m, 4H), 1.76 – 1.72 (m, 1H), 1.45 – 1.328 (m, 4H), 1.29 – 1.19 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ145.34, 135.36, 129.14, 126.86, 44.33, 34.75, 27.13, 26.36, 21.17.



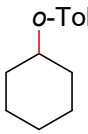
2b

Cyclohexylbenzene (**2b**). Yield 86% (34.46 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.31 – 7.27 (m, 2H), 7.22– 7.15 (m, 3H), 2.52 – 2.46 (m, 1H), 1.89 – 1.82 (m, 4H), 1.77 – 1.72 (m, 1H), 1.44 – 1.36 (m, 4H), 1.30 – 1.22 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 148.28, 128.45, 127.00, 125.94, 44.77, 34.64, 27.10, 26.35.



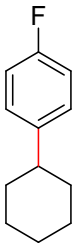
2c

1-Cyclohexyl-4-methoxybenzene (**2c**). Yield 96% (45.67 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.13 (d, J = 8.4 Hz, 2H), 6.83 (d, J = 8.7 Hz, 2H), 3.78 (s, 3H), 2.48 – 2.41 (m, 1H), 1.86 – 1.81 (m, 4H), 1.76 – 1.71 (m, 1H), 1.40 – 1.35 (m, 4H), 1,29 – 1.21 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.63, 140.38, 127.63, 113.64, 55.24, 43.69, 34.73, 26.97, 26.19.



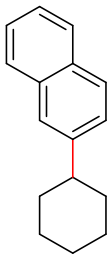
2d

1-Cyclohexyl-2-methylbenzene (**2d**). Yield 71% (30.94 mg). White solid**. ^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.24 – 7.05 (m, 4H), 2.73 – 2.67 (m, 1H), 2.33 (s, 3H), 1.87 – 1.74 (m, 5H), 1.44 – 1.38 (m, 4H), 1.29 – 1.26 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 146.09, 135.29, 130.36, 126.26, 125.63, 125.54, 40.26, 33.82, 27.36, 26.52, 19.54.



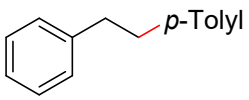
2e

1-Cyclohexyl-4-fluorobenzene (**2e**). Yield 85% (37.85 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.17 – 7.13 (m, 2H), 6.99 – 6.93 (m, 2H), 2.50 – 2.45 (m, 1H), 1.86 – 1.83 (m, 4H), 1.76 – 1.72 (m, 1H), 1.43 – 1.35 (m, 4H), 1.29 – 1.21 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.28 (d, J^F = 243.2 Hz), 143.90 (d, J^F = 3.4 Hz), 128.24 (d, J^F = 7.6 Hz), 115.08 (d, J^F = 20.9 Hz), 44.01, 34.83, 27.04, 26.27.



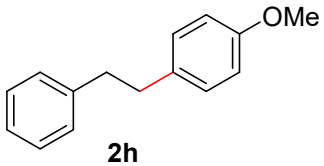
2f

2-Cyclohexylnaphthalene (**2f**). Yield 96% (50.48 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.79 – 7.75 (m, 3H), 7.62 (s, 1H), 7.45 – 7.35 (m, 3H), 2.69 – 2.62 (m, 1H), 1.98 – 1.94 (m, 2H), 1.89 – 1.85 (m, 2H), 1.80 – 1.75 (m, 1H), 1.57 – 1.38 (m. 4H), 1.34 – 1.25 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 145.74, 133.83, 132.26, 127.88, 127.76, 127.72, 126.38, 125.93, 125.18, 124.69, 44.84, 34.59, 27.12, 26.40.



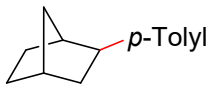
2g

1-Methyl-4-phenethylbenzene (**2g**). Yield 51% (25.06 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.30 – 7.26 (m, 2H), 7.21 – 7.17 (m, 3H), 7.09 (s, 4H), 2.89 (s, 4H), 2.32 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 142.10, 138.91, 135.53, 129.20, 128.62, 128.49, 126.05, 38.28, 37.70, 21.21.



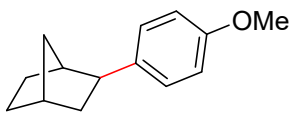
2h

1-Methoxy-4-phenethylbenzene (**2h**). Yield 72% (38.21 mg). Off-white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.30 – 7.26 (m, 2H), 7.21 – 7.16 (m, 3H), 7.09 (d, J = 8.7 Hz, 2H), 6.82 (d, J = 8.7 Hz, 2H), 7.39 (s, 3H), 2.92 – 2.83 (m, 4H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.97, 142.03, 134.05, 129.52, 128.65, 128.48, 126.04, 113.88, 55.42, 38.40, 37.22.



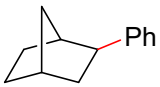
2i

2-(p-Tolyl)bicyclo[2.2.1]heptane (**2i**). Yield 98% (45.64 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.12 – 7.07 (m, 4H), 2.72 – 2.68 (m, 1H), 2.31 (s, 3H), 1.77 – 1.71 (m, 1H), 1.67 – 1.51 (m, 4H), 1.37 – 1.22 (m, 2H), 1.18 – 1.14 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 144.80, 134.94, 129.05, 127.15, 47.10, 43.25, 39.27, 36.97, 36.19, 30.75, 29.10, 21.08.



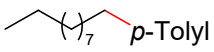
2j

2-(4-methoxyphenyl)bicyclo[2.2.1]heptane (**2j**). Yield 87% (44.00 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.13 (d, J = 8.4 Hz, 2H), 6.83 (d, J = 8.8 Hz, 2H), 3.78 (s, 3H), 2.69 (dd, J = 8.8, 5.6 Hz, 1H), 2.33 – 2.30 (m, 2H), 1.77 – 1.71 (m, 1H), 1.65 – 1.49 (m, 4H), 1.37 – 1.14 (m, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.53, 139.98, 128.11, 113.71, 55.41, 46.69, 43.35, 39.36, 36.96, 36.11, 30.70, 29.09.



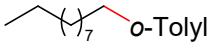
2k

2-phenylbicyclo[2.2.1]heptane (**2k**). Yield 92% (39.61 mg) colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.29 – 7.12 (m, 5H), 2.74 (dd, *J* = 8.8, 5.8 Hz, 1H), 2.36 – 2.34 (m, 2H), 1.79 – 1.73 (m, 1H), 1.69 – 1.51 (m, 4H), 1.38 – 1.32 (m, 2H), 1.29 – 1.23 (m, 2H), 1.20 – 1.15 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 147.79, 128.37, 127.24, 125.53, 47.49, 43.07, 39.31, 37.00, 36.25, 30.77, 29.09.



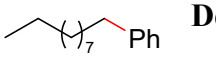
2l

1-Decyl-4-methylbenzene (**2l**). Yield 84% (48.81 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.10 – 7.05 (m, 4H), 2.55 (t, *J* = 7.8 Hz, 2H), 2.31 (s, 3H), 1.62 – 1.54 (m, 2H), 1.33 – 1.25 (m, 14H), 0.88 (t, *J* = 6.7 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 140.07, 135.10, 129.08, 128.45, 35.72, 32.10, 31.87, 29.83, 29.80, 29.73, 29.54, 22.89, 21.18, 14.32.



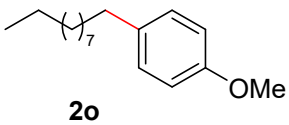
2m

1-Decyl-2-methylbenzene (**2m**). Yield 82% (47.64 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.13 – 7.06 (m, 4H), 2.60 – 2.56 (m, 2H), 2.30 (m, 3H), 1.59 – 1.52 (m, 2H), 1.37 – 1.26 (m, 14H), 0.88 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 141.32, 136.00, 130.24, 128.95, 126.00, 125.87, 33.54, 32.11, 30.50, 29.94, 29.83, 29.77, 29.55, 22.89, 19.48, 14.33.



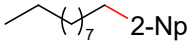
2n

Decylbenzene (**2n**). Yield 61% (33.30 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.29 – 7.25 (m, 2H), 7.19 – 7.15 (m, 3H), 2.60 (t, *J* = 7.7 Hz, 2H), 1.64 – 1.57 (m, 2H), 1.31 – 1.26 (m, 14H), 0.88 (t, *J* = 7.06 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 143.16, 128.58, 128.39, 125.71, 36.19, 32.10, 31.74, 29.82, 29.79, 29.72, 29.54, 22.88, 14.32.



2o

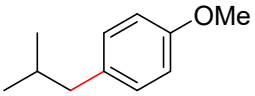
1-Decyl-4-methoxybenzene (**2o**). Yield 76% (47.20 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.09 (d, *J* = 8.6 Hz, 2H), 6.82 (d, *J* = 8.7 Hz, 2H), 3.78 (s, 3H), 2. 54 (t, *J* = 7.9 Hz, 2H), 1.59 – 1.53 (m, 2H), 1.30 – 1.25 (m, 14H), 0.88 (t, *J* = 6.7 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.73, 135.25, 129.42, 113.79, 55.42, 35.23, 32.10, 31.98, 29.81, 29.72, 29.53, 29.48, 22.88, 14.32.



2p

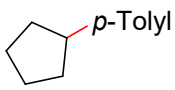
2-Decylnaphthalene (**2p**). Yield 95% (63.75 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.80 – 7.74 (m, 3H), 7.60 (s, 1H), 7.41 (qd, *J* = 6.9, 1.5 Hz, 2H),

7.32 (dd, *J* = 8.4, 1.7 Hz, 1H), 2.75 (t, *J* = 7.8 Hz, 2H), 1.73 – 1.65 (m, 2H), 1.39 – 1.25 (m, 14H), 0.87 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 140.49, 133.62, 131.90, 127.71, 127.59, 127.47, 127.39, 126.28, 125.79, 124.97, 36.14, 31.92, 31.42, 29.65, 29.63, 29.57, 29.36, 22.71, 14.15.



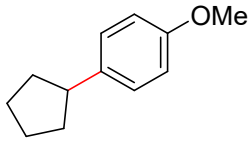
2q

1-Isobutyl-4-methoxybenzene (**2q**). Yield 86% (35.31 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.06 (d, *J* = 8.7 Hz, 2H), 6.82 (d, *J* = 8.7 Hz, 2H), 3.79 (s, 3H), 2.41 (d, *J* = 7.2 Hz, 2H), 1.86 – 1.76 (m, 1H), 0.89 (d, *J* = 6.7 Hz, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.80, 134.00, 130.14, 113.64, 55.41, 44.70, 30.56, 22.49.



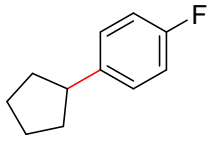
2r

1-Cyclopentyl-4-methylbenzene (**2r**). Yield 94% (37.66 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** 7.15 – 7.09 (m, 4H), 2.99 – 2.91 (m, 1H), 2.32 (s, 3H), 2.08 – 2.01 (m 2H), 1.81 – 1.76 (m, 2H), 1.70 – 1.64 (m, 2H), 1.61 – 1.54 (m, 2H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 143.63, 135.28, 129.09, 127.16, 45.75, 34.86, 25.67, 21.15.



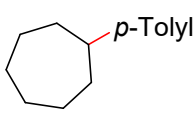
2s

1-Cyclopentyl-4-methoxybenzene (**2s**). Yield 81% (35.69 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.16 (d, *J* = 8.3 Hz, 2H), 6.84 (d, *J* = 8.7 Hz, 2H), 3.79 (s, 3H), 2.98 – 2.89 (m, 1H), 2.08 – 2.00 (m, 2H), 1.81 – 1,75 (m, 2H), 1.70 – 1.63 (m, 2H), 1.59 – 1.49 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.78, 138.72, 128.11, 113.79, 55.45, 45.33, 34.91, 25.59.



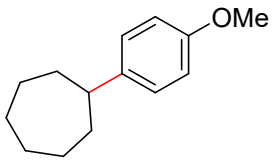
2t

1-Cyclopentyl-4-fluorobenzene (**2t**). Yield 61% (25.04 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.20 – 7.15 (m, 2H), 6.98 – 6.92 (m, 2H), 3.00 – 2.91 (m, 1H), 2.09 – 2.01 (m, 2H), 1.83 – 1.75 (m, 2H), 1.70 – 1.63 (m, 2H), 1.58 – 1.49 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.28 (d, J^F = 242.9 Hz), 142.22 (d, J^F = 3.1 Hz), 128.51 (d, J^F = 7.7 Hz), 115.03 (d, J^F = 20.9 Hz), 45.39, 34.90, 25.58.



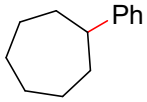
2u

***p*-Tolylcycloheptane** (**2u**). Yield 80% (37.66 mg). Colorless oil **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.08 (s, 4H), 2.66 – 2.59 (m, 1H), 2.31 (s, 3H), 1.92 – 1.86 (m, 2H), 1.81 – 1.74 (m, 2H), 1.71 – 1.51 (m, 8H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 147.25, 135.06, 129.14, 126.72, 46.82, 37.10, 28.13, 27.36, 21.15.



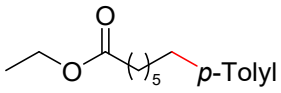
2v

(**4-Methoxyphenyl)cycloheptane** (**2v**). Yield 50% (25.54 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** 7.11 (d, *J* = 8.5 Hz, 2H), 6.82 (d, *J* = 8.7 Hz, 2H), 3.78 (s, 3H), 2.65 – 2.58 (m, 1H), 1.91 – 1.86 (m, 2H), 1.80 – 1.73 (m, 2H), 1.71 – 1.64 (m, 2H), 1.63 – 1.48 (m, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.57, 142.48, 127.66, 113.79, 55.41, 46.37, 37.23, 28.11, 27.30.



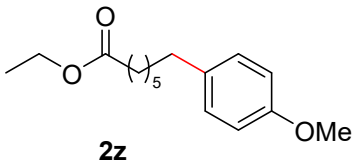
2x

Phenylcycloheptane (**2x**). Yield 81% (35.29 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.28 – 7.24 (m, 2H), 7.20 – 7.13 (m, 3H), 2.69 – 2.62 (m, 1H), 1.94 – 1.88 (m 2H), 1.82 – 1.75 (m, 2H), 1.72 – 1.49 (m, 8H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 150.20, 128.46, 126.86, 125.67, 47.24, 37.00, 28.13, 27.41.



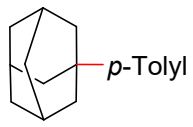
2y

Ethyl 6-(p-tolyl)hexanoate (**2y**). Yield 53% (31.05 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.09 – 7.04 (m, 4H), 4.11 (q, *J* = 7.1 Hz, 2H), 2.57 (t, *J* = 7.7 Hz, 2H), 2.31 – 2.26 (m, 5H), 1.69 – 1.57 (m, 4H), 1.39 – 1.32 (m, 2H), 1.24 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 173.98, 139.60, 135.22, 129.11, 128.42, 60.35, 35.43, 34.46, 31.39, 28.91, 25.01, 21.15, 14.41.



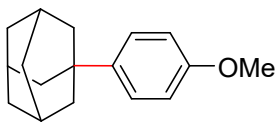
2z

Ethyl 6-(4-methoxyphenyl)hexanoate (**2z**). Yield 60% (37.55 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.08 (d, *J* = 8.7 Hz, 2H), 6.82 (d, *J* = 8.7 Hz, 2H), 4.12 (q, *J* = 7.1 H, 2H), 3.78 (s, 3H), 2.55 (t, *J* = 7.6 Hz, 2H), 2.28 (t, *J* = 7.5 Hz, 2H), 1.69 – 1.56 (m, 4H), 1.39 – 1.31 (m, 2H), 1.24 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 174.00, 157.82, 134.79, 129.41, 113.84, 60.36, 55.42, 34.95, 34.47, 31.51, 28.86, 25.01, 14.42.



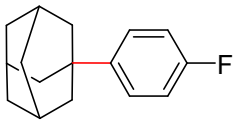
2aa

1,4-Di-*p*-tolylnaphthalene (**2aa**). Yield 89% (50.36 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ7.26 (d, *J* = 8.2 Hz, 2H), 7.13 (d, *J* = 8.3 Hz, 2H), 2.32 (s, 3H), 2.08 (bs, 3H), 1.90 (d, *J* = 2.7 Hz, 6H), 1.80 – 1.72 (m, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 148.64, 135.07, 128.98, 124.90, 43.44, 37.01, 35.99, 29.17, 21.06.



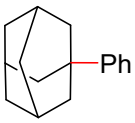
2ab

1-(4-Methoxyphenyl)adamantane (**2ab**). Yield 93% (56.35 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.28 (d, *J* = 9.0 Hz, 2H), 6.86 (d, *J* = 8.9 Hz, 2H), 3.79 (s, 3H), 2.08 (bs, 3H), 1.89 (d, *J* = 2.7 Hz, 6H), 1.80 – 1.72 (m, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.48, 143.88, 125.96, 113.54, 55.38, 43.55, 36.97, 35.70, 29.15.



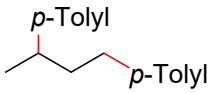
2ac

1-(4-Fluorophenyl)adamantane (**2ac**). Yield 64% (51.25 mg). Pale yellow oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.32 – 7.29 (m, 2H), 7.02 – 6.95 (m, 2H), 2.09 (bs, 3H), 1.89 (d, *J* = 2.6 Hz, 6H), 1.77 – 1.72 (m, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.03 (d, J^F = 243.2 Hz), 147.23 (d, J^F = 3.0 Hz), 126.49 (d, J^F = 7.5 Hz), 114.81 (d, J^F = 20.7 Hz), 43.51, 36.88, 36.01, 29.10.



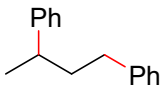
2ad

1-Phenyladamantane (**2ad**). Yield 81% (43.00 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.38 – 7.29 (m, 4H), 7.20 – 7.15 (m, 1H), 2.10 (bs, 3H), 1.92 (d, *J* = 2.8 Hz, 6H), 1.81 – 1.73 (m, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.50, 128.27, 125.68, 125.02, 43.33, 36.98, 36.34, 29.13.



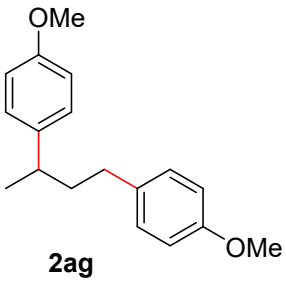
2ae

4,4'-(Butane-1,3-diyl)bis(methylbenzene) (**2ae**). Yield 61% (36.35 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.12 –7.00 (m, 8H), 2.67 (dd, *J* = 14.6, 7.0 Hz, 1H), 2.46 (t, *J* = 7.7 Hz, 2H), 2.31 (d, *J* = 9.9 Hz, 6H), 1.94 – 1.79 (m, 2H), 1.24 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 144.49, 139.70, 135.48, 135.16, 129.25, 129.11, 128.43, 127.12, 40.30, 39.21, 33.65, 22.85, 21.19, 21.17.



2af

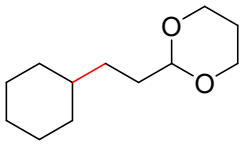
Butane-1,3-diyldibenzene (**2af**). Yield 63% (33.13 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.36 – 7.11 (m, 10H), 2.76 – 2.67 (m, 1H), 2.56 – 2.45 (m, 2H), 1.98 – 1.83 (m, 2H), 1.27 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 147.47, 142.73, 128.58, 128.55, 128.44, 127.26, 126.14, 125.82, 40.16, 39.68, 34.11, 22.69.



2ag

4,4'-(Butane-1,3-diyl)bis(methoxybenzene) (**2ag**). Yield 68% (45.96 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.12 (d, *J* = 8.6 Hz, 2H), 7.04 (d, *J* = 8.6 Hz, 2H), 6.83 (dd, *J* = 20.2, 8.7 Hz, 4H), 3.79 (d, *J* = 8.5 Hz, 6H), 2.65 (dt, *J* = 14.0, 7.0 Hz, 1H), 2.46 – 2.42 (m, 2H), 1.87 – 1.81

(m, 2H), 1.23 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.92, 157.78, 139.64, 134.86, 129.41, 128.09, 113.92, 113.84, 55.43, 40.56, 38.72, 33.14, 22.91.



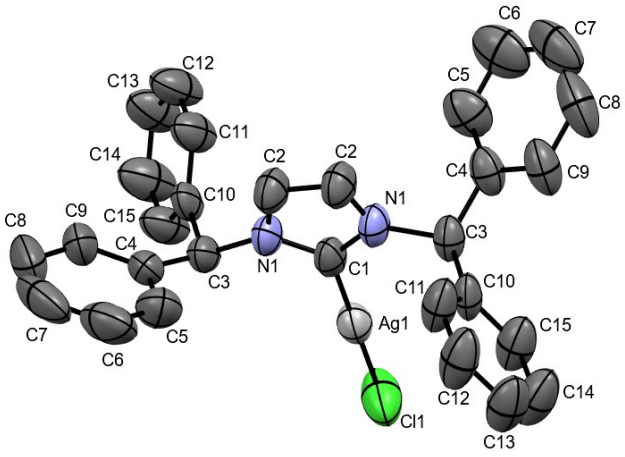
2ah

2-**(2-cyclohexylethyl)-1,3-dioxane** (**2ah**). Yield 78 % (38.67 mg). Colorless oil. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 4.49 (t, *J* = 5.2 Hz, 1H), 4.10 (ddd, *J* = 11.7, 4.9, 1.2 Hz, 2H), 3.79 – 3.73 (m, 2H), 2.14 – 2.02 (m, 1H), 1.71 – 1.65 (m, 4H), 1.62 – 1.57 (m, 2H), 1.36 – 1.31 (m, 1H), 1.27 – 1.07 (m, 7H), 0.87 (d, *J* = 11.1 Hz, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 103.11, 67.11, 33.42, 32.87, 31.69, 26.85, 26.53, 26.05.

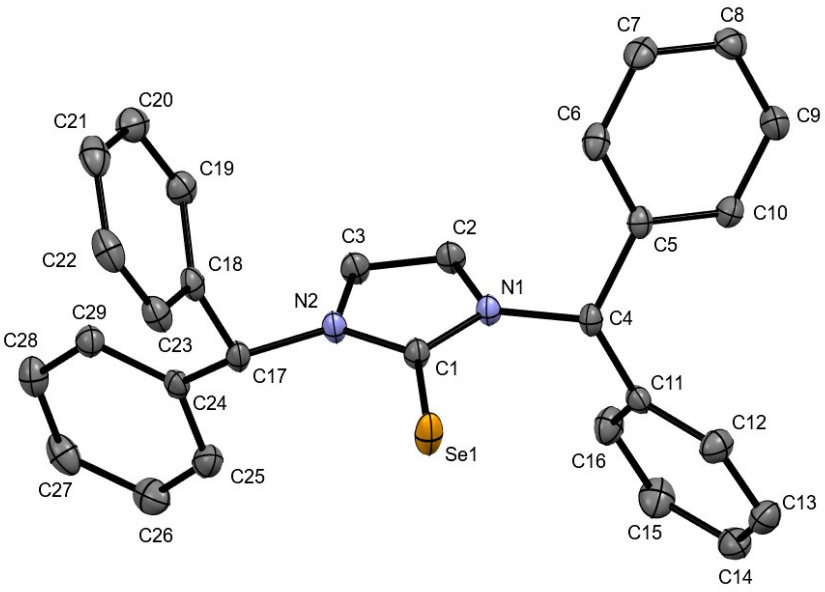
Crystallographic Analysis

The single crystals of the complex [Ag(IBzH)Cl] was collected on a Kuma KM4 diffractometer equipped with Eos CCD detector (graphite monochromatic, MoKα radiation, λ = 0.71073 Å) at room temperature. The single crystal of the complex [Se(IBzH)] were collected on a Rigaku Oxford Diffraction XtaLAB SynergyR DW diffractometer equipped with a HyPix ARC 150° Hybrid Photon Counting (HPC) detector using CuKα (λ = 1.54184 Å) at 100 K. The corrections to the Lorentz and polarization factors were applied to the reflection intensities.[25] Data were processed using the CrysAlisPro software. The structures were solved by direct methods using SHELXS and refined by full-matrix least-squares methods based F^2 using SHELXL.[26, 27] The hydrogen atoms were determined from the geometric concepts and refined in a riding model with isotropic temperature factors of 1.2 times the Ueq value of the parent atom. All non-hydrogen atoms were located from difference Fourier synthesis and refined by least squares method in the full-matrix anisotropic approximation. The crystallographic data for compounds and details of X-ray experiment are collected in the Supplementary information Tables. The structure drawings in ESI were prepared by using Mercury program.[28] The coordinates of atoms and other parameters for structures were deposited with the Cambridge Crystallographic Data Centre: 2393080 for [Ag(IBzH)Cl], 2393081 for [Se(IBzH)]; 12 Union Road, Cambridge CB2 1EZ, UK (Fax,_44-(1223)336-033, E-mail deposit@ccdc.cam.ac.uk).

Figure S1 The molecular structure of complexes [Ag(IBzH)Cl] and [Se(IBzH)]. Hydrogen atoms and solvent molecules have been omitted for clarity.



[Ag(IBzH)Cl]



[Se(IBzH)]

Crystallographic data

Table 1 Experimental details for compound [Ag(IBzH)Cl] and [Se(IBzH)].

	[Ag(IBzH)Cl]	**[Se(IBzH)]**
	Crystal data	
Chemical formula	$C_{29}H_{24}AgClN_2$	$C_{29}H_{24}N_2Se$
M_r	543.82	479.46
Crystal system, space group	Monoclinic, *C*2/*c*	Monoclinic, $P2_1/n$
Temperature (K)	293	100
a, *b*, *c* (Å)	13.0868 (11), 15.0378 (14), 12.4442 (9)	8.3091 (1), 25.5056 (2), 11.3577 (1)
β (°)	91.317 (7)	107.935 (1)
V (Å^3)	2448.3 (4)	2290.06 (4)
Radiation type	Mo *K*α	Cu *K*α
μ (mm^{-1})	0.95	2.35
Crystal size (mm)	0.4 × 0.25 × 0.1	0.2 × 0.15 × 0.1
	Data collection	
Diffractometer	KM4 with Eos CCD	XtaLAB Synergy R, DW

		system, HyPix-Arc 150
T_{min}, T_{max}	0.752, 1.000	0.687, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4664, 2408, 1716	17831, 4442, 4302
R_{int}	0.031	0.017
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617	0.621
	Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.083, 1.03	0.024, 0.063, 1.06
No. of reflections	2408	4442
No. of parameters	151	290
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.28, -0.37	0.33, -0.50

For all structures: Z = 4. Absorption was corrected for by multi-scan methods, SCALE3 ABSPACK (Rigaku Oxford Diffraction, 2015).. H-atom parameters were constrained.

Table 2 Selected geometric parameters (Å, º).

[Ag(IBzH)Cl]			
Ag1—Cl1	2.3065 (18)	C9—H9	0.9300
Ag1—C1	2.066 (5)	C9—C8	1.404 (7)
N1—C1	1.355 (4)	C8—H8	0.9300
N1—C2	1.381 (5)	C8—C7	1.362 (8)
N1—C3	1.480 (4)	C7—H7	0.9300
C1—N1^{i}	1.355 (4)	C10—C11	1.372 (5)
C2—C2^{i}	1.351 (7)	C10—C15	1.373 (5)
C2—H2	0.9300	C11—H11	0.9300
C3—H3	0.9800	C11—C12	1.375 (6)
C3—C4	1.524 (5)	C12—H12	0.9300
C3—C10	1.515 (5)	C12—C13	1.354 (6)
C6—H6	0.9300	C13—H13	0.9300
C6—C5	1.363 (7)	C13—C14	1.363 (6)
C6—C7	1.360 (8)	C14—H14	0.9300
C5—H5	0.9300	C14—C15	1.383 (6)
C5—C4	1.380 (6)	C15—H15	0.9300
C4—C9	1.374 (5)		
C1—Ag1—Cl1	180.0	C4—C9—C8	119.9 (5)
C1—N1—C2	111.1 (3)	C8—C9—H9	120.0
C1—N1—C3	122.7 (3)	C9—C8—H8	120.0
C2—N1—C3	126.1 (3)	C7—C8—C9	120.0 (5)
N1—C1—Ag1	127.8 (2)	C7—C8—H8	120.0
N1^{i}—C1—Ag1	127.8 (2)	C6—C7—C8	120.1 (6)

N1^{i}—C1—N1	104.5 (4)	C6—C7—H7	120.0
N1—C2—H2	126.7	C8—C7—H7	120.0
C2^{i}—C2—N1	106.65 (18)	C11—C10—C3	123.4 (4)
C2^{i}—C2—H2	126.7	C11—C10—C15	118.3 (4)
N1—C3—H3	106.9	C15—C10—C3	118.3 (4)
N1—C3—C4	109.6 (3)	C10—C11—H11	119.6
N1—C3—C10	111.2 (3)	C10—C11—C12	120.9 (4)
C4—C3—H3	106.9	C12—C11—H11	119.6
C10—C3—H3	106.9	C11—C12—H12	119.9
C10—C3—C4	114.9 (3)	C13—C12—C11	120.2 (4)
C5—C6—H6	120.0	C13—C12—H12	119.9
C7—C6—H6	120.0	C12—C13—H13	119.9
C7—C6—C5	120.0 (6)	C12—C13—C14	120.2 (5)
C6—C5—H5	119.1	C14—C13—H13	119.9
C6—C5—C4	121.8 (5)	C13—C14—H14	120.2
C4—C5—H5	119.1	C13—C14—C15	119.7 (5)
C5—C4—C3	119.3 (3)	C15—C14—H14	120.2
C9—C4—C3	122.5 (4)	C10—C15—C14	120.8 (4)
C9—C4—C5	118.1 (4)	C10—C15—H15	119.6
C4—C9—H9	120.0	C14—C15—H15	119.6
N1—C3—C4—C5	-45.7 (5)	C6—C5—C4—C3	-178.3 (4)
N1—C3—C4—C9	137.2 (4)	C6—C5—C4—C9	-1.1 (7)
N1—C3—C10—C11	-41.6 (5)	C5—C6—C7—C8	0.1 (9)
N1—C3—C10—C15	138.6 (4)	C5—C4—C9—C8	0.5 (6)
C1—N1—C2—C2^{i}	-0.6 (5)	C4—C3—C10—C11	83.7 (4)
C1—N1—C3—C4	141.3 (3)	C4—C3—C10—C15	-96.1 (5)
C1—N1—C3—C10	-90.5 (4)	C4—C9—C8—C7	0.5 (8)
C2—N1—C1—Ag1	-179.8 (2)	C9—C8—C7—C6	-0.8 (9)
C2—N1—C1—N1^{i}	0.2 (2)	C7—C6—C5—C4	0.8 (8)
C2—N1—C3—C4	-43.6 (5)	C10—C3—C4—C5	-171.8 (4)
C2—N1—C3—C10	84.6 (4)	C10—C3—C4—C9	11.1 (5)
C3—N1—C1—Ag1	-4.0 (3)	C10—C11—C12—C13	-0.3 (8)
C3—N1—C1—N1^{i}	176.0 (3)	C11—C10—C15—C14	-1.3 (7)
C3—N1—C2—C2^{i}	-176.2 (4)	C11—C12—C13—C14	0.0 (8)
C3—C4—C9—C8	177.6 (4)	C12—C13—C14—C15	-0.3 (9)
C3—C10—C11—C12	-178.8 (4)	C13—C14—C15—C10	1.0 (8)
C3—C10—C15—C14	178.5 (4)	C15—C10—C11—C12	1.0 (7)

[Se(IBzH)]

Se1—C1	1.8400 (14)	C14—H14	0.9500
N1—C1	1.3619 (18)	C14—C15	1.382 (2)
N1—C2	1.3885 (18)	C15—H15	0.9500
N1—C4	1.4717 (16)	C15—C16	1.392 (2)
N2—C1	1.3590 (17)	C16—H16	0.9500
N2—C3	1.3888 (18)	C17—H17	1.0000
N2—C17	1.4776 (17)	C17—C18	1.516 (2)
C2—H2	0.9500	C17—C24	1.5266 (19)
C2—C3	1.343 (2)	C18—C19	1.395 (2)
C3—H3	0.9500	C18—C23	1.391 (2)
C4—H4	1.0000	C19—H19	0.9500
C4—C5	1.5313 (18)	C19—C20	1.389 (2)
C4—C11	1.5200 (19)	C20—H20	0.9500
C5—C6	1.3969 (19)	C20—C21	1.389 (2)
C5—C10	1.3906 (19)	C21—H21	0.9500
C6—H6	0.9500	C21—C22	1.387 (2)

C6—C7	1.384 (2)	C22—H22	0.9500
C7—H7	0.9500	C22—C23	1.395 (2)
C7—C8	1.386 (2)	C23—H23	0.9500
C8—H8	0.9500	C24—C25	1.397 (2)
C8—C9	1.387 (2)	C24—C29	1.388 (2)
C9—H9	0.9500	C25—H25	0.9500
C9—C10	1.392 (2)	C25—C26	1.383 (2)
C10—H10	0.9500	C26—H26	0.9500
C11—C12	1.391 (2)	C26—C27	1.391 (2)
C11—C16	1.390 (2)	C27—H27	0.9500
C12—H12	0.9500	C27—C28	1.386 (2)
C12—C13	1.389 (2)	C28—H28	0.9500
C13—H13	0.9500	C28—C29	1.396 (2)
C13—C14	1.383 (2)	C29—H29	0.9500
C1—N1—C2	109.77 (11)	C15—C14—H14	120.2
C1—N1—C4	124.26 (11)	C14—C15—H15	119.7
C2—N1—C4	125.96 (12)	C14—C15—C16	120.56 (14)
C1—N2—C3	109.89 (11)	C16—C15—H15	119.7
C1—N2—C17	123.79 (11)	C11—C16—C15	120.36 (14)
C3—N2—C17	126.31 (11)	C11—C16—H16	119.8
N1—C1—Se1	127.09 (10)	C15—C16—H16	119.8
N2—C1—Se1	127.19 (10)	N2—C17—H17	106.3
N2—C1—N1	105.71 (12)	N2—C17—C18	112.50 (11)
N1—C2—H2	126.3	N2—C17—C24	110.02 (11)
C3—C2—N1	107.34 (12)	C18—C17—H17	106.3
C3—C2—H2	126.3	C18—C17—C24	114.86 (11)
N2—C3—H3	126.4	C24—C17—H17	106.3
C2—C3—N2	107.27 (12)	C19—C18—C17	121.80 (13)
C2—C3—H3	126.4	C23—C18—C17	119.18 (13)
N1—C4—H4	106.7	C23—C18—C19	118.94 (14)
N1—C4—C5	109.66 (11)	C18—C19—H19	119.7
N1—C4—C11	112.11 (11)	C20—C19—C18	120.56 (14)
C5—C4—H4	106.7	C20—C19—H19	119.7
C11—C4—H4	106.7	C19—C20—H20	119.9
C11—C4—C5	114.58 (11)	C21—C20—C19	120.20 (14)
C6—C5—C4	119.38 (12)	C21—C20—H20	119.9
C10—C5—C4	121.97 (12)	C20—C21—H21	120.2
C10—C5—C6	118.59 (13)	C22—C21—C20	119.60 (15)
C5—C6—H6	119.6	C22—C21—H21	120.2
C7—C6—C5	120.82 (13)	C21—C22—H22	119.9
C7—C6—H6	119.6	C21—C22—C23	120.20 (14)
C6—C7—H7	119.9	C23—C22—H22	119.9
C6—C7—C8	120.26 (13)	C18—C23—C22	120.44 (14)
C8—C7—H7	119.9	C18—C23—H23	119.8
C7—C8—H8	120.3	C22—C23—H23	119.8
C7—C8—C9	119.47 (14)	C25—C24—C17	117.66 (12)
C9—C8—H8	120.3	C29—C24—C17	123.32 (13)
C8—C9—H9	119.8	C29—C24—C25	118.88 (13)
C8—C9—C10	120.32 (14)	C24—C25—H25	119.5
C10—C9—H9	119.8	C26—C25—C24	121.09 (14)
C5—C10—C9	120.52 (13)	C26—C25—H25	119.5
C5—C10—H10	119.7	C25—C26—H26	120.1
C9—C10—H10	119.7	C25—C26—C27	119.87 (14)
C12—C11—C4	118.42 (12)	C27—C26—H26	120.1
C16—C11—C4	123.10 (12)	C26—C27—H27	120.3

C16—C11—C12	118.46 (13)	C28—C27—C26	119.47 (14)
C11—C12—H12	119.4	C28—C27—H27	120.3
C13—C12—C11	121.18 (14)	C27—C28—H28	119.7
C13—C12—H12	119.4	C27—C28—C29	120.66 (14)
C12—C13—H13	120.1	C29—C28—H28	119.7
C14—C13—C12	119.84 (14)	C24—C29—C28	120.01 (14)
C14—C13—H13	120.1	C24—C29—H29	120.0
C13—C14—H14	120.2	C28—C29—H29	120.0
C15—C14—C13	119.60 (14)		
N1—C2—C3—N2	0.14 (16)	C7—C8—C9—C10	-0.4 (2)
N1—C4—C5—C6	45.10 (16)	C8—C9—C10—C5	-0.4 (2)
N1—C4—C5—C10	-137.66 (13)	C10—C5—C6—C7	-0.2 (2)
N1—C4—C11—C12	-151.42 (13)	C11—C4—C5—C6	172.19 (12)
N1—C4—C11—C16	30.27 (18)	C11—C4—C5—C10	-10.57 (18)
N2—C17—C18—C19	55.63 (17)	C11—C12—C13—C14	-0.9 (2)
N2—C17—C18—C23	-127.61 (13)	C12—C11—C16—C15	0.3 (2)
N2—C17—C24—C25	61.56 (16)	C12—C13—C14—C15	0.5 (2)
N2—C17—C24—C29	-122.74 (14)	C13—C14—C15—C16	0.3 (2)
C1—N1—C2—C3	0.35 (16)	C14—C15—C16—C11	-0.7 (2)
C1—N1—C4—C5	-138.01 (13)	C16—C11—C12—C13	0.5 (2)
C1—N1—C4—C11	93.52 (15)	C17—N2—C1—Se1	2.8 (2)
C1—N2—C3—C2	-0.59 (17)	C17—N2—C1—N1	-178.11 (12)
C1—N2—C17—C18	93.16 (16)	C17—N2—C3—C2	178.27 (13)
C1—N2—C17—C24	-137.40 (13)	C17—C18—C19—C20	174.65 (13)
C2—N1—C1—Se1	178.37 (10)	C17—C18—C23—C22	-175.00 (13)
C2—N1—C1—N2	-0.70 (16)	C17—C24—C25—C26	173.95 (13)
C2—N1—C4—C5	43.45 (18)	C17—C24—C29—C28	-174.04 (13)
C2—N1—C4—C11	-85.01 (16)	C18—C17—C24—C25	-170.29 (12)
C3—N2—C1—Se1	-178.27 (11)	C18—C17—C24—C29	5.41 (19)
C3—N2—C1—N1	0.79 (16)	C18—C19—C20—C21	0.3 (2)
C3—N2—C17—C18	-85.55 (16)	C19—C18—C23—C22	1.9 (2)
C3—N2—C17—C24	43.88 (18)	C19—C20—C21—C22	1.8 (2)
C4—N1—C1—Se1	-0.4 (2)	C20—C21—C22—C23	-2.0 (2)
C4—N1—C1—N2	-179.44 (12)	C21—C22—C23—C18	0.2 (2)
C4—N1—C2—C3	179.06 (13)	C23—C18—C19—C20	-2.1 (2)
C4—C5—C6—C7	177.18 (13)	C24—C17—C18—C19	-71.27 (16)
C4—C5—C10—C9	-176.59 (13)	C24—C17—C18—C23	105.49 (14)
C4—C11—C12—C13	-177.89 (13)	C24—C25—C26—C27	0.7 (2)
C4—C11—C16—C15	178.63 (14)	C25—C24—C29—C28	1.6 (2)
C5—C4—C11—C12	82.76 (16)	C25—C26—C27—C28	0.9 (2)
C5—C4—C11—C16	-95.55 (16)	C26—C27—C28—C29	-1.2 (2)
C5—C6—C7—C8	-0.6 (2)	C27—C28—C29—C24	-0.1 (2)
C6—C5—C10—C9	0.7 (2)	C29—C24—C25—C26	-1.9 (2)
C6—C7—C8—C9	0.9 (2)		

Symmetry code(s): (i) -*x*+1, *y*, -*z*+3/2.

Computational Methods

Computational Methods. All of the calculations were performed using Gaussian 09 suite of programs. All of the geometry optimizations were performed at the B3LYP level of theory in the gas phase with the 6-311++G(d,p) basis set. For geometry optimizations, we employed the X-ray structures of 1,3-dibenzhydryl-1*H*-imidazol-3-ium and 1,3-dibenzyl-1*H*-imidazol-3-ium and their linear metal complexes as the starting geometry and performed full optimization. The absence of imaginary frequencies was used to characterize the structures as minima on the potential energy surface. All of the optimized geometries were verified as minima (no imaginary frequencies). Energetic parameters were calculated under standard conditions (298.15 K and 1 atm). Structural representations were generated using CYLview software (Legault, C. Y. CYLview version 1.0 BETA, University of Sherbrooke). All other representations were generated using GaussView (GaussView, version 5, Dennington, R.; Keith, T.; Millam, J. Semichem Inc., Shawnee Mission, KS, 2009) or ChemCraft software (Andrienko, G. L. ChemCraft version b562a, https://www.chemcraftprog.com).

Full Reference for Gaussian 09

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Chart SI–1 HOMO and LUMO Energy Levels of IBzH and Related NHC Ligands Calculated at the B3LYP 6-311++g(d,p) Level[a,b]

entry	compound	orbital	E [au]	E [eV]	E [kcal/mol]	ΔE [eV]
1	IBzH	HOMO-1	-0.2339	-6.36	-146.77	
2	IBzH	HOMO	-0.2201	-5.99	-138.11	
3[a]	IBzH	LUMO+3	-0.0264	-0.72	-16.57	-5.27
4	IBn	HOMO-1	-0.2362	-6.43	-148.22	
5	IBn	HOMO	-0.2208	-6.01	-138.55	
6[b]	IBn	LUMO+1	-0.0234	-0.64	-14.68	-5.37
7	IPr	HOMO-1	-0.2406	-6.55	-150.98	
8	IPr	HOMO	-0.2210	-6.01	-139.78	
9[b]	IPr	LUMO+1	-0.0177	-0.48	-12.21	-5.53

[a]LUMO+3 due to required orbital symmetry. [b]LUMO+1 due to required orbital symmetry. See, Falivene, L.; Cavallo, L. *Coord. Chem. Rev.* **2017**, *344*, 101-114.

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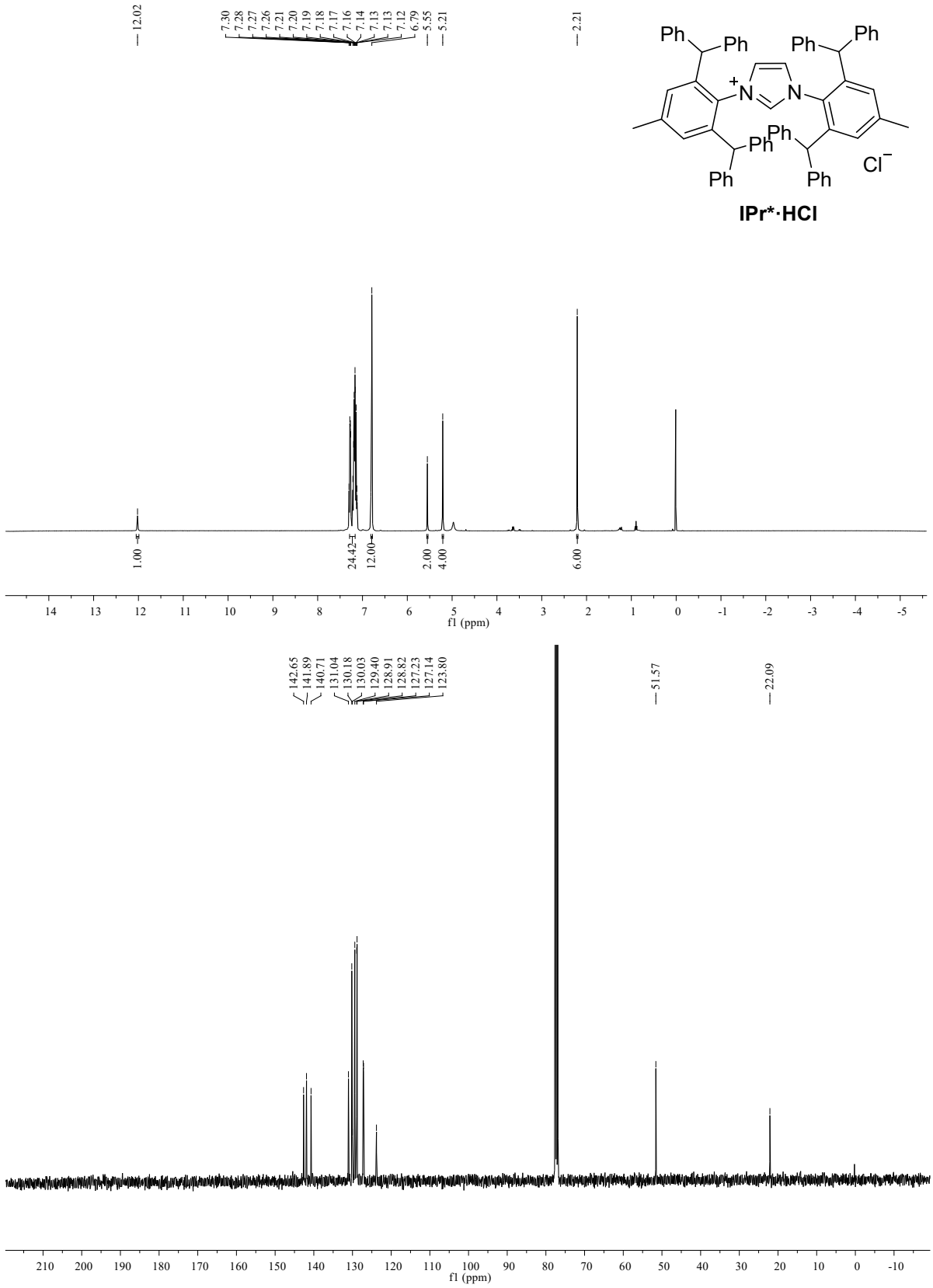
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7.20
7.19
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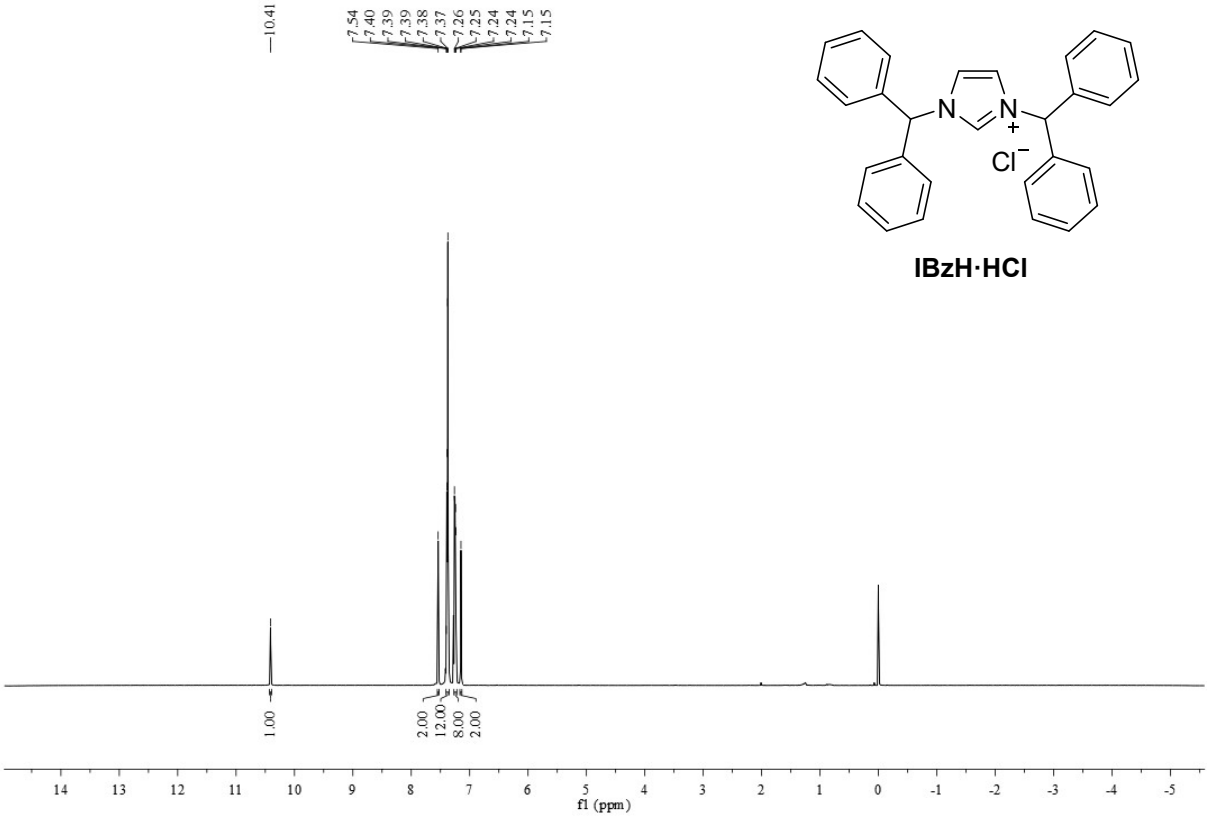
7.17
7.16
7.14
7.13
7.13
7.12
6.79
5.55
5.21
2.21
Ph
Ph
Ph
Ph
N
N
Ph
Ph
Ph
Ph
Cl⁻
IPr*·HCl
1.00
24.42
12.00
2.00
4.00
6.00
f1 (ppm)
142.65
141.89
140.71
131.04
130.18
130.03
129.40
128.91
128.82
127.23
127.14
123.80
51.57
22.09
f1 (ppm)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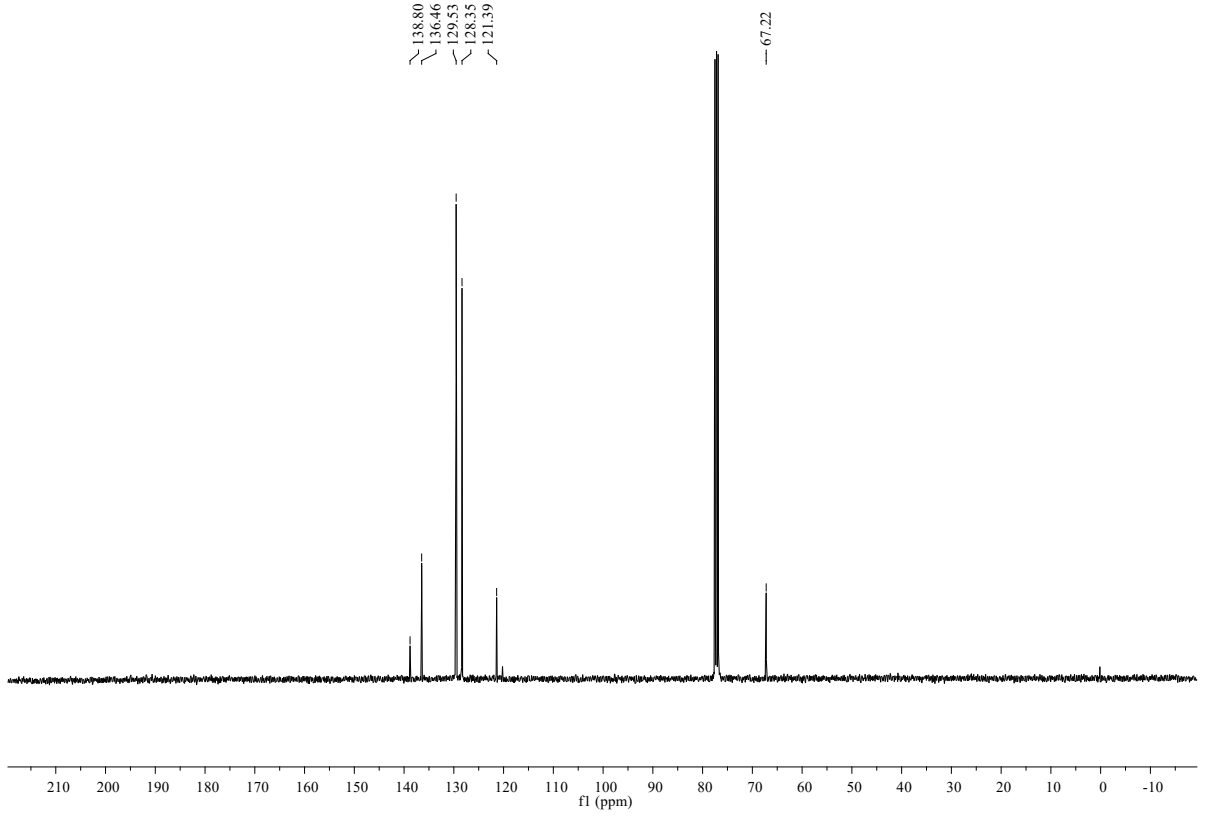
7.26
7.25
7.24
7.24
7.15
7.15
1.00
2.00
12.00
8.00
2.00
f1 (ppm)

N
N
+
Cl⁻

IBzH·HCl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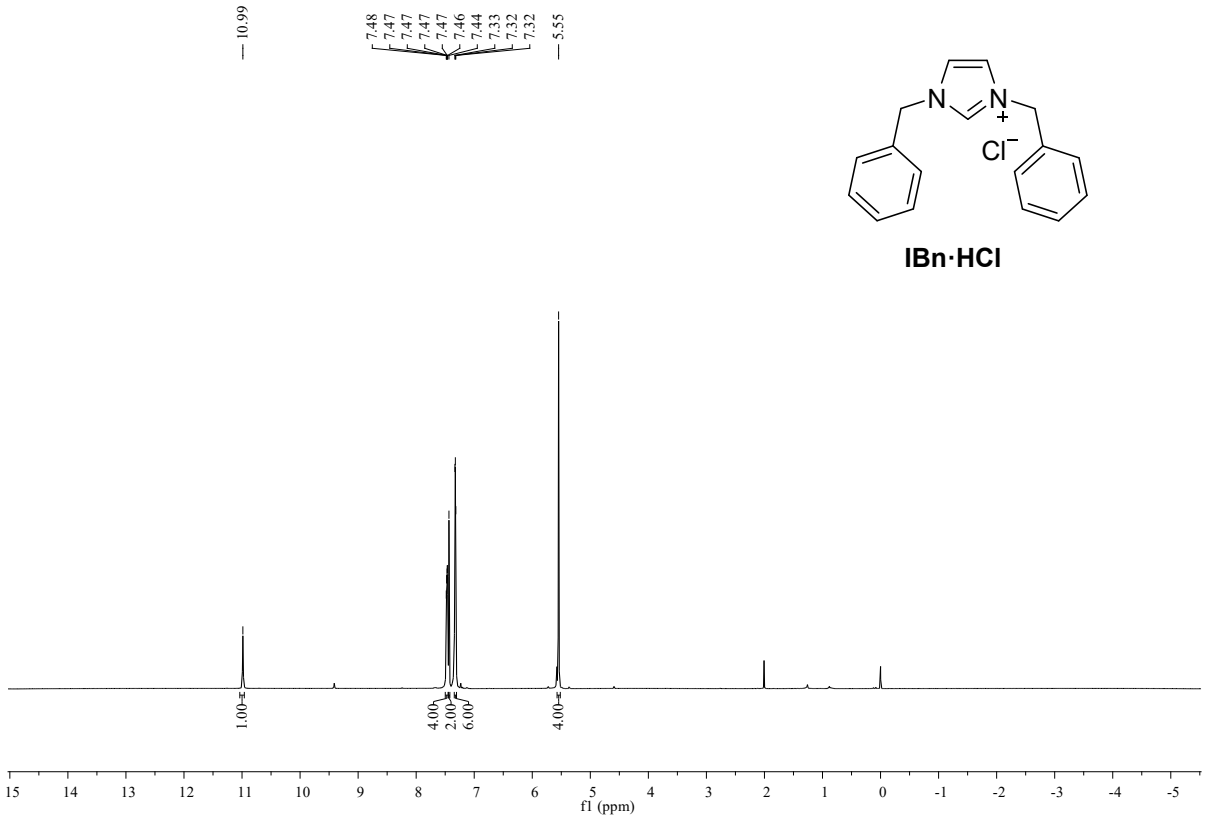
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7.32
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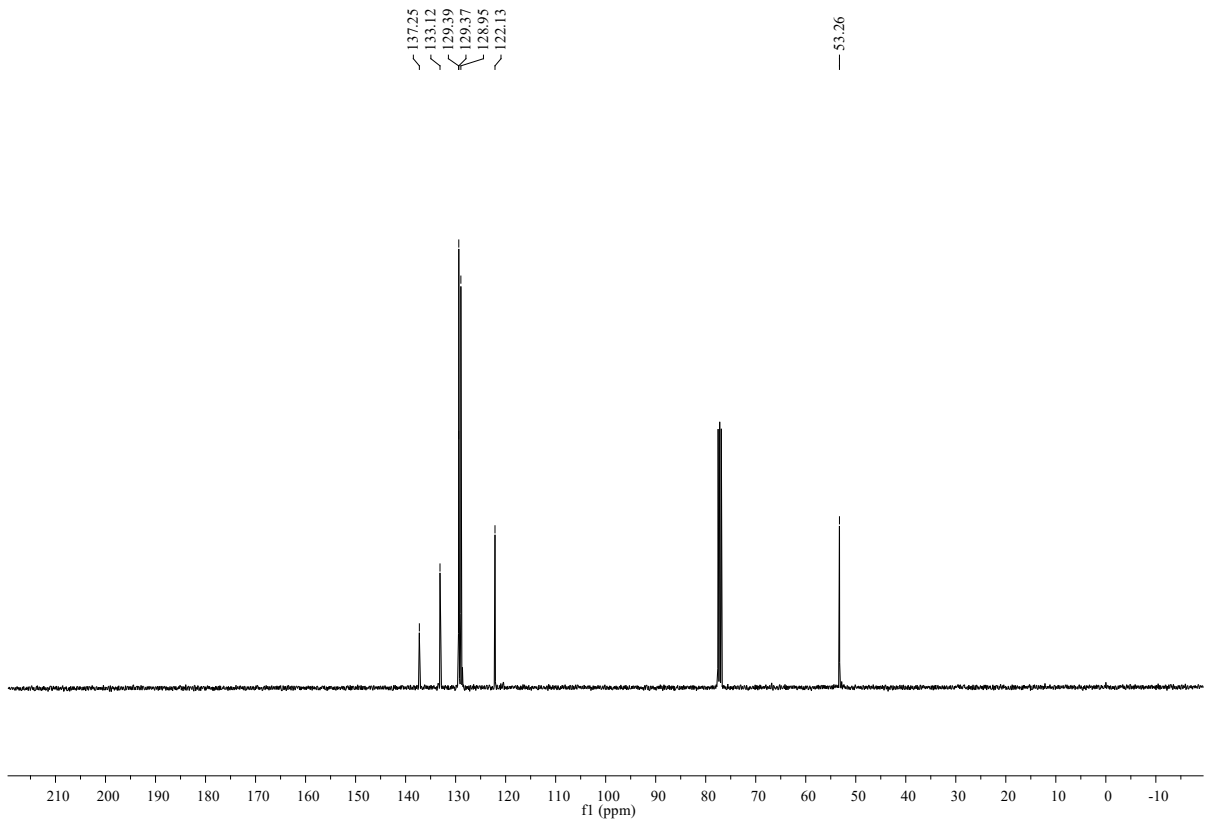
4.00
2.00
6.00
4.00
f1 (ppm)

N
N
Cl⁻

IBn·HCl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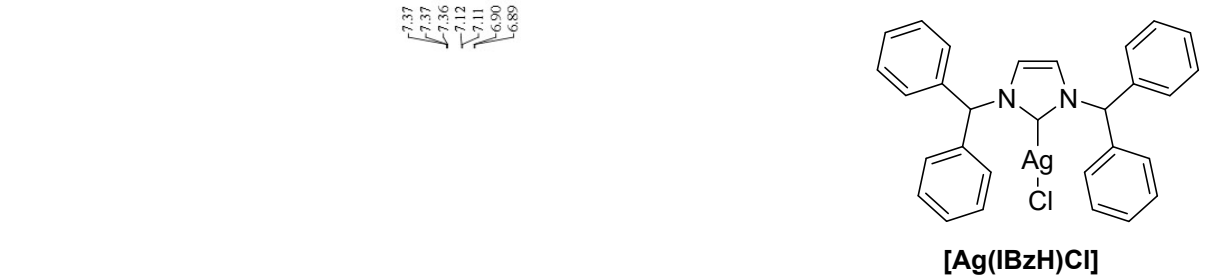
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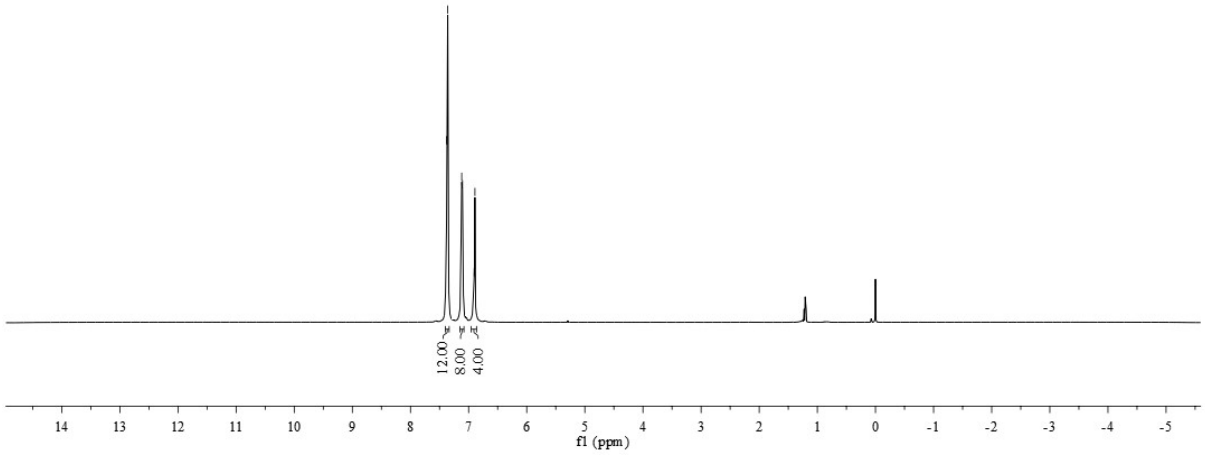
N
N
Ag
Cl

[Ag(IBzH)Cl]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4.00
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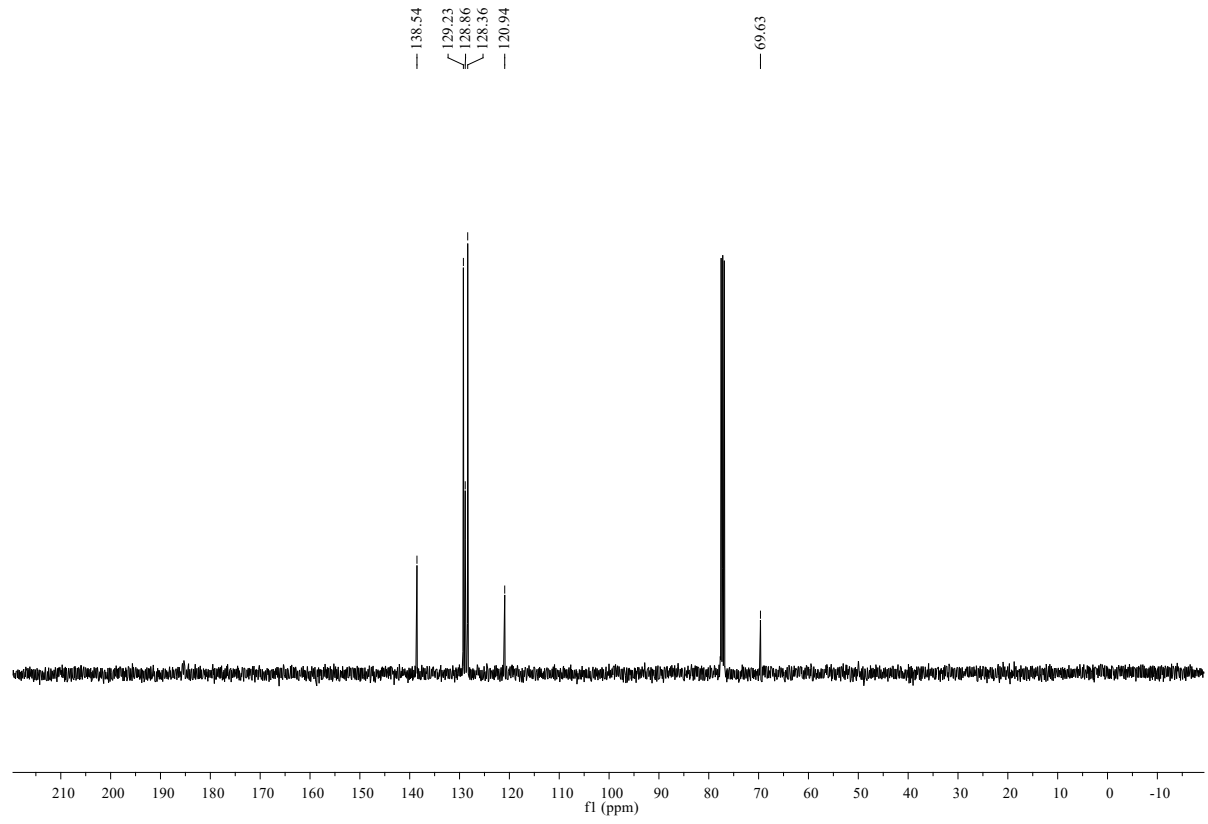
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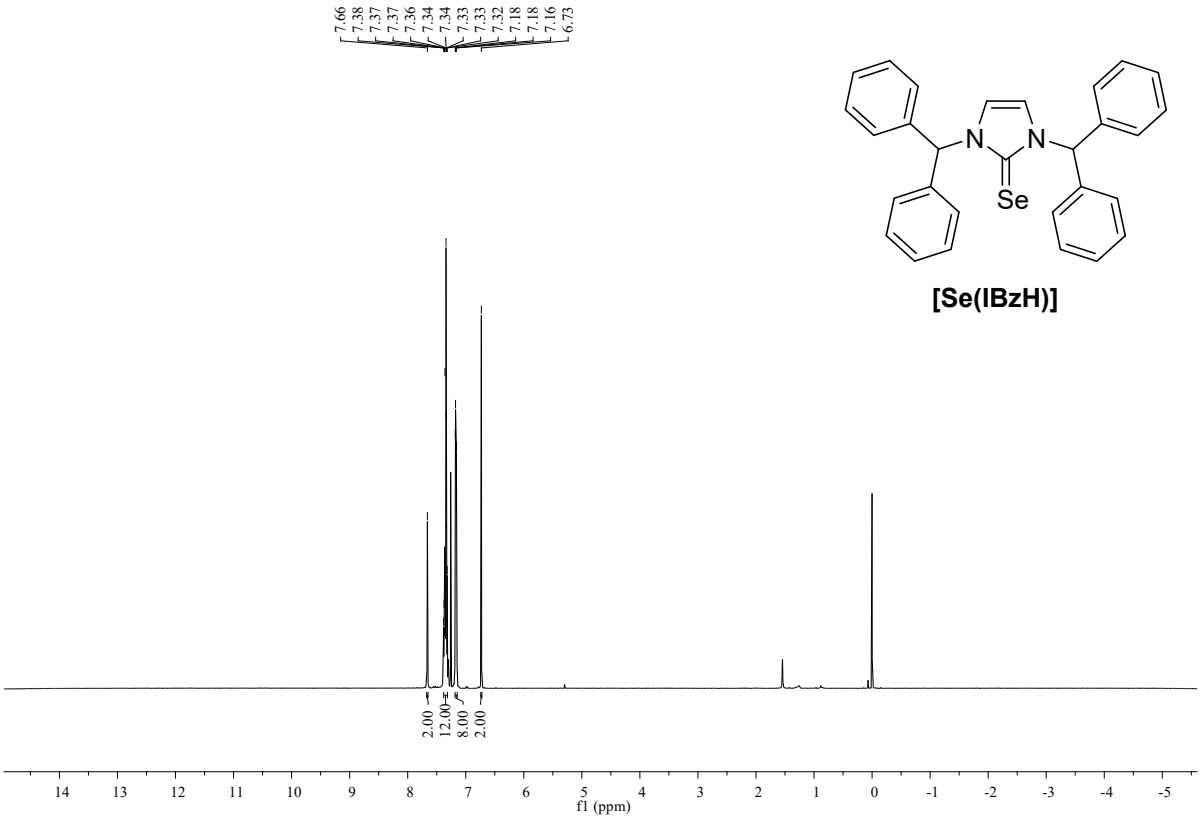
f1 (ppm)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7.32
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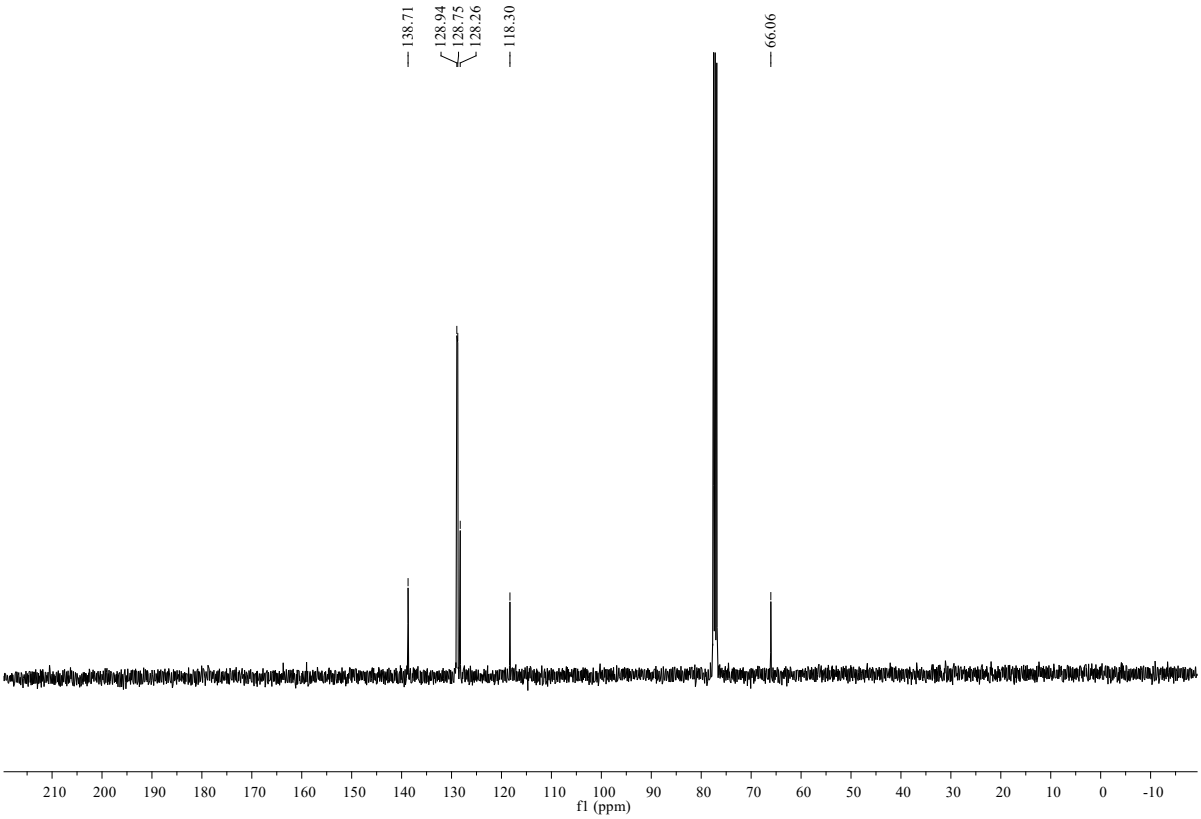
6.73
N
N
Se
[Se(IBzH)]
2.00
12.00
8.00
2.00
f1 (ppm)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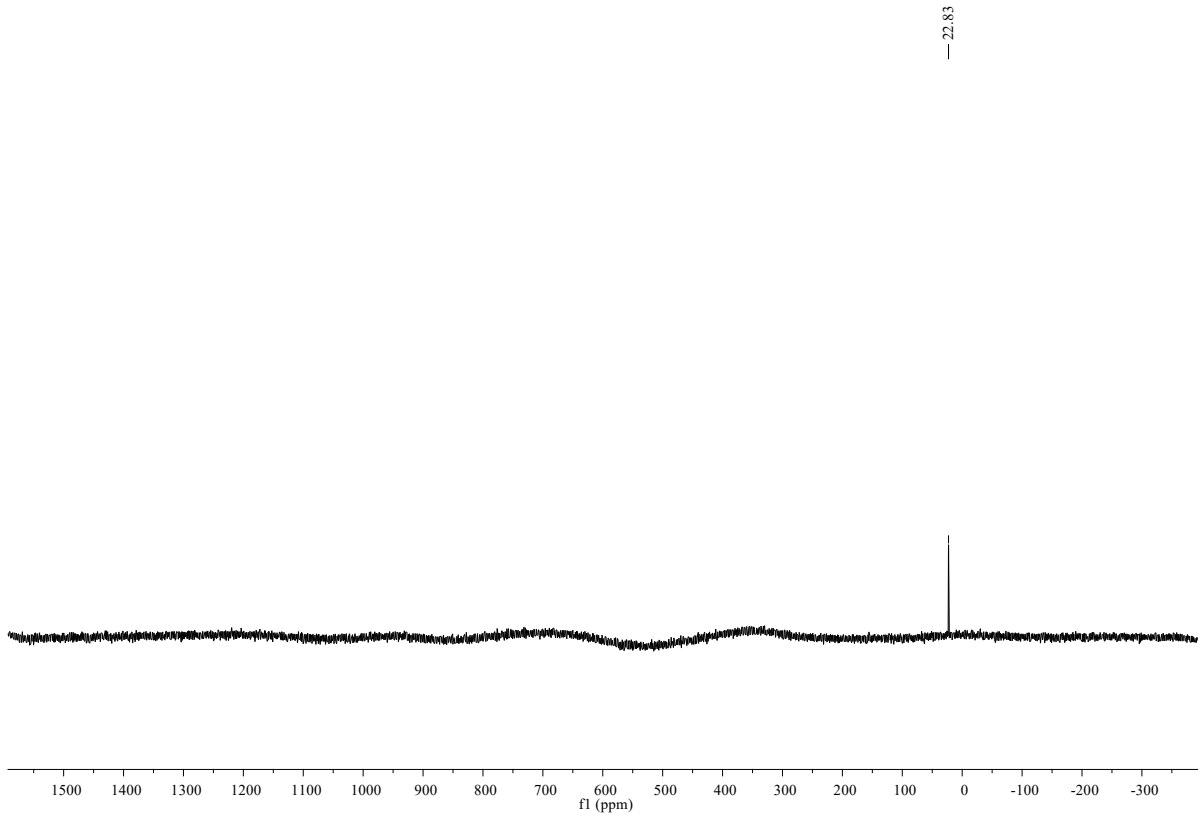
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500
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200
100
0
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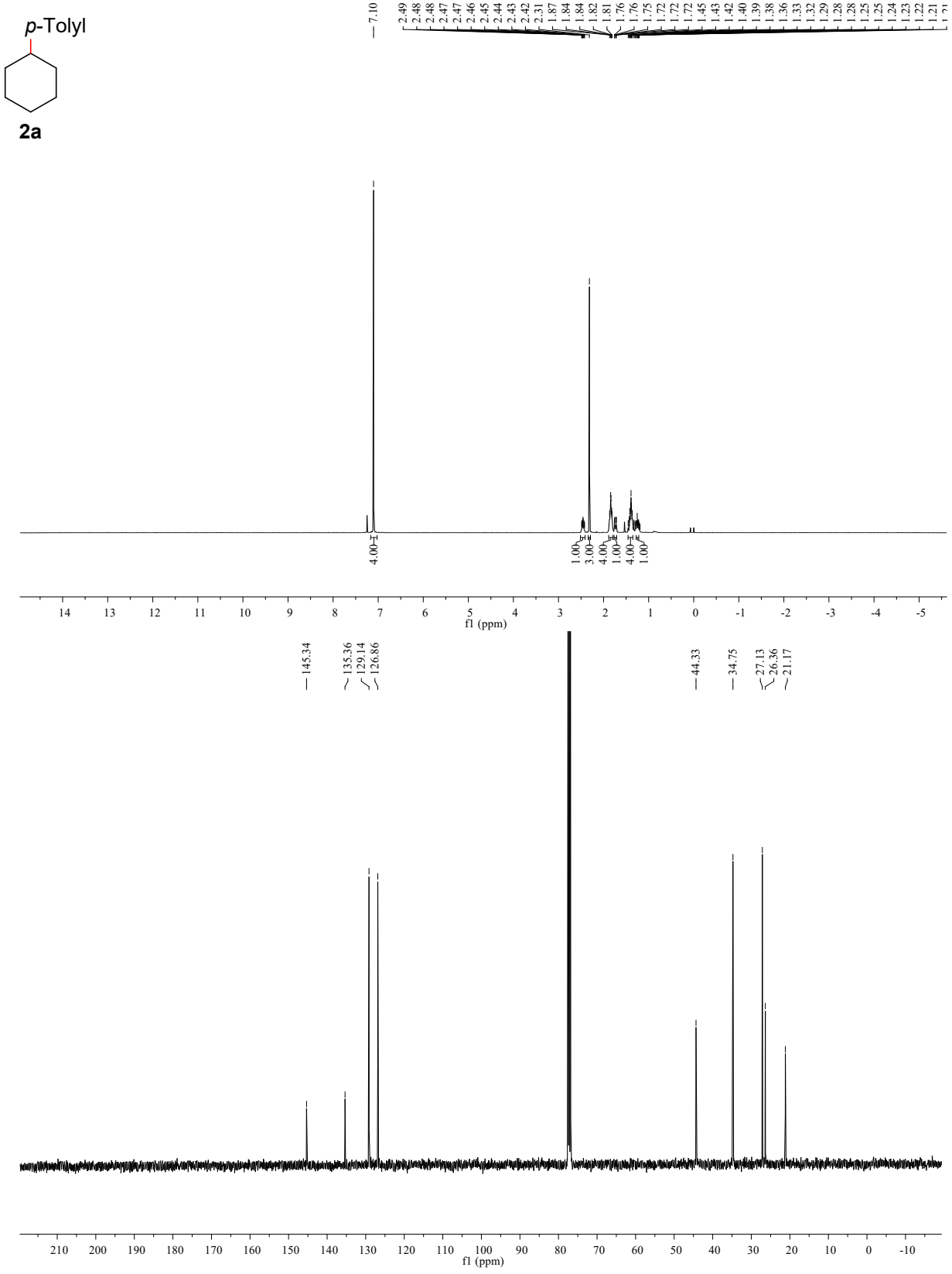
-200
-300
f1 (ppm)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4.00
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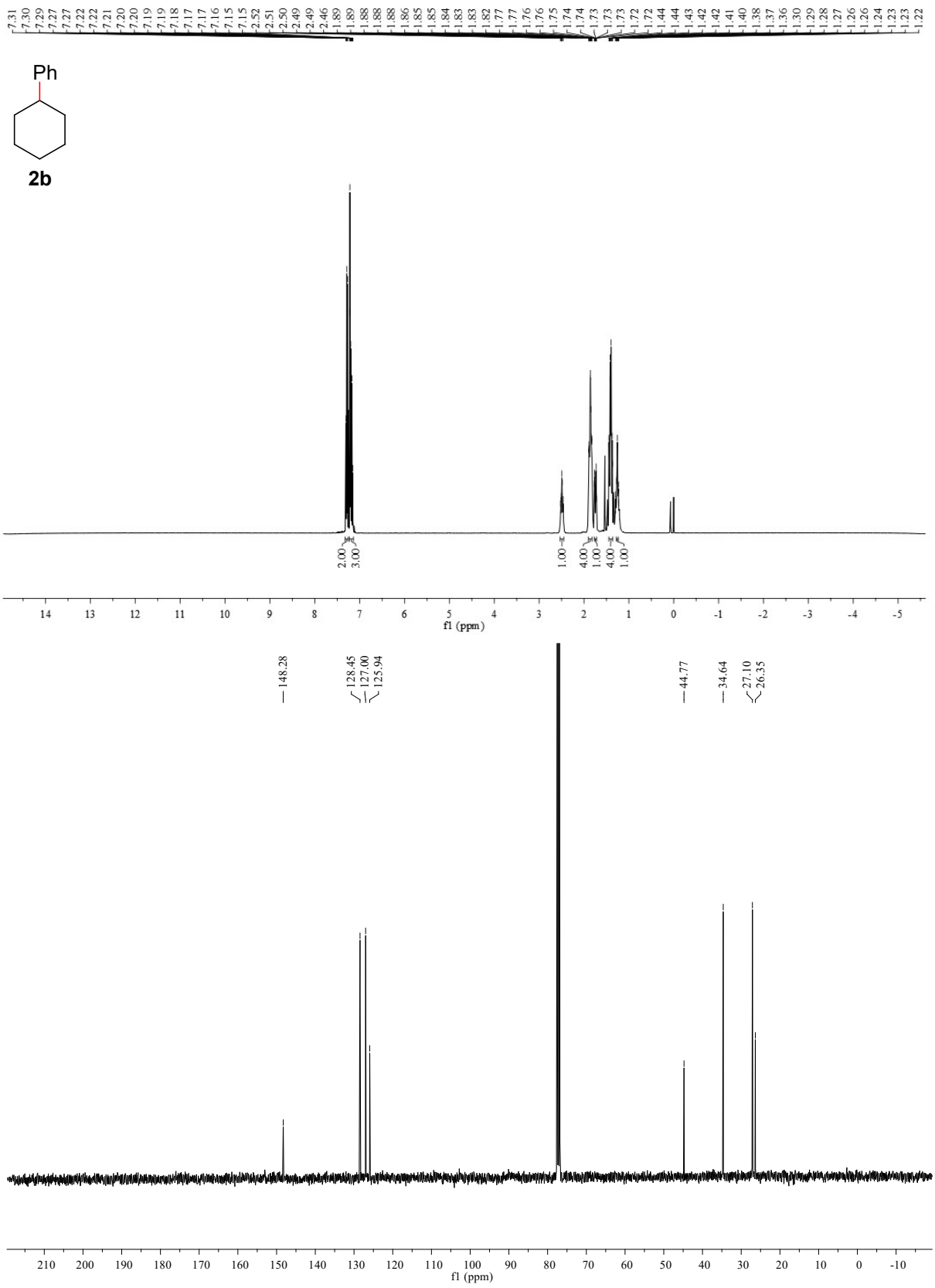
f1 (ppm)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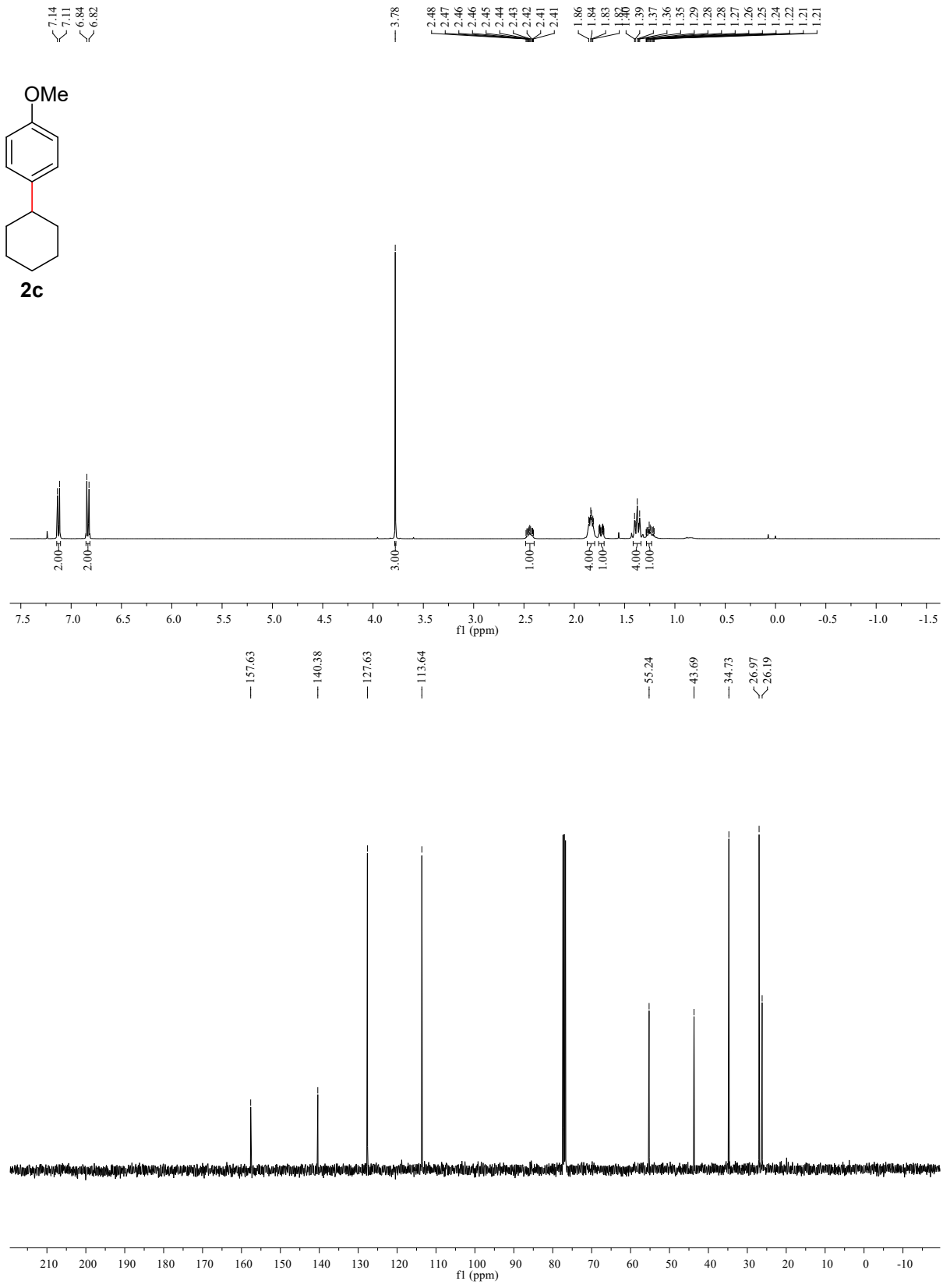
f1 (ppm)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1.35
1.29
1.28
1.28
1.27
1.26
1.25
1.24
1.22
1.21
1.21
OMe
2c
2.00
2.00
3.00
1.00
4.00
1.00
4.00
1.00
f1 (ppm)
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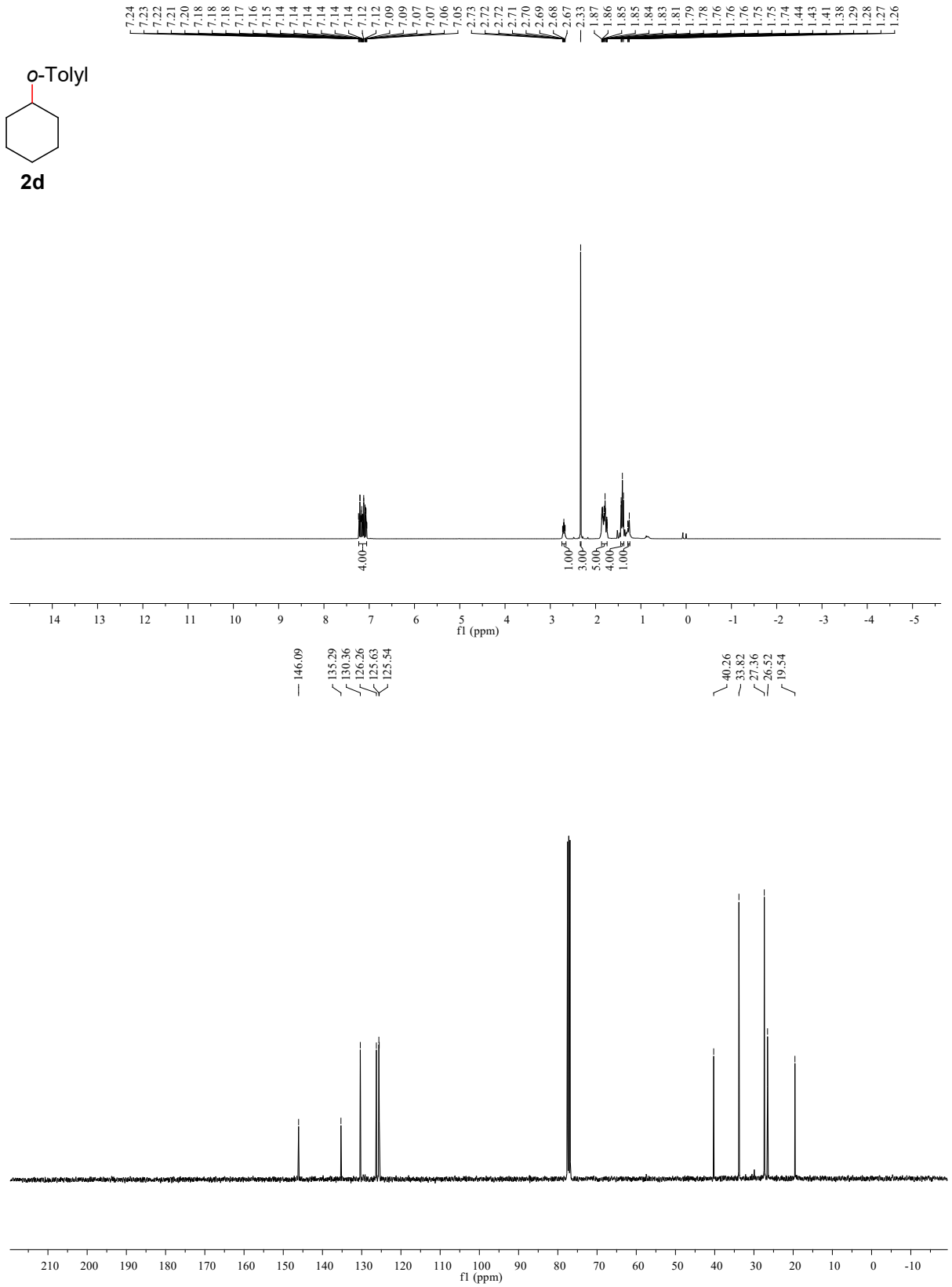
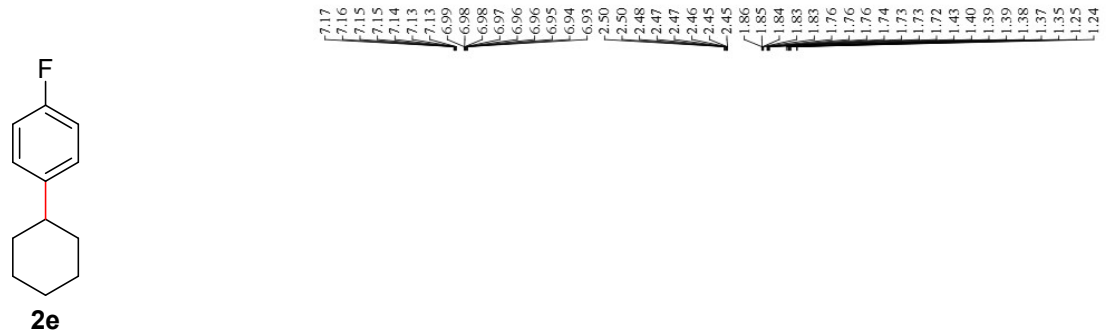
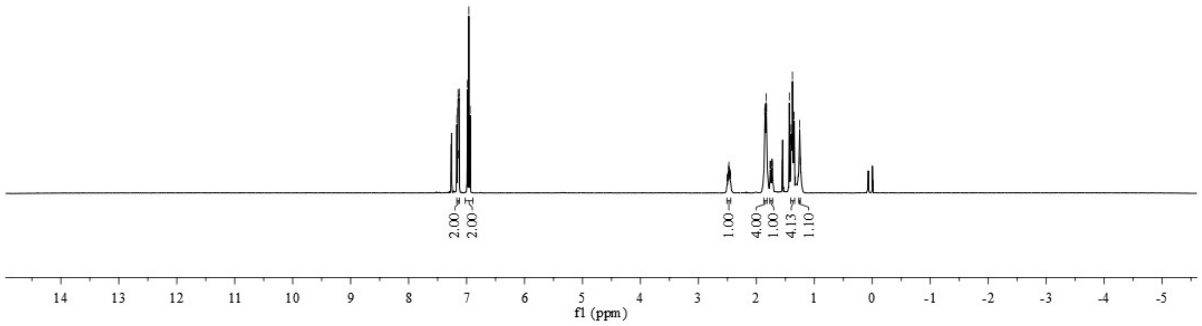
26.19
f1 (ppm)


o-Tolyl
2d
f1 (ppm)
f1 (ppm)


F

2e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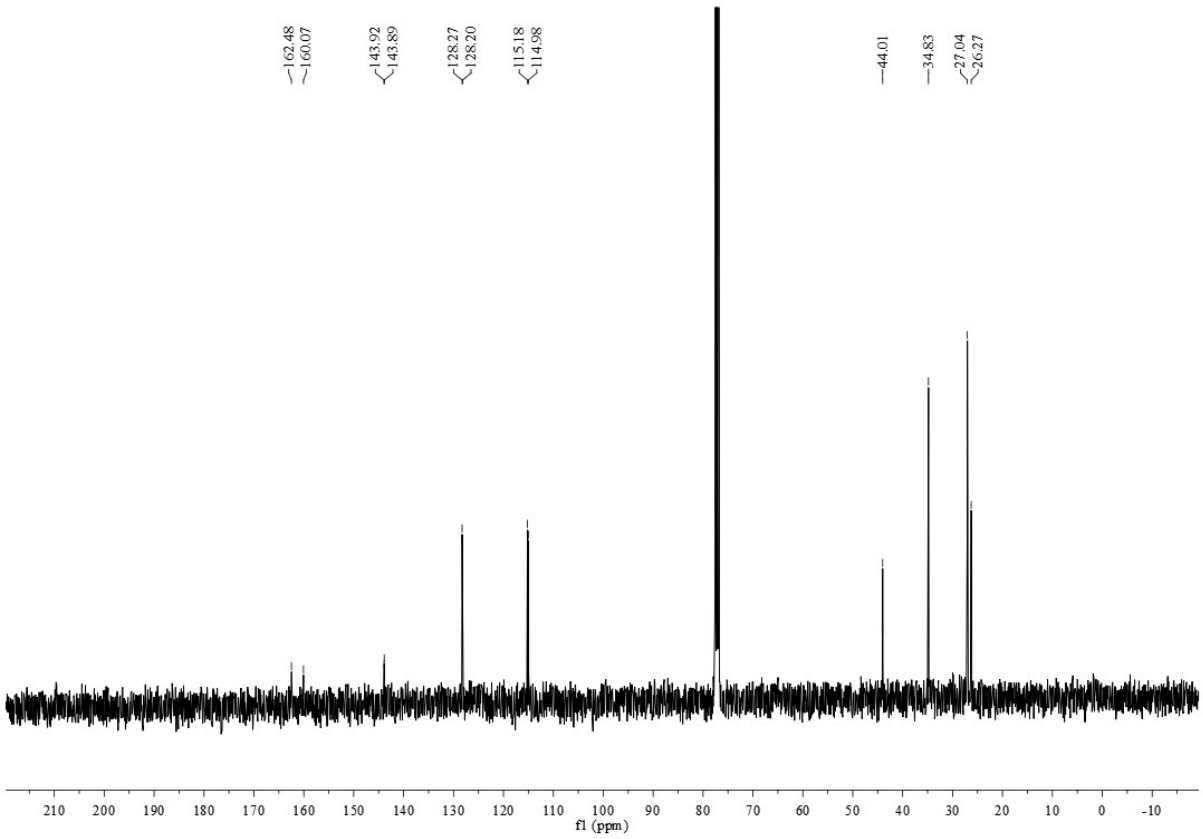
1.00
4.00
1.00
4.13
1.10
f1 (ppm)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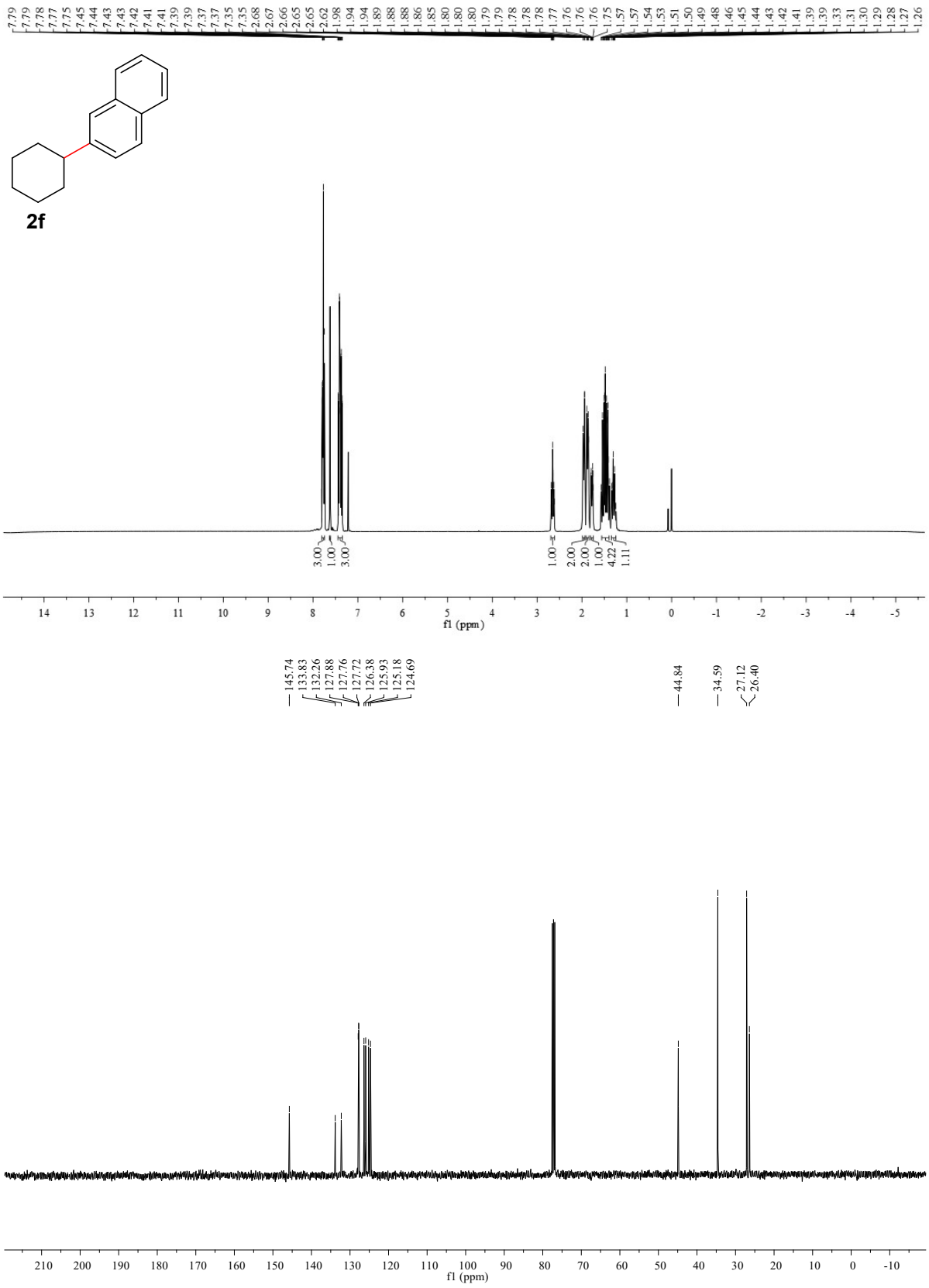
115.18
114.98
44.01
34.83
27.04
26.27
f1 (ppm)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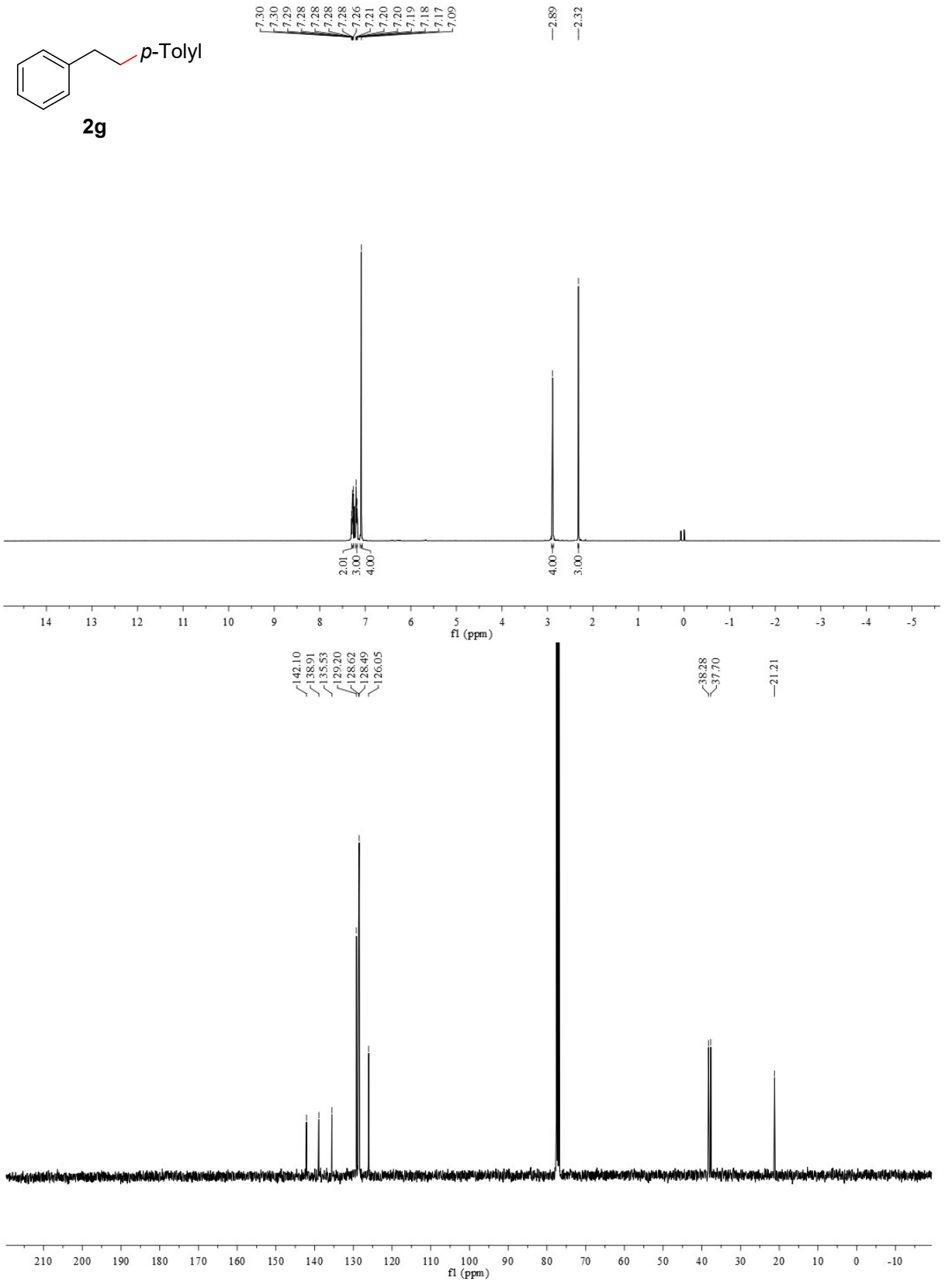
2f
3.00 1.00 3.00 1.00 2.00 2.00 1.00 4.22 1.11
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5
f1 (ppm)
145.74 133.83 132.26 127.88 127.76 127.72 126.38 125.93 125.18 124.69
44.84 34.59 27.12 26.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.20
7.19
7.18
7.17
7.09
2.89
2.32
2.01
3.00
4.00
4.00
3.00
f1 (ppm)
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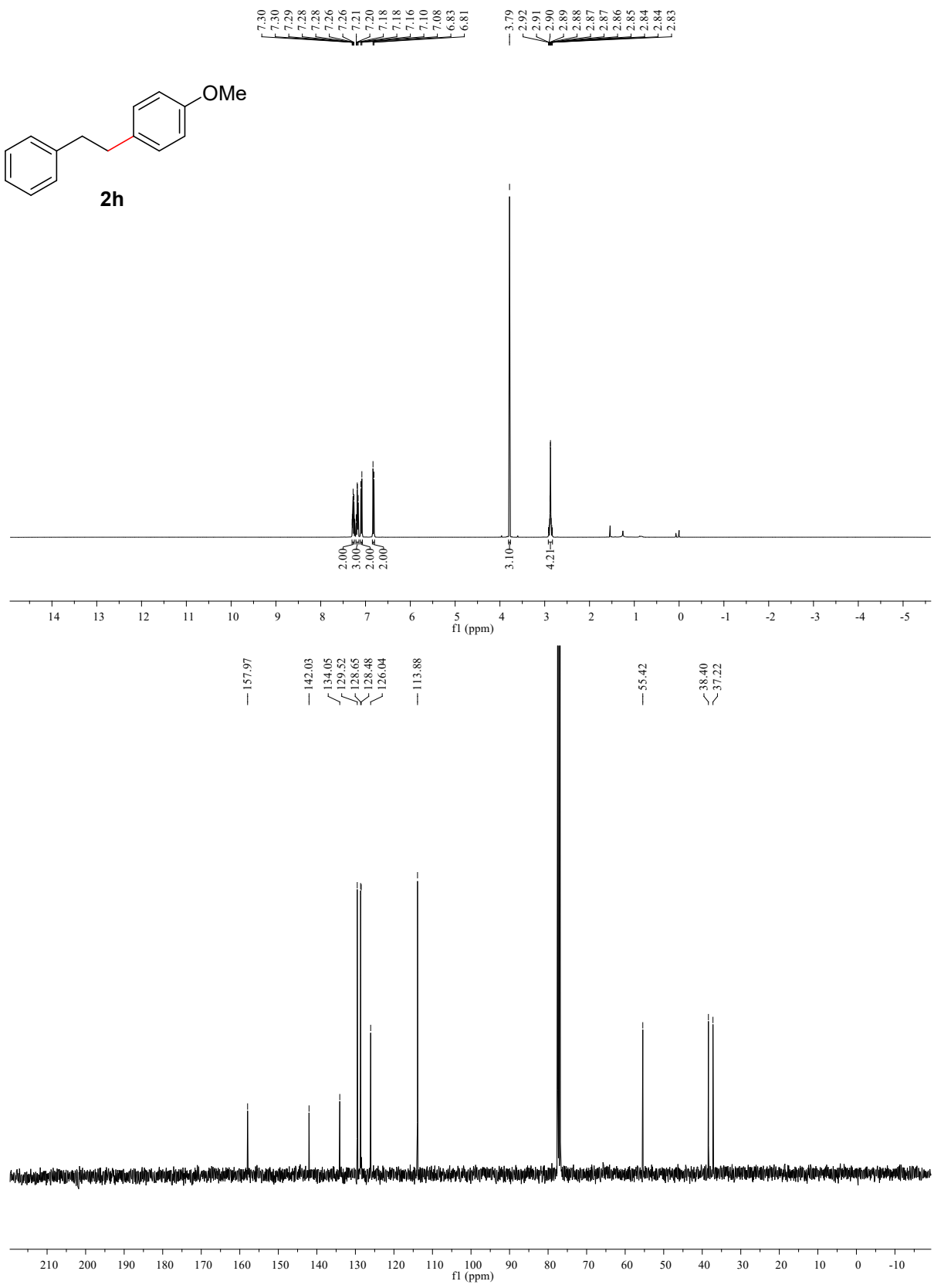
f1 (ppm)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7.08
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2.85
2.84
2.84
2.83
OMe
2h
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3.00
2.00
2.00
3.10
4.21
f1 (ppm)
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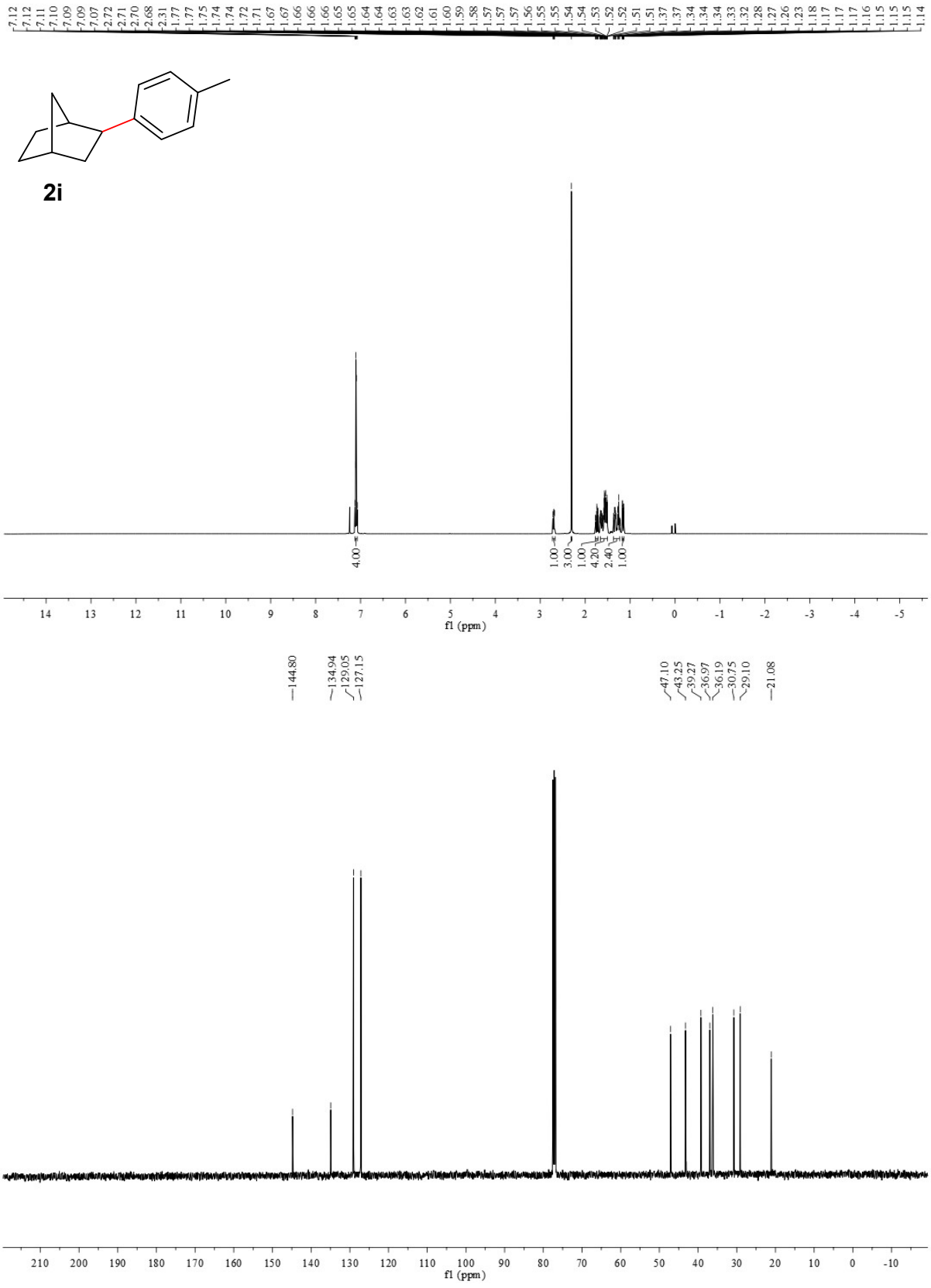
37.22
f1 (ppm)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2i
4.00 1.00 3.00 1.00 4.20 2.40 1.00
f1 (ppm)
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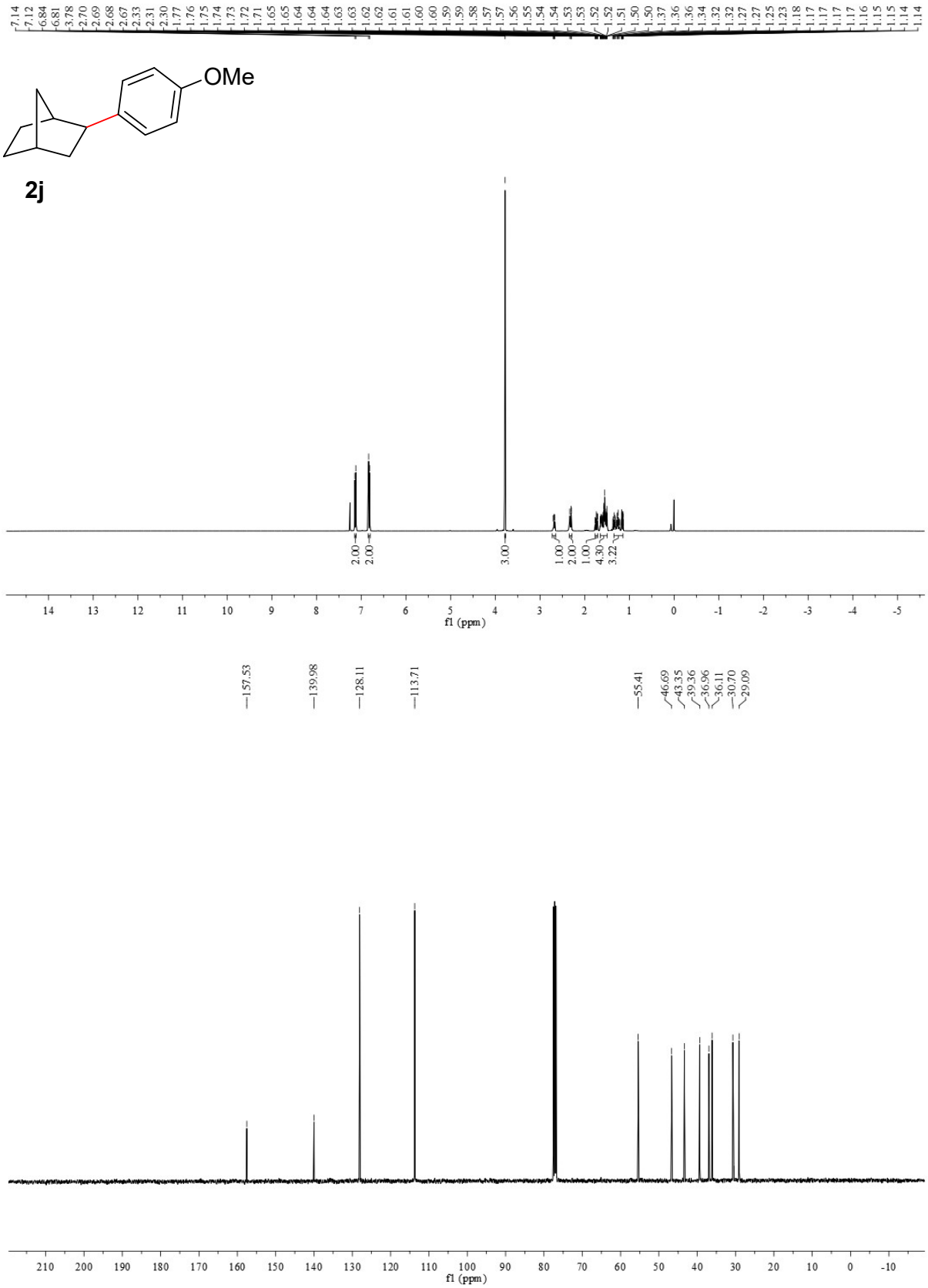
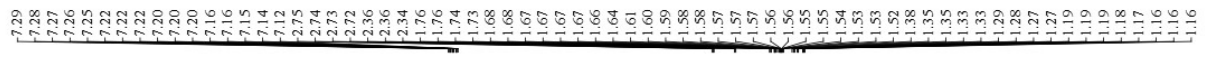
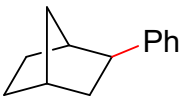
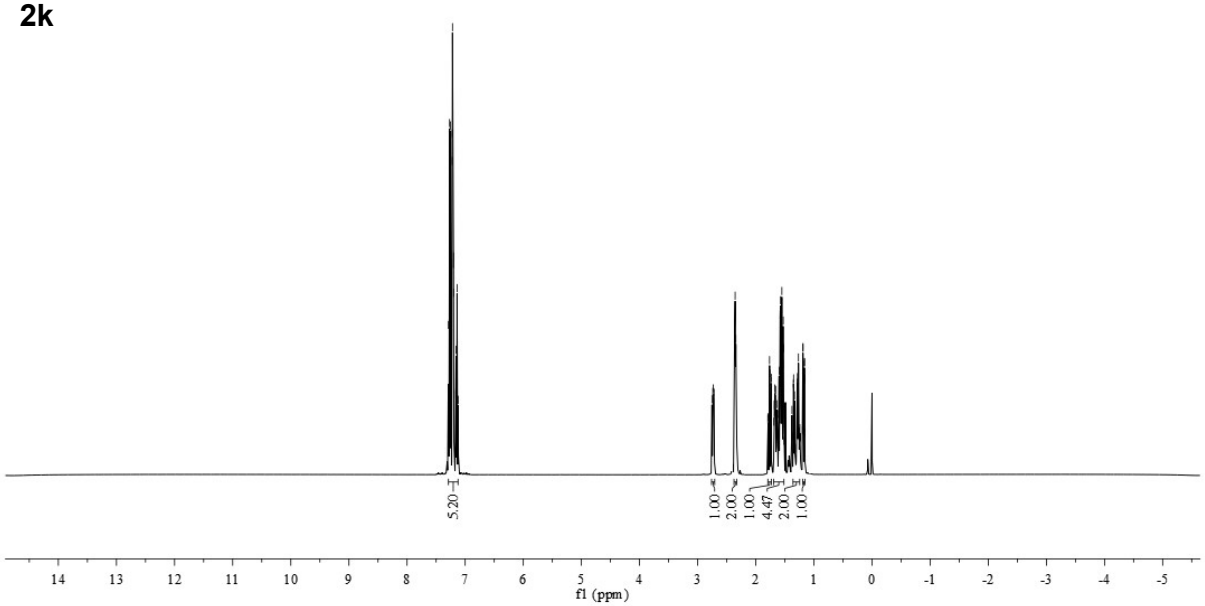
f1 (ppm)

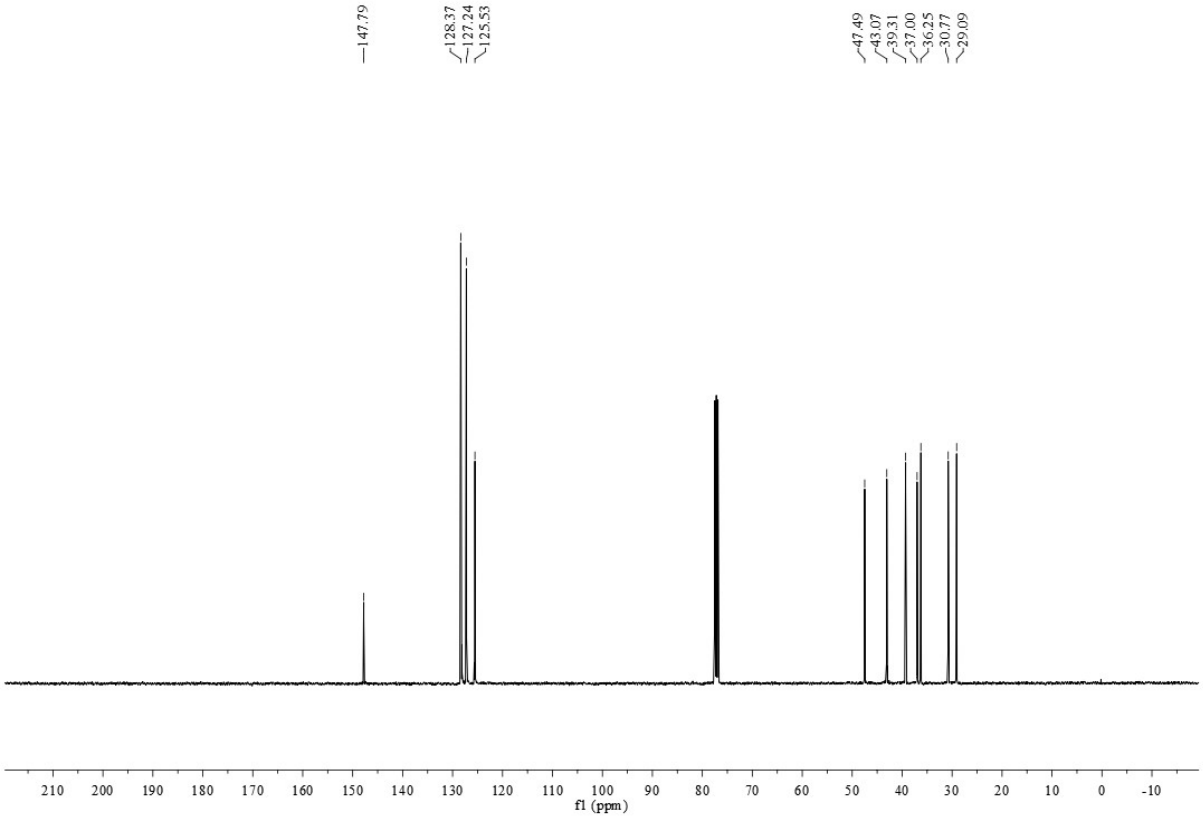

OMe
2j
f1 (ppm)
f1 (ppm)

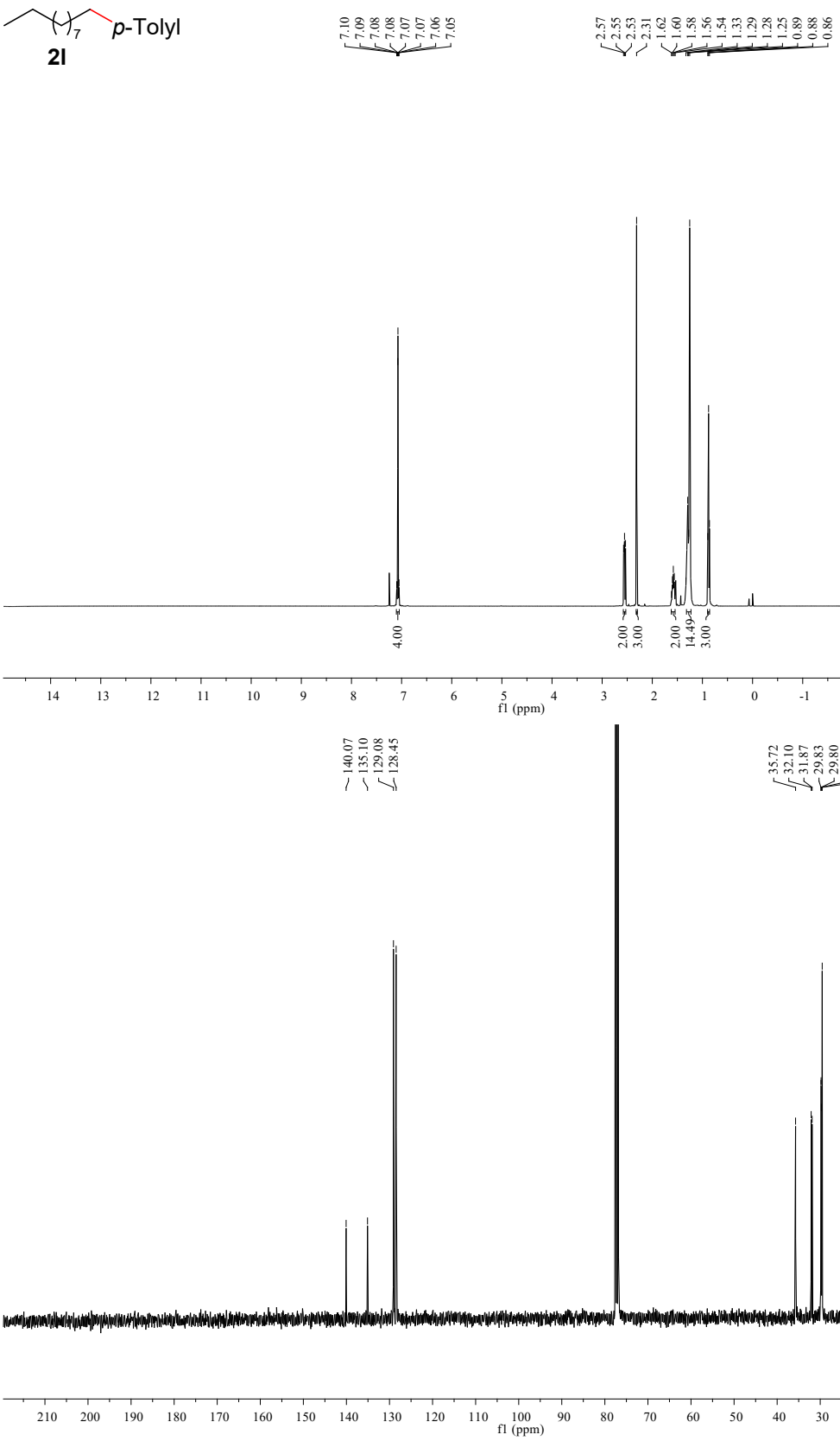


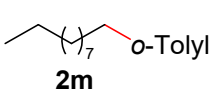

Ph

2k

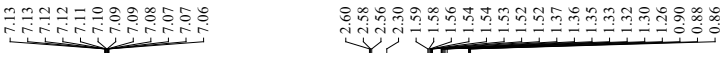

5.20
1.00
2.00
1.00
4.47
2.00
1.00
f1 (ppm)

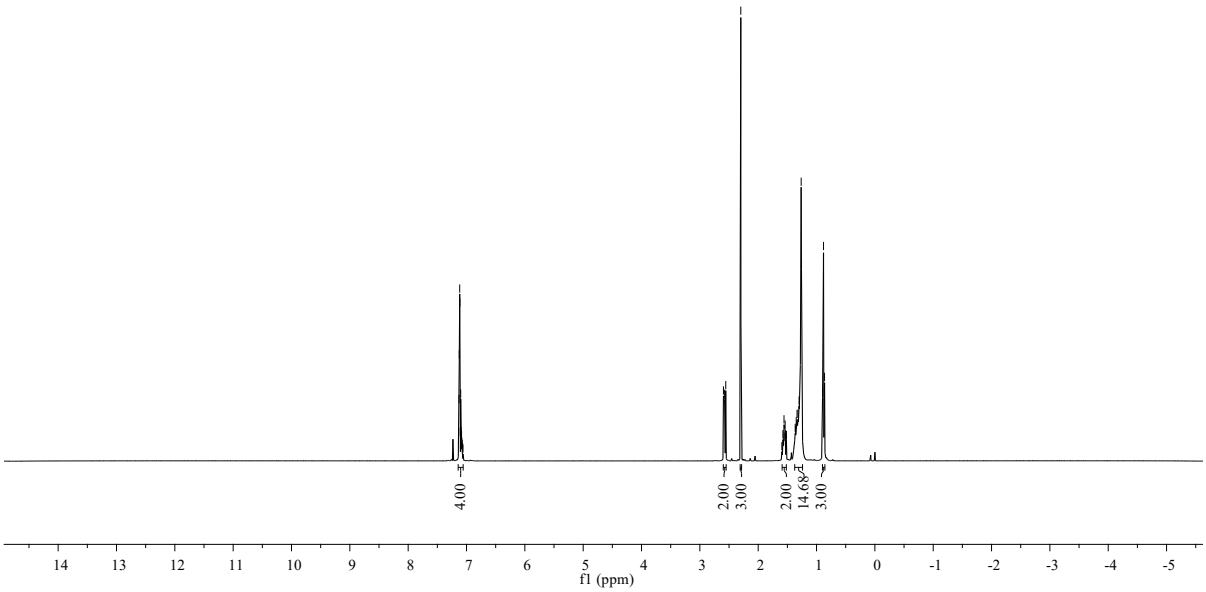

147.79
128.37
127.24
125.53
47.49
43.07
39.31
37.00
36.25
30.77
29.09
f1 (ppm)


p-Tolyl
7
2l
7.10
7.09
7.08
7.08
7.07
7.07
7.06
7.05
2.57
2.55
2.53
2.31
1.62
1.60
1.58
1.56
1.54
1.33
1.29
1.28
1.25
0.89
0.88
0.86
4.00
2.00
3.00
2.00
14.49
3.00
f1 (ppm)
140.07
135.10
129.08
128.45
35.72
32.10
31.87
29.83
29.80
29.73
29.54
22.89
21.18
14.32
f1 (ppm)


o-Tolyl
7

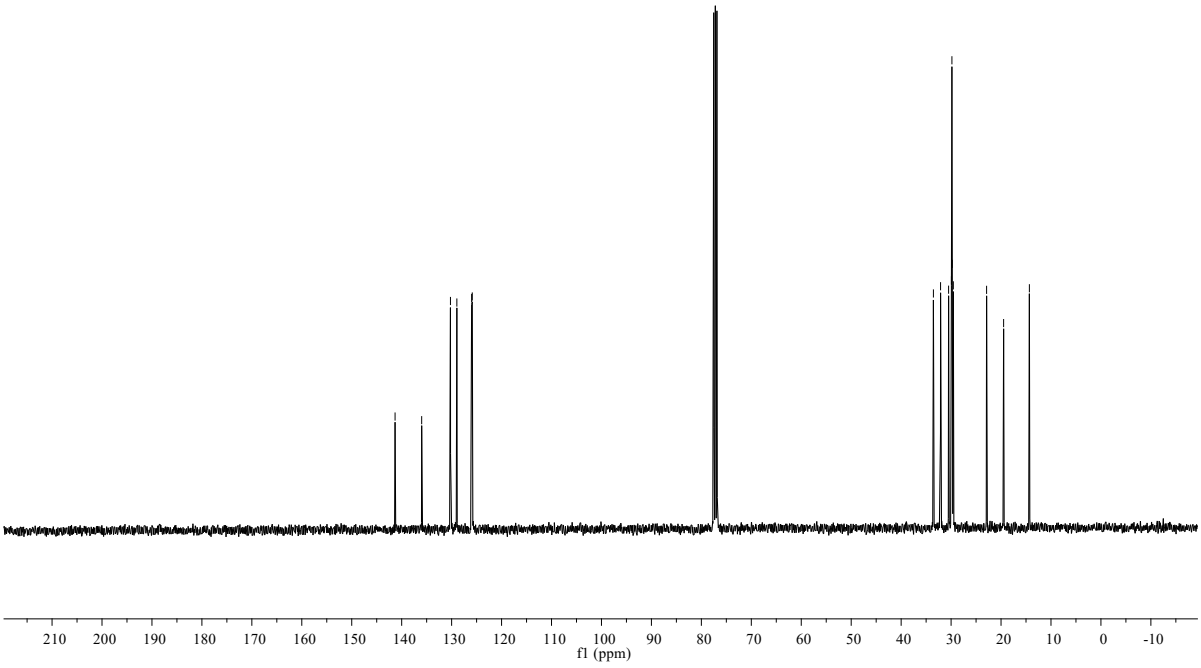
2m

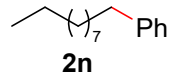

7.13
7.13
7.12
7.12
7.11
7.10
7.09
7.09
7.08
7.07
7.07
7.06
2.60
2.58
2.56
2.30
1.59
1.58
1.56
1.54
1.54
1.53
1.52
1.52
1.37
1.36
1.35
1.33
1.32
1.30
1.26
0.90
0.88
0.86


4.00
2.00
3.00
2.00
14.68
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5
f1 (ppm)


141.32
136.00
130.24
128.95
126.00
125.87

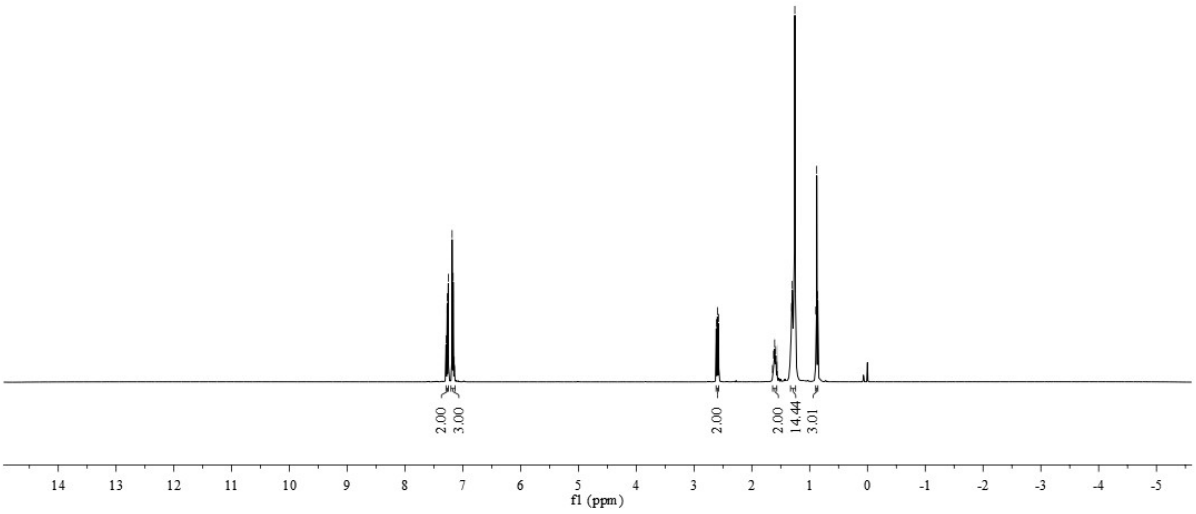
33.54
32.11
30.50
29.94
29.83
29.77
29.55
22.89
19.48
14.33

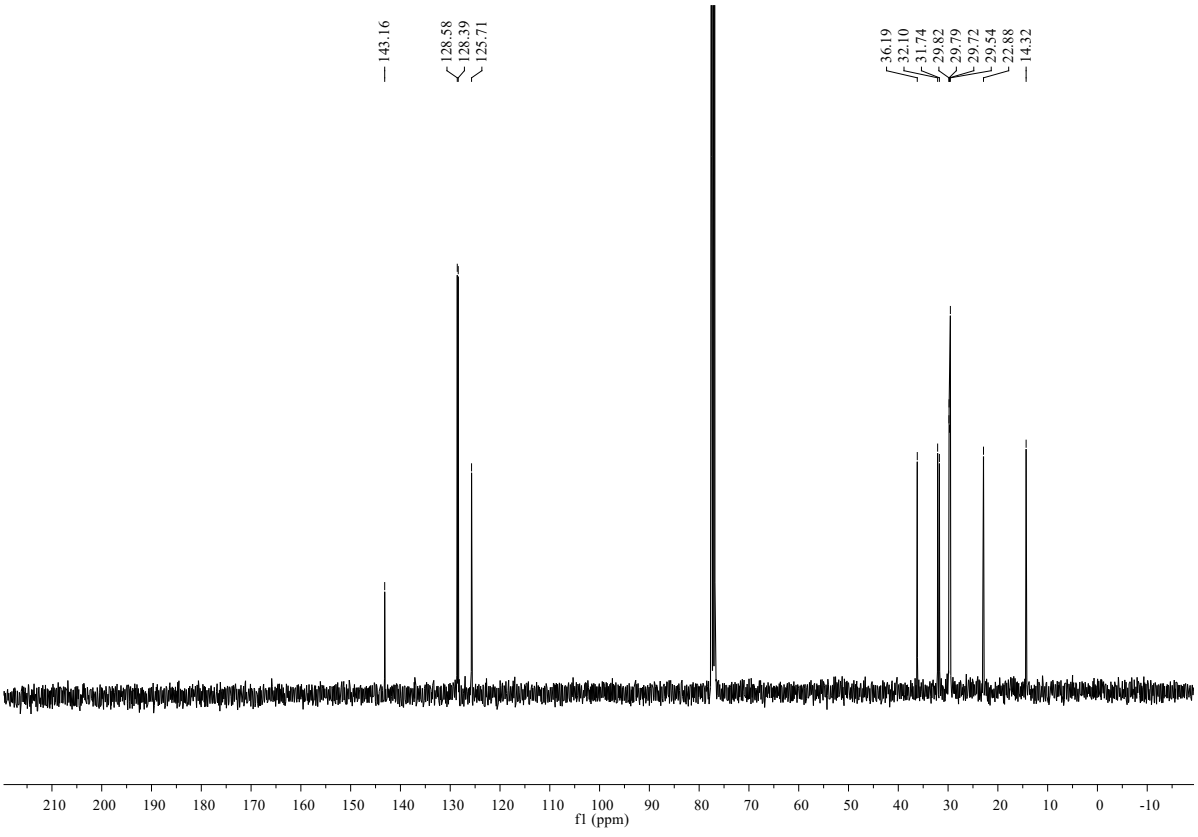

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

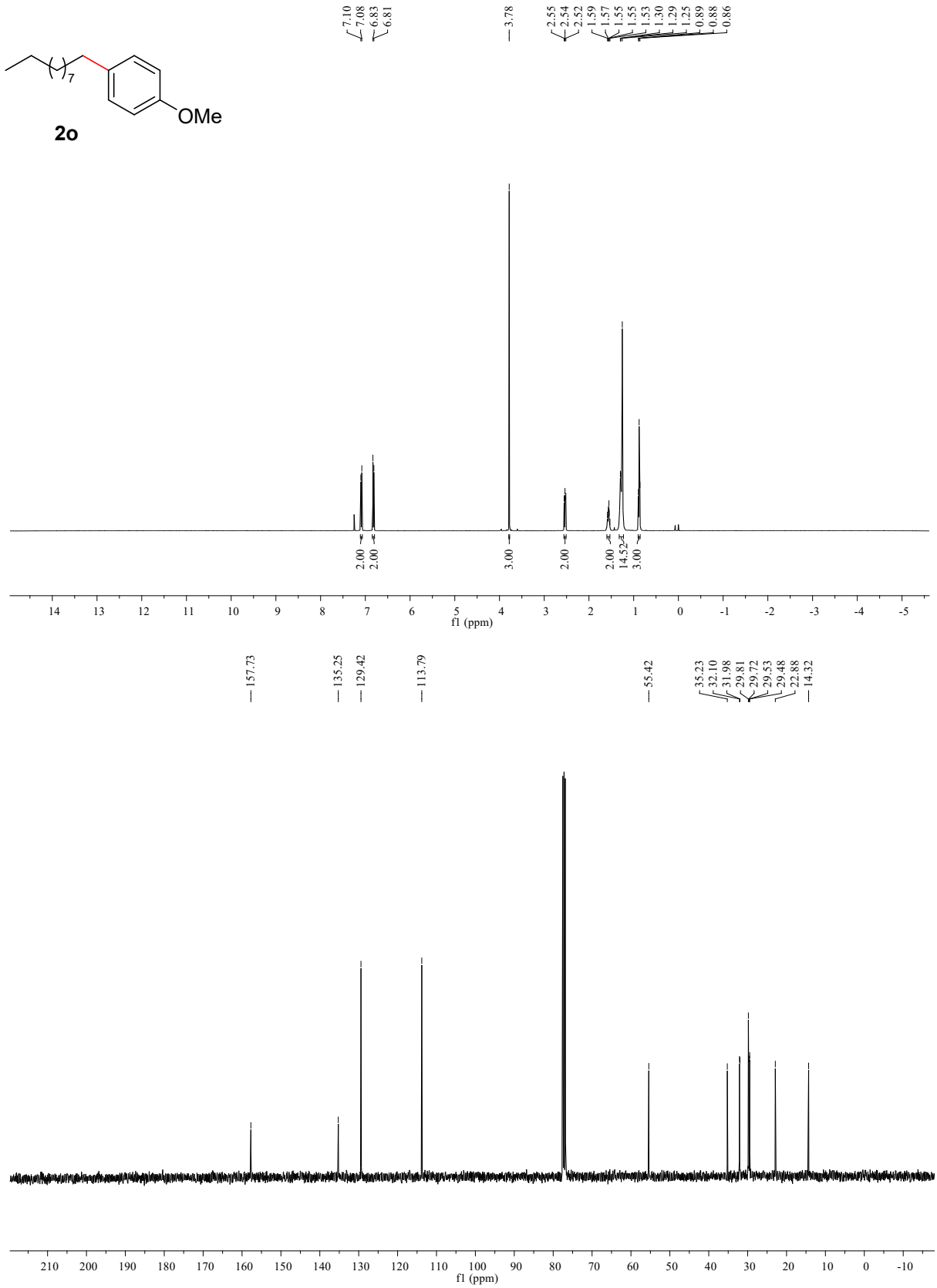

Ph
7

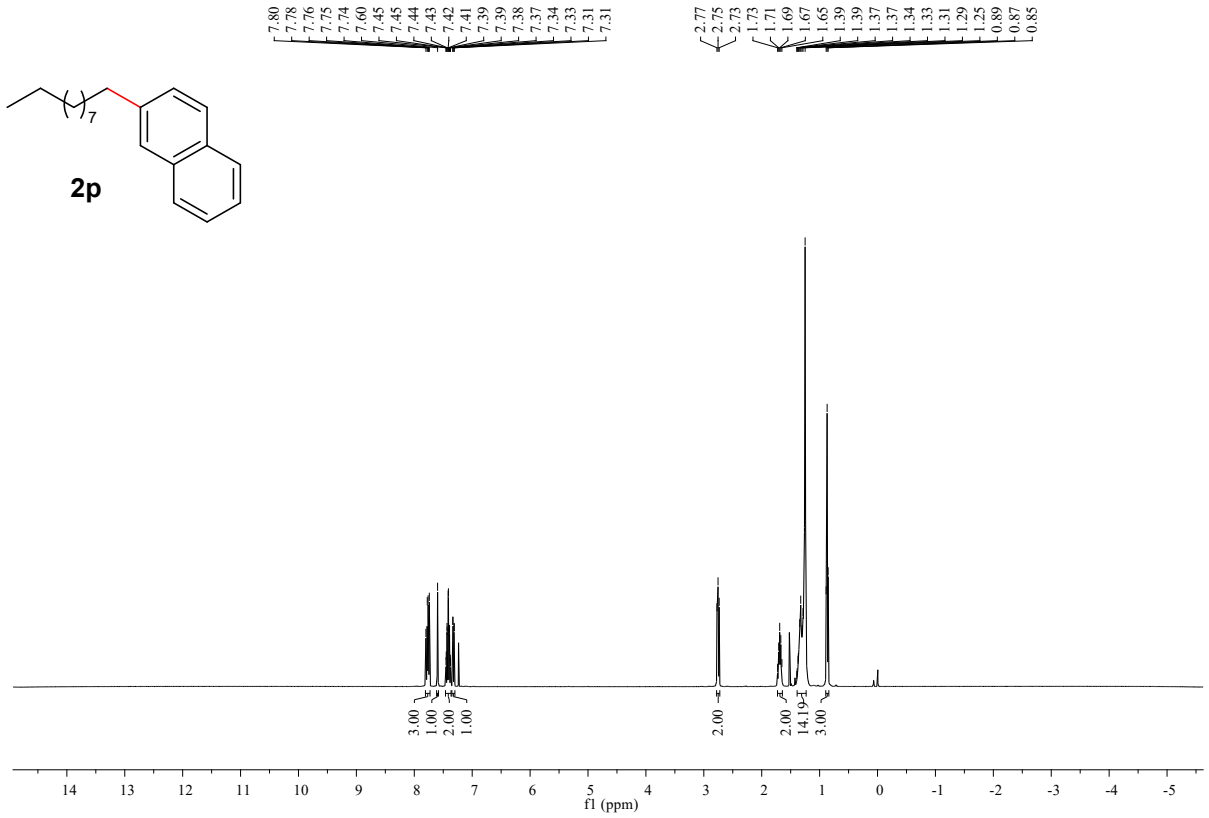
2n

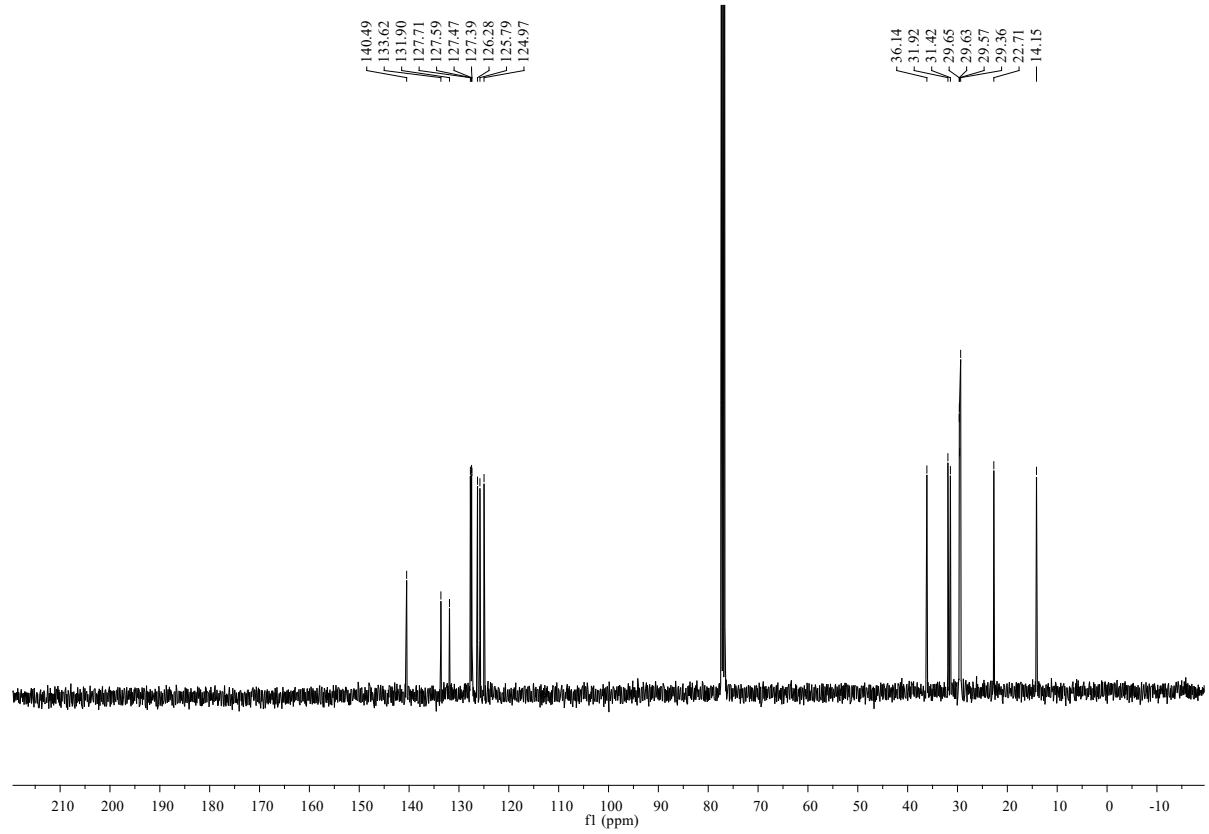

7.29
7.29
7.28
7.27
7.27
7.26
7.25
7.19
7.18
7.17
7.15
7.15
7.15
2.62
2.60
2.58
1.64
1.62
1.61
1.59
1.57
1.31
1.30
1.26
0.89
0.88
0.86

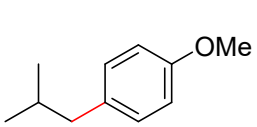

2.00
3.00
2.00
2.00
14.44
3.01
f1 (ppm)


143.16
128.58
128.39
125.71
36.19
32.10
31.74
29.82
29.79
29.72
29.54
22.88
14.32
f1 (ppm)


7.10
7.08
6.83
6.81
3.78
2.55
2.54
2.52
1.59
1.57
1.55
1.55
1.53
1.30
1.29
1.25
0.89
0.88
0.86
OMe
2o
2.00
2.00
3.00
2.00
2.00
14.52
3.00
f1 (ppm)
157.73
135.25
129.42
113.79
55.42
35.23
32.10
31.98
29.81
29.72
29.53
29.48
22.88
14.32
f1 (ppm)

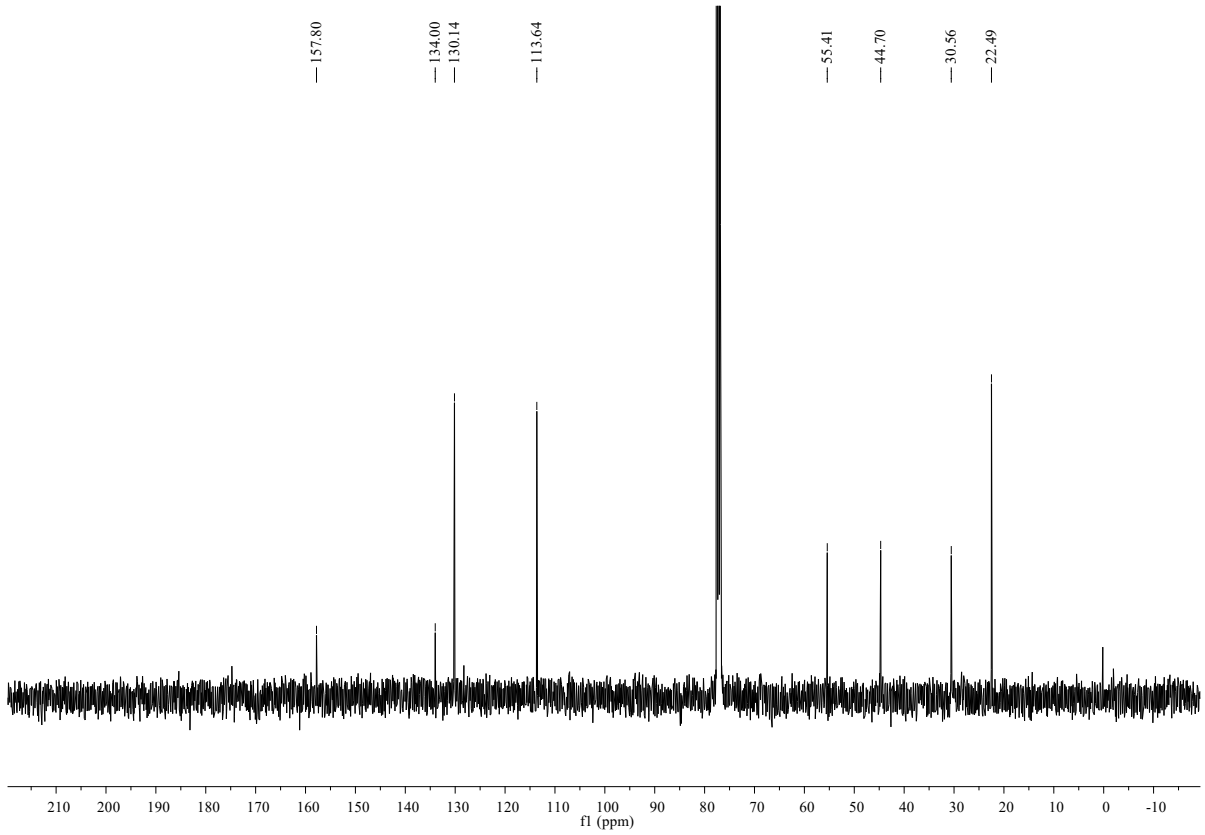

7.80
7.78
7.76
7.75
7.74
7.60
7.45
7.45
7.44
7.43
7.42
7.41
7.39
7.39
7.38
7.37
7.34
7.33
7.31
7.31
2.77
2.75
2.73
1.73
1.71
1.69
1.67
1.65
1.39
1.39
1.37
1.37
1.34
1.33
1.31
1.29
1.25
0.89
0.87
0.85
7
2p
3.00
1.00
2.00
1.00
2.00
2.00
14.19
3.00
f1 (ppm)

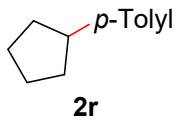

140.49
133.62
131.90
127.71
127.59
127.47
127.39
126.28
125.79
124.97
36.14
31.92
31.42
29.65
29.63
29.57
29.36
22.71
14.15
f1 (ppm)


OMe

2q

7.07
7.04
6.83
6.81
3.79
2.42
2.40
1.84
1.82
1.81
1.79
1.77
0.88
2.00
2.00
3.00
2.00
1.00
6.00
f1 (ppm)


157.80
134.00
130.14
113.64
55.41
44.70
30.56
22.49
f1 (ppm)


p-Tolyl

2r

7.15
7.13
7.11
7.09
2.95
2.32
2.06
2.06
2.05
2.05
2.05
2.04
2.04
2.04
2.03
2.03
2.02
1.81
1.81
1.80
1.80
1.79
1.78
1.78
1.78
1.76
1.69
1.68
1.67
1.66
1.65
1.65
1.59
1.58
1.58
1.58
1.57
1.57
1.56
1.56
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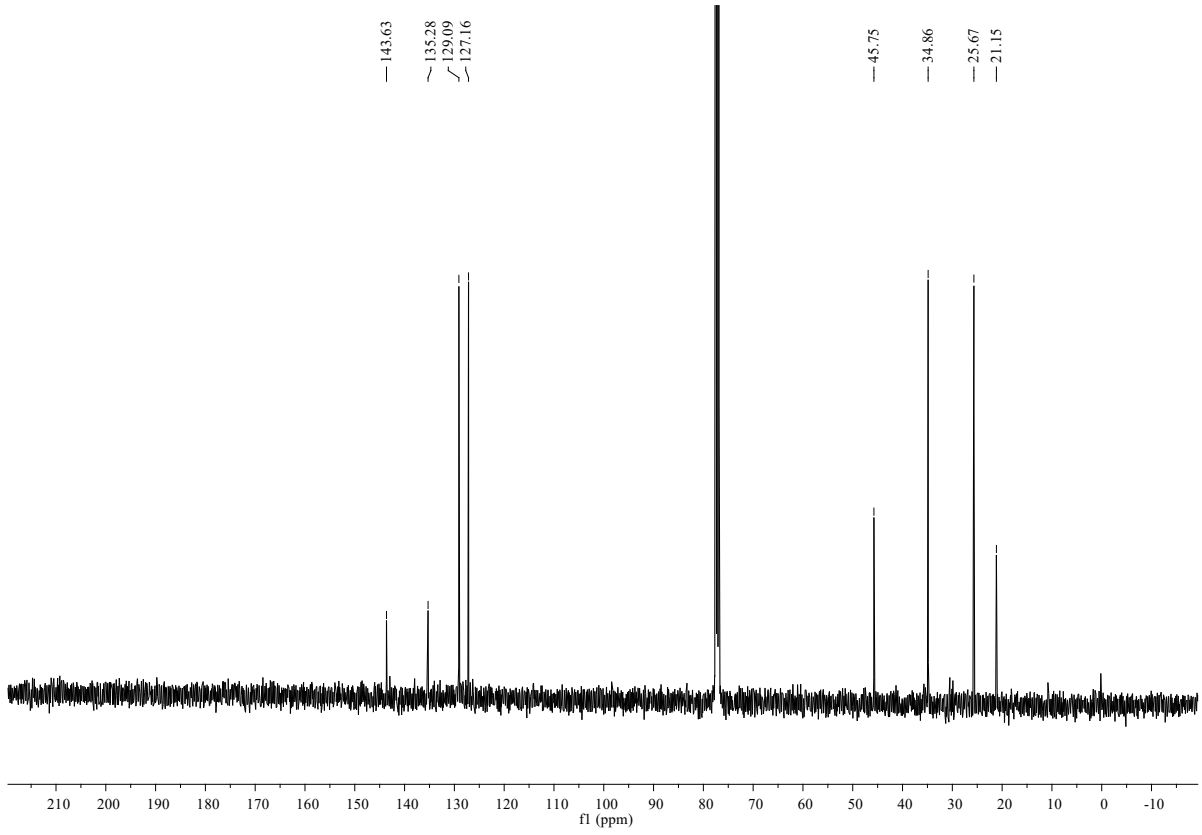
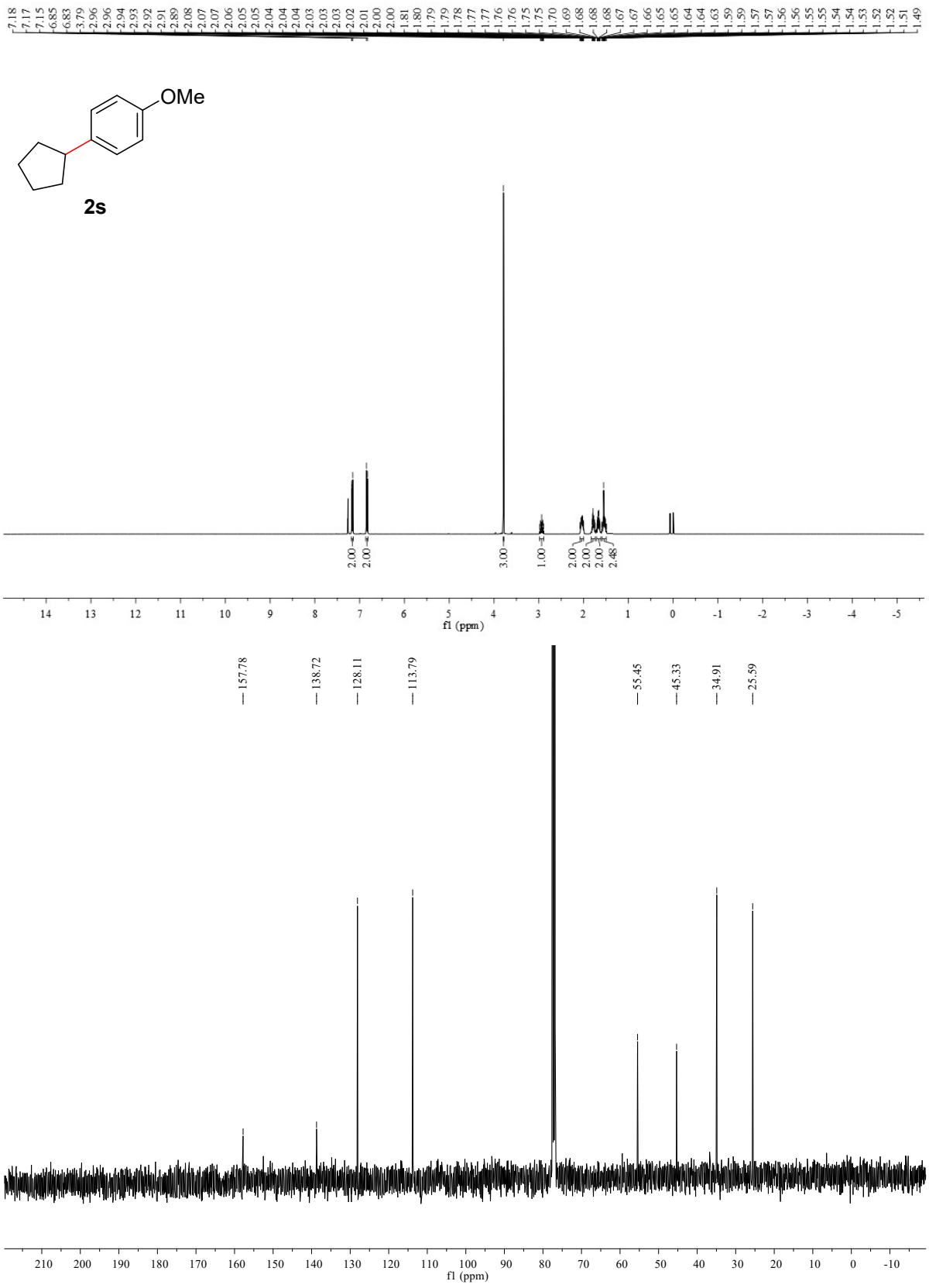
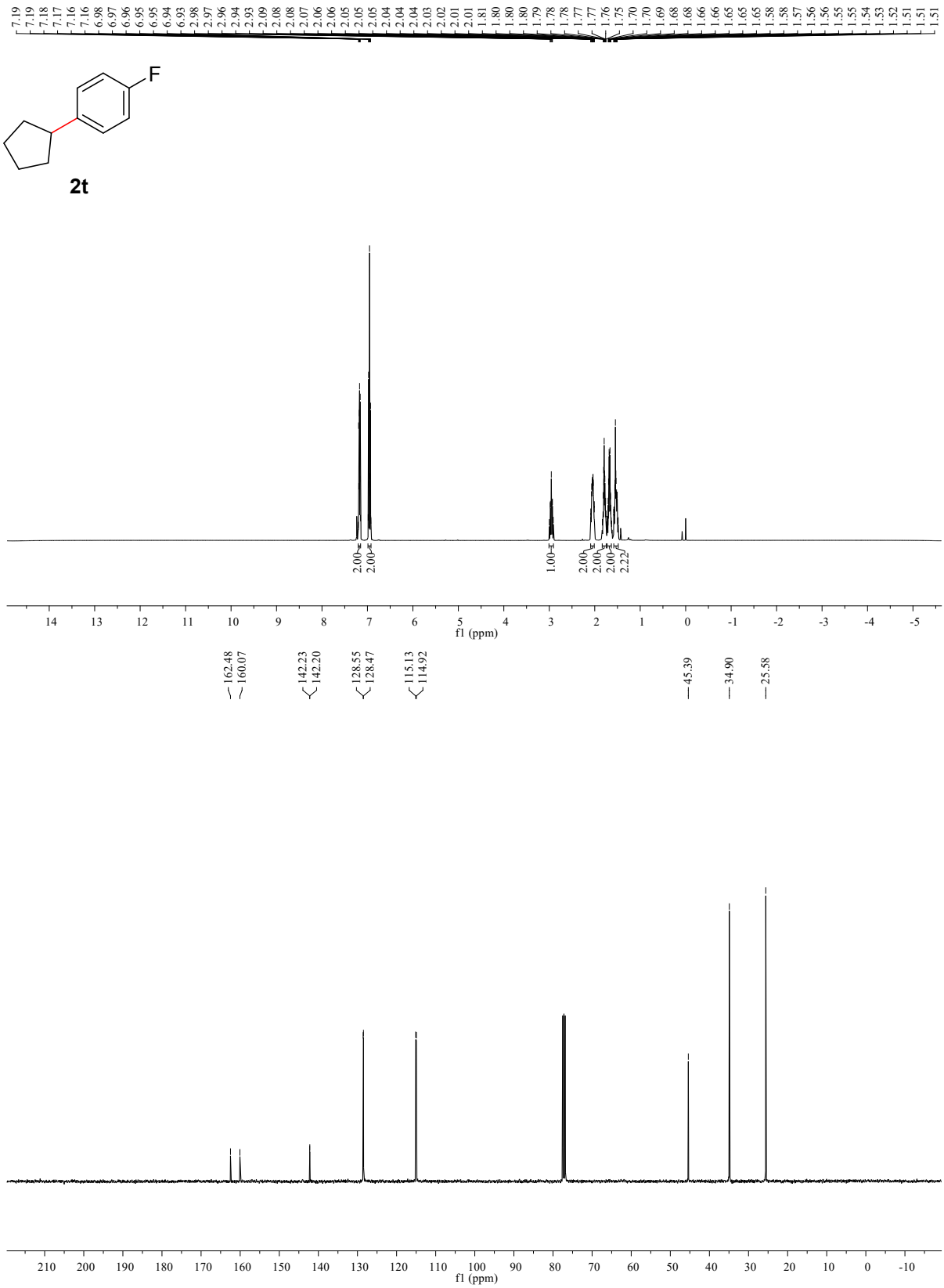
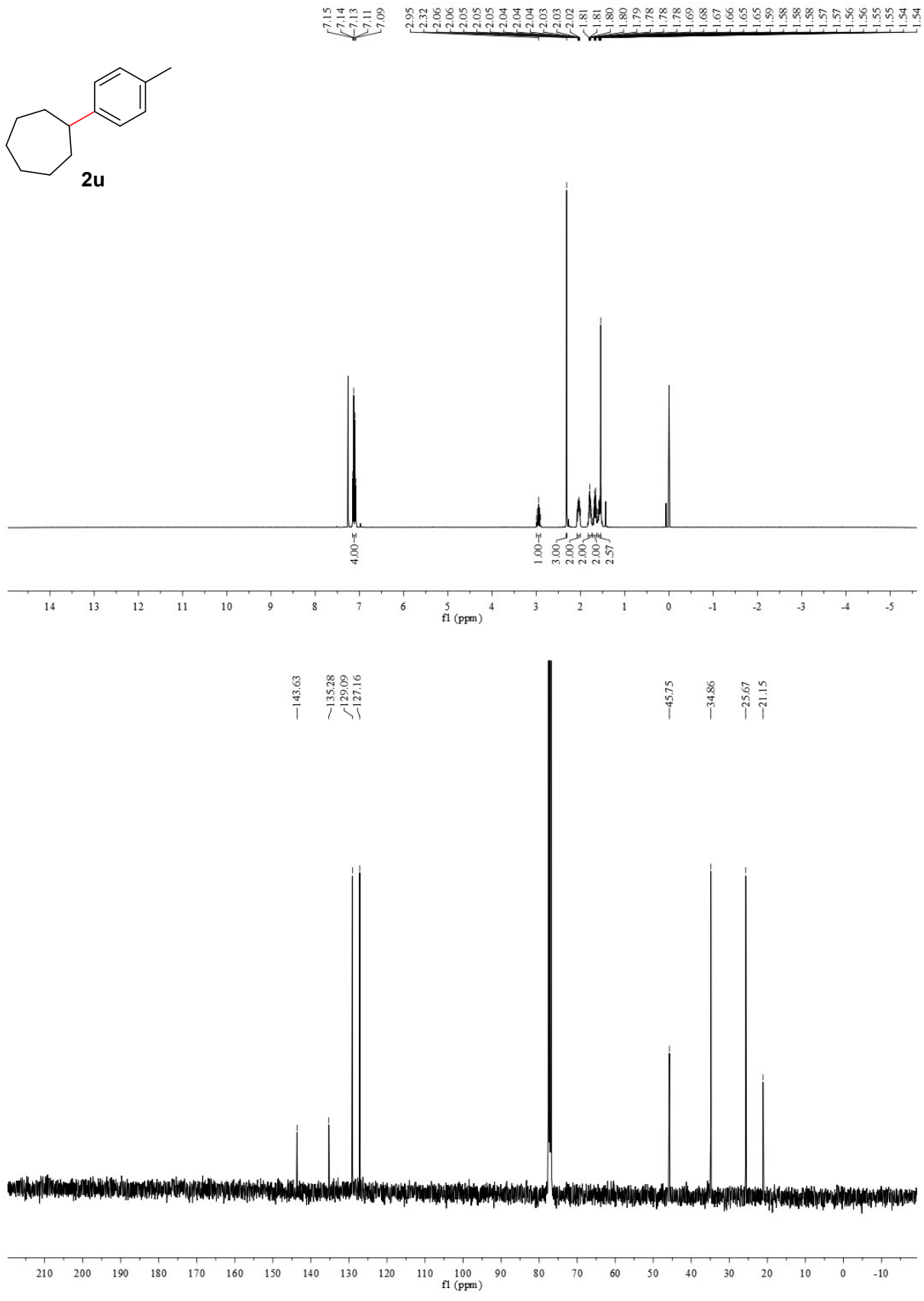
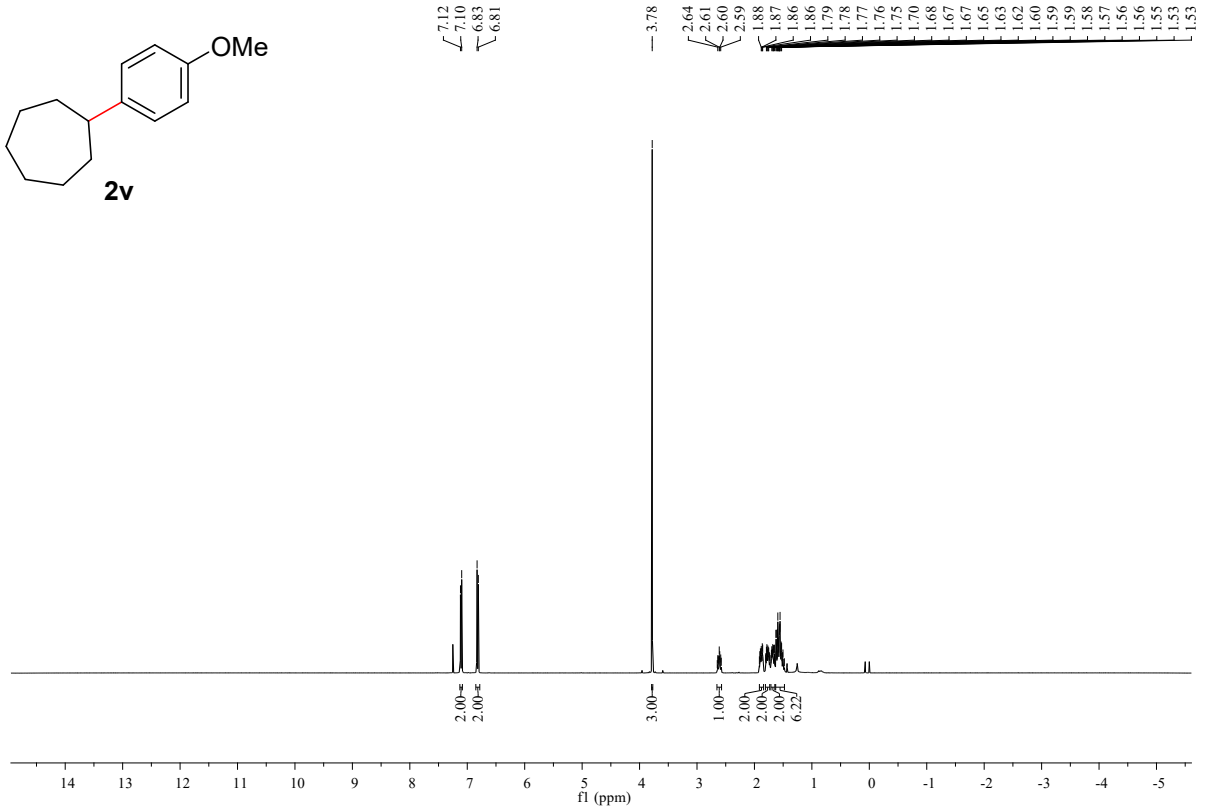
2.00
2.00
2.00
2.57
f1 (ppm)

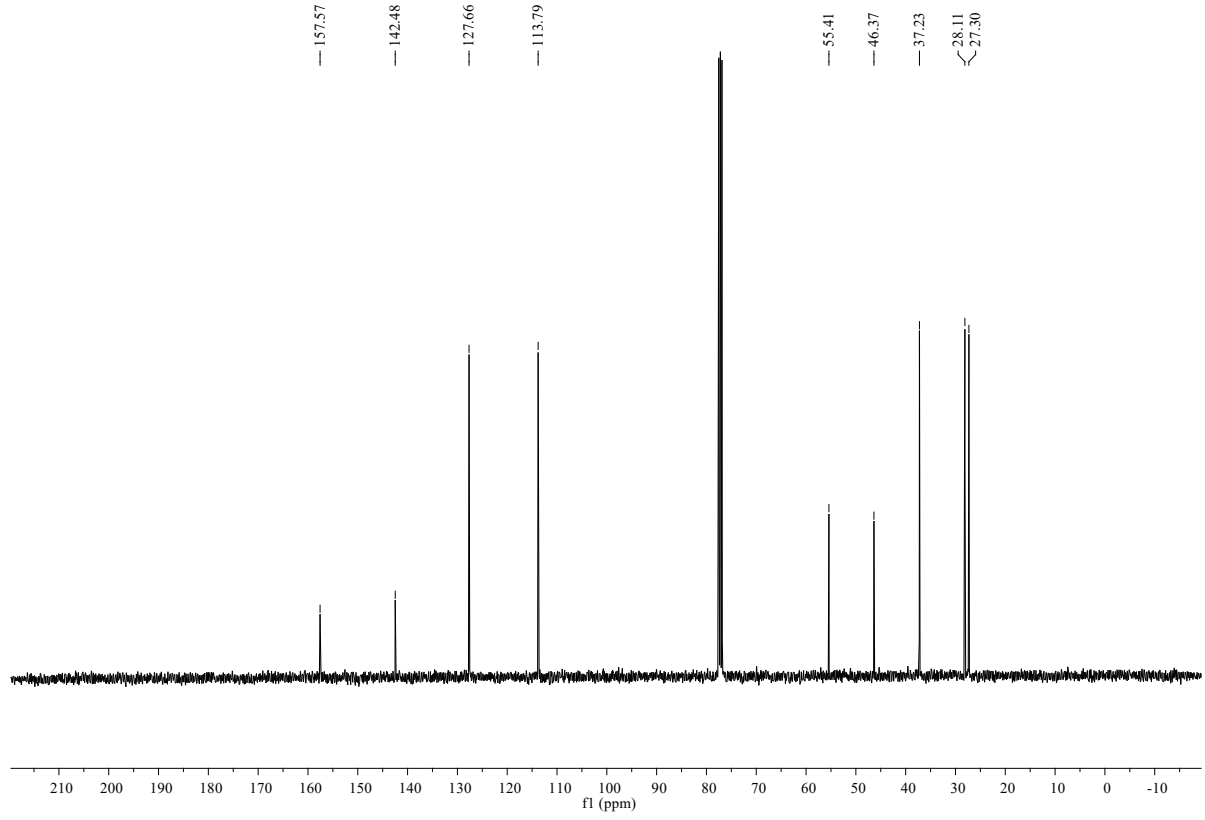

143.63
135.28
129.09
127.16
45.75
34.86
25.67
21.15
f1 (ppm)

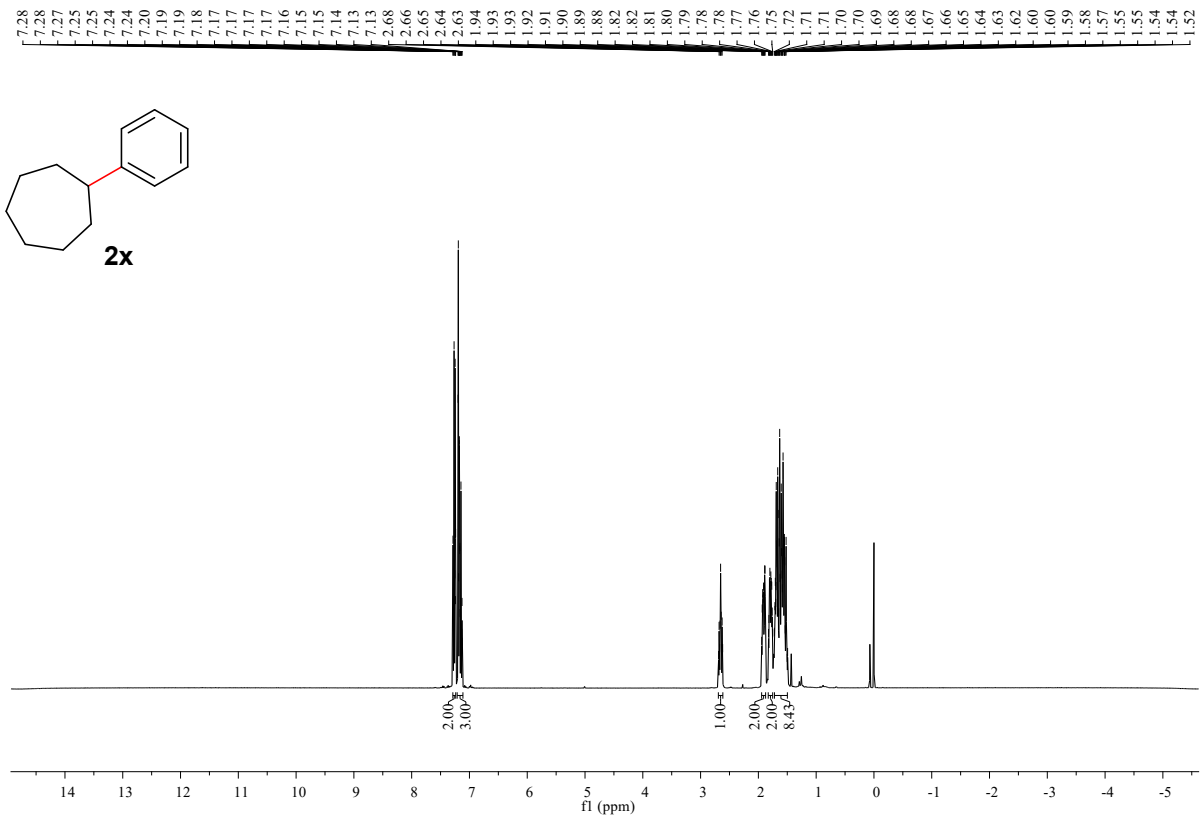

OMe
2s
f1 (ppm)
157.78
138.72
128.11
113.79
55.45
45.33
34.91
25.59
f1 (ppm)

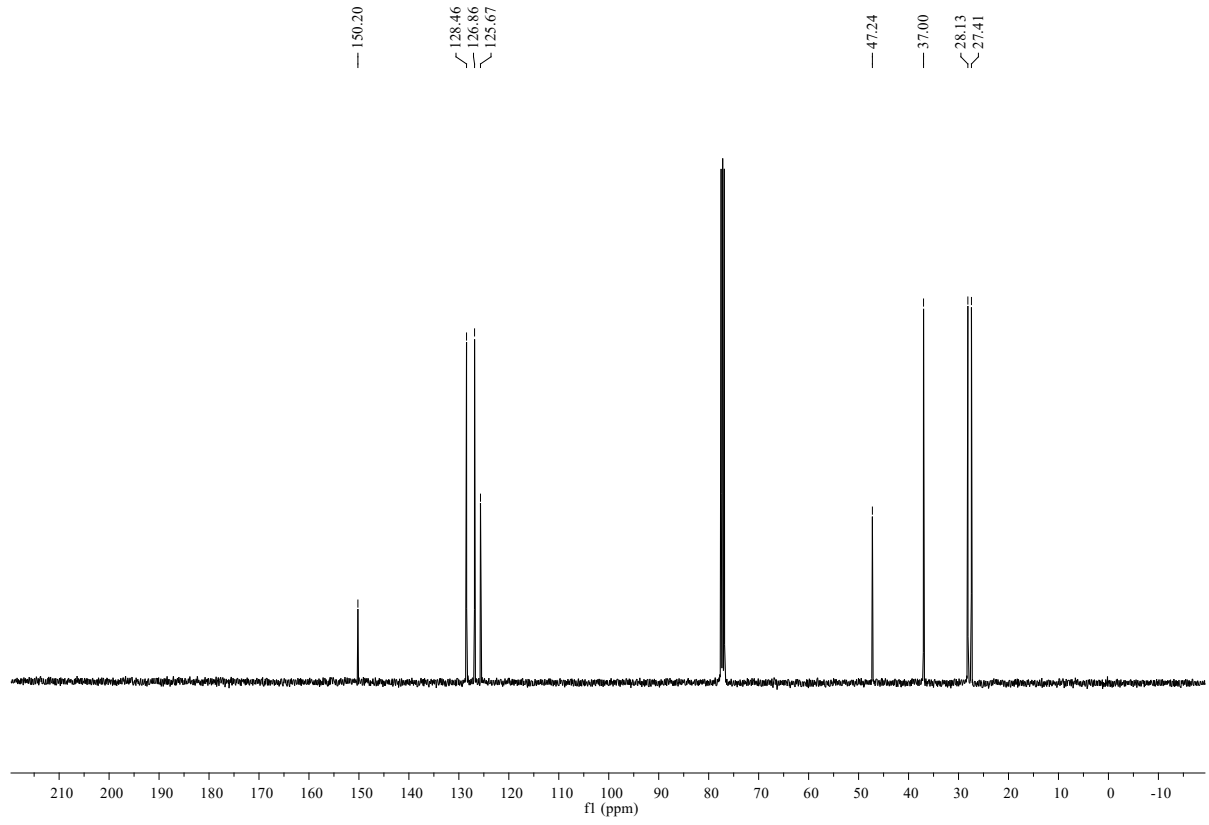

7.19 7.19 7.18 7.17 7.16 7.16 6.98 6.97 6.96 6.95 6.95 6.94 6.93 2.98 2.97 2.96 2.94 2.93 2.09 2.08 2.08 2.07 2.06 2.06 2.05 2.05 2.05 2.04 2.04 2.04 2.03 2.02 2.01 2.01 1.81 1.80 1.80 1.80 1.79 1.78 1.78 1.77 1.77 1.76 1.75 1.70 1.70 1.69 1.68 1.68 1.66 1.66 1.65 1.65 1.65 1.58 1.58 1.57 1.56 1.56 1.55 1.55 1.54 1.53 1.52 1.51 1.51 1.51
F
2t
2.00 2.00 1.00 2.00 2.00 2.00 2.22
f1 (ppm)
162.48 160.07 142.23 142.20 128.55 128.47 115.13 114.92 45.39 34.90 25.58
f1 (ppm)

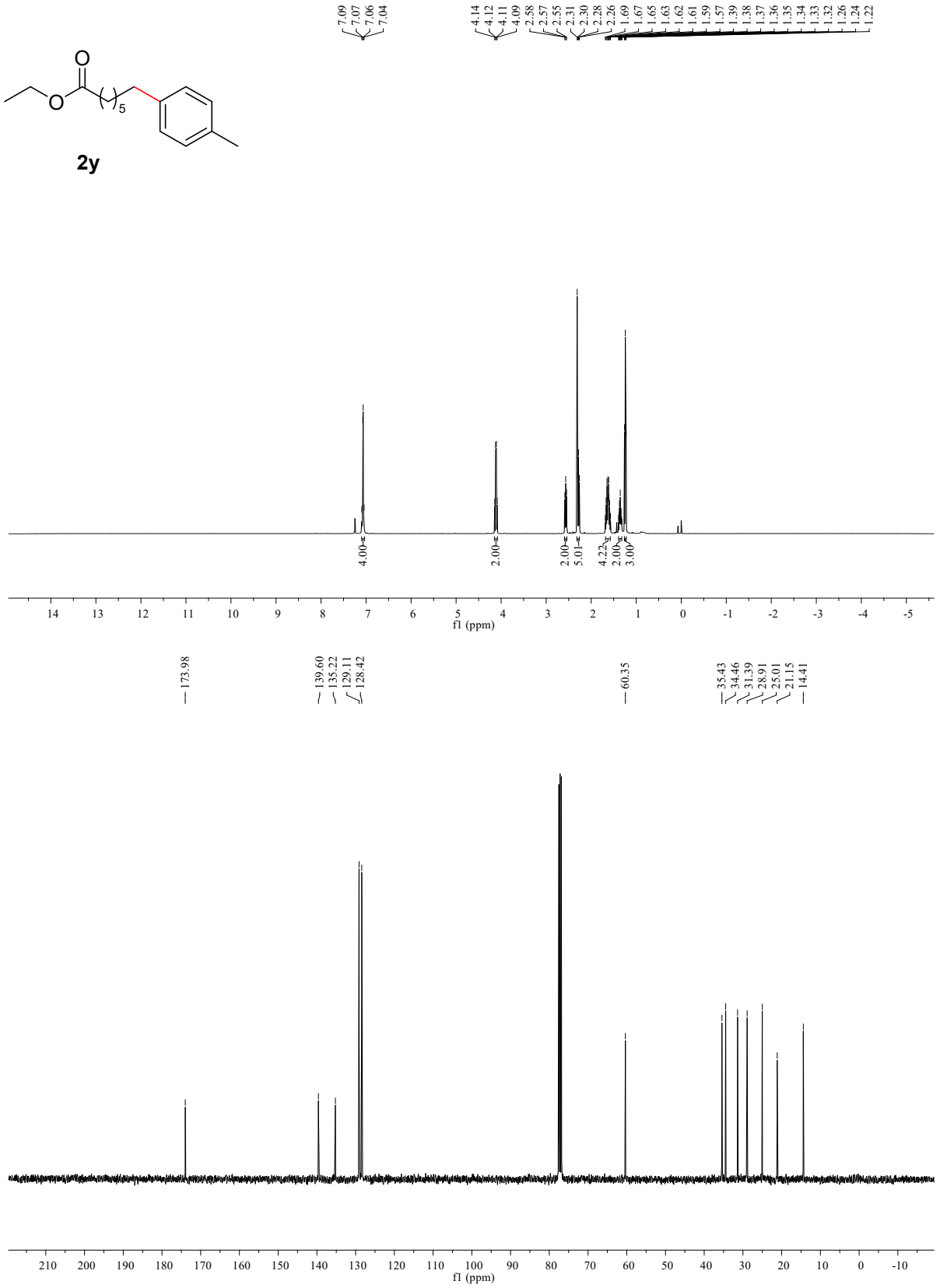

7.15
7.14
7.13
7.11
7.09
2.95
2.32
2.06
2.06
2.05
2.05
2.05
2.04
2.04
2.04
2.03
2.03
2.02
1.81
1.81
1.80
1.80
1.79
1.78
1.78
1.78
1.69
1.68
1.67
1.66
1.65
1.65
1.59
1.58
1.58
1.58
1.57
1.57
1.56
1.56
1.55
1.55
1.54
1.54
2u
4.00
1.00
3.00
2.00
2.00
2.00
2.57
f1 (ppm)
143.63
135.28
129.09
127.16
45.75
34.86
25.67
21.15
f1 (ppm)

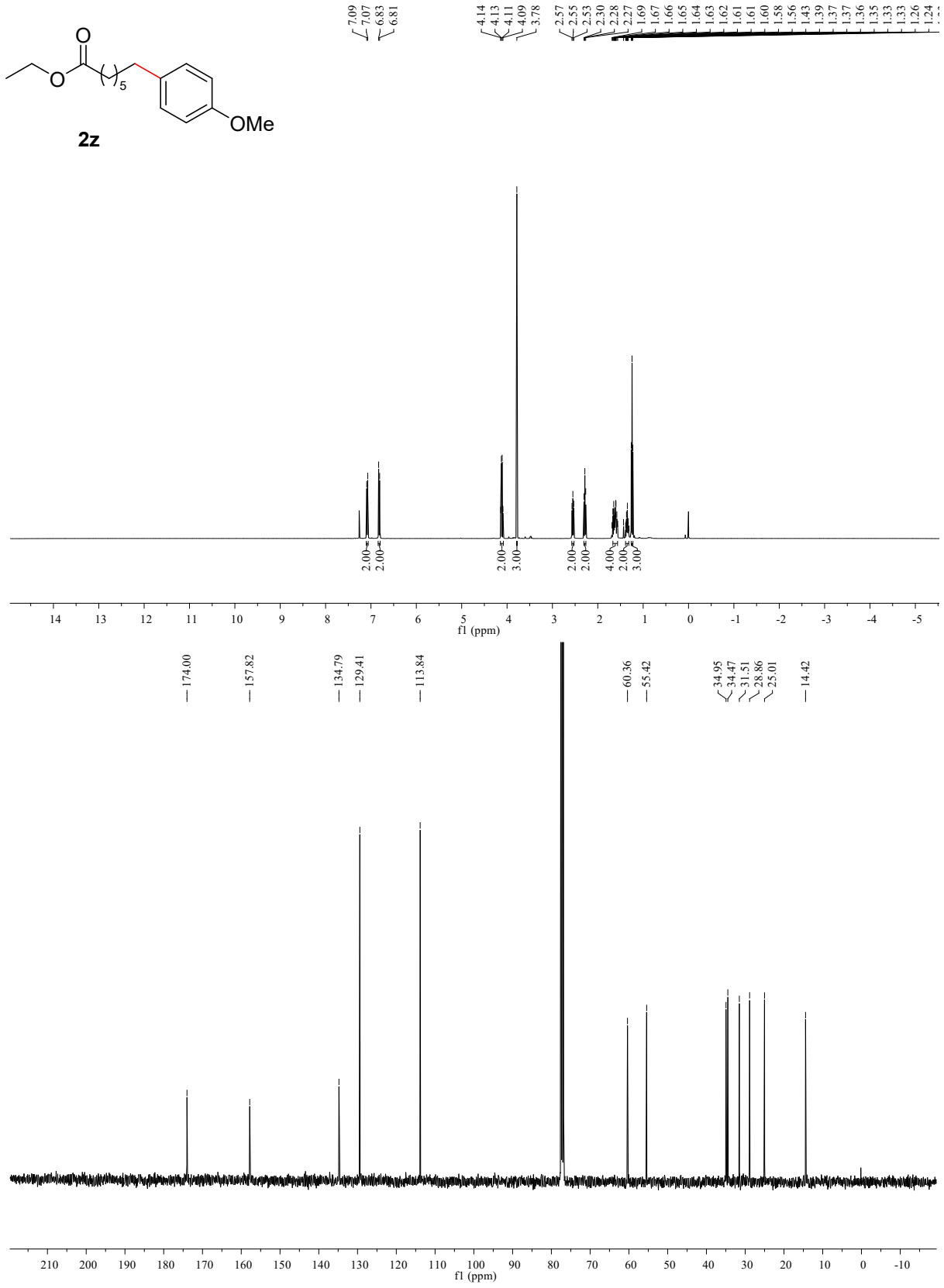

OMe
2v
7.12
7.10
6.83
6.81
3.78
2.64
2.61
2.60
2.59
1.88
1.87
1.86
1.86
1.79
1.78
1.77
1.76
1.75
1.70
1.68
1.67
1.67
1.65
1.63
1.62
1.60
1.59
1.59
1.58
1.57
1.56
1.56
1.55
1.53
1.53
2.00
2.00
3.00
1.00
2.00
2.00
2.00
6.22
f1 (ppm)

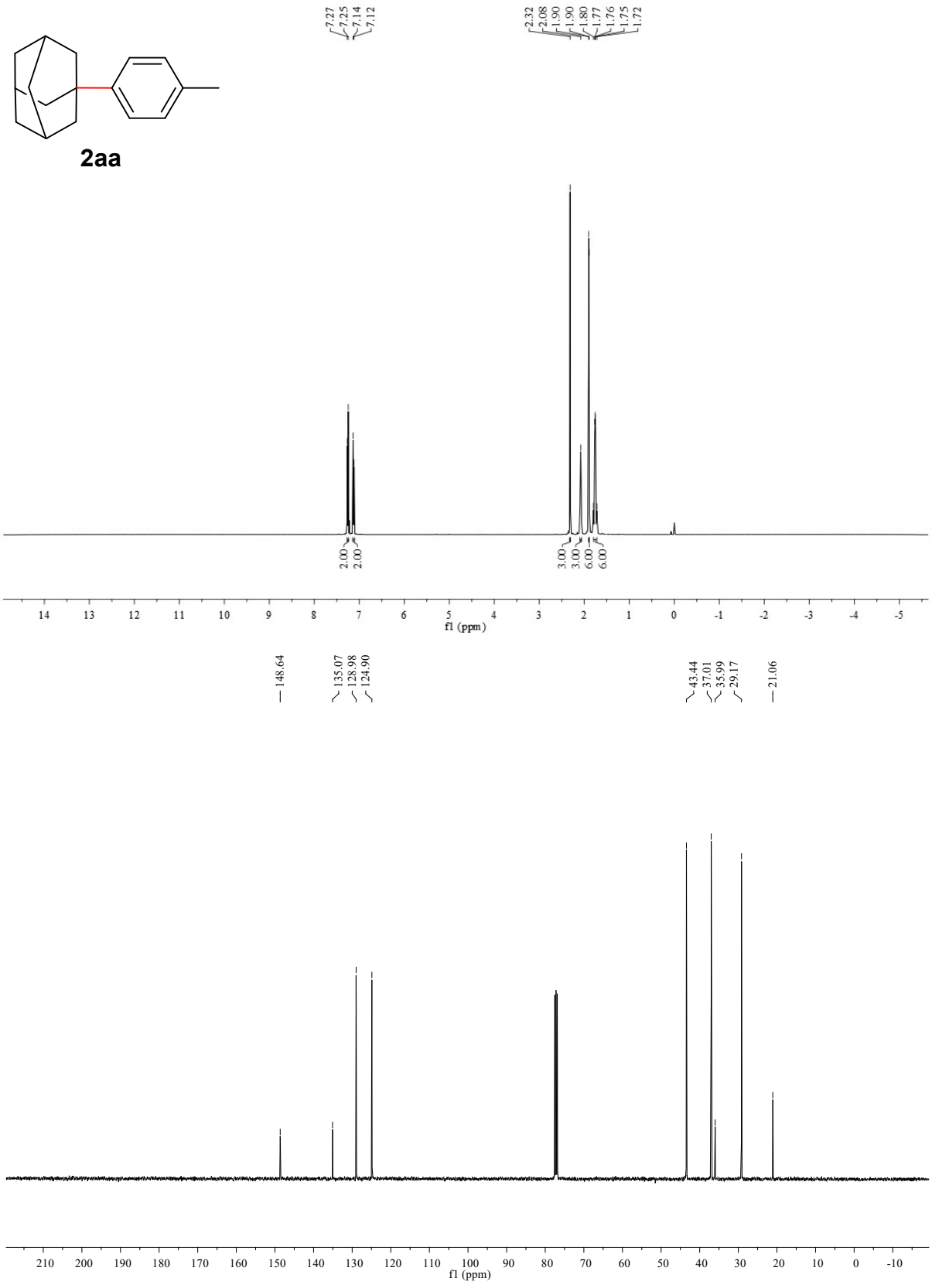

157.57
142.48
127.66
113.79
55.41
46.37
37.23
28.11
27.30
f1 (ppm)

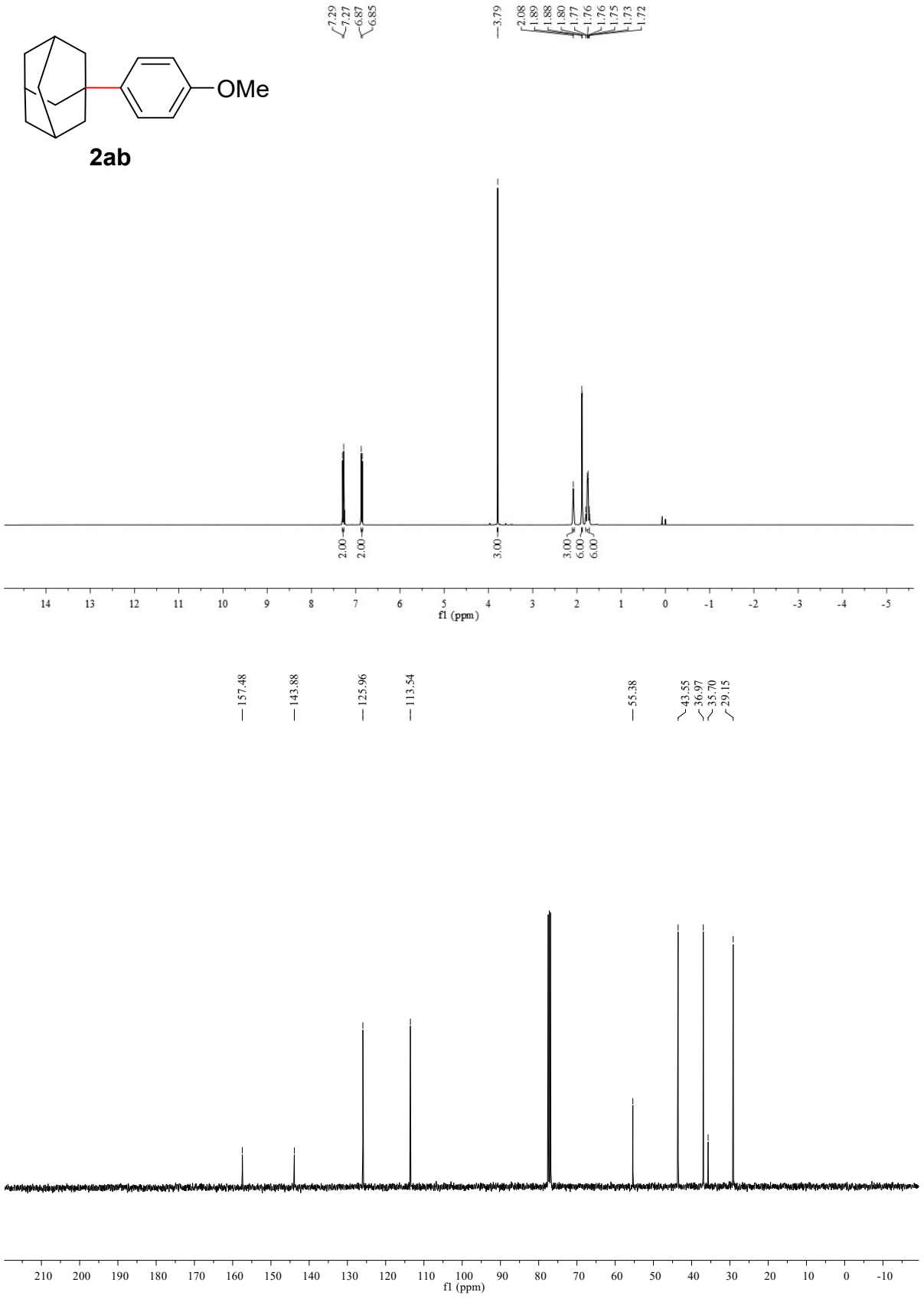

7.28 7.28 7.27 7.25 7.25 7.24 7.24 7.20 7.19 7.18 7.17 7.17 7.17 7.17 7.16 7.15 7.15 7.14 7.13 7.13 2.68 2.66 2.65 2.64 2.63 1.94 1.93 1.92 1.91 1.90 1.89 1.88 1.82 1.82 1.81 1.80 1.79 1.78 1.78 1.77 1.76 1.75 1.72 1.71 1.71 1.70 1.70 1.69 1.68 1.68 1.67 1.66 1.65 1.64 1.63 1.62 1.60 1.60 1.59 1.58 1.57 1.55 1.55 1.54 1.54 1.52
2x
2.00 3.00 1.00 2.00 2.00 8.43
f1 (ppm)

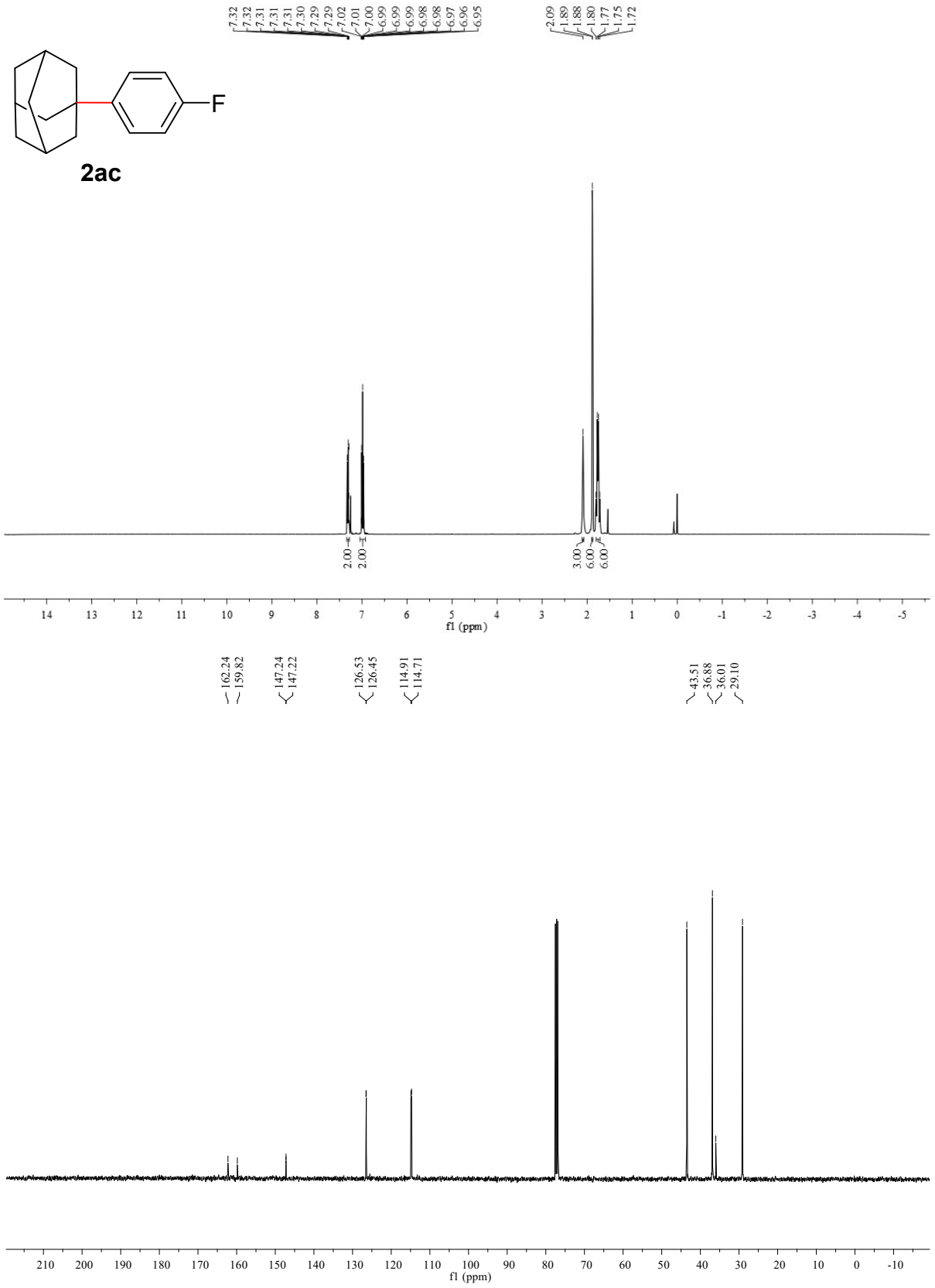

150.20 128.46 126.86 125.67 47.24 37.00 28.13 27.41
f1 (ppm)

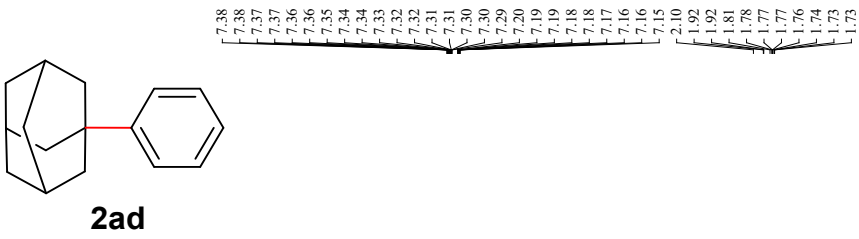

7.09
7.07
7.06
7.04
4.14
4.12
4.11
4.09
2.58
2.57
2.55
2.31
2.30
2.28
2.26
1.69
1.67
1.65
1.63
1.62
1.61
1.59
1.57
1.39
1.38
1.37
1.36
1.35
1.34
1.33
1.32
1.26
1.24
1.22
O
O
5
2y
4.00
2.00
2.00
5.01
4.22
2.00
3.00
f1 (ppm)
173.98
139.60
135.22
129.11
128.42
60.35
35.43
34.46
31.39
28.91
25.01
21.15
14.41
f1 (ppm)


7.09
7.07
6.83
6.81
4.14
4.13
4.11
4.09
3.78
2.57
2.55
2.53
2.30
2.28
2.27
1.69
1.67
1.66
1.65
1.64
1.63
1.62
1.61
1.61
1.60
1.58
1.56
1.43
1.39
1.37
1.37
1.36
1.35
1.33
1.33
1.26
1.24
O
O
5
OMe
2z
2.00
2.00
2.00
3.00
2.00
2.00
4.00
2.00
3.00
f1 (ppm)
174.00
157.82
134.79
129.41
113.84
60.36
55.42
34.95
34.47
31.51
28.86
25.01
14.42
f1 (ppm)

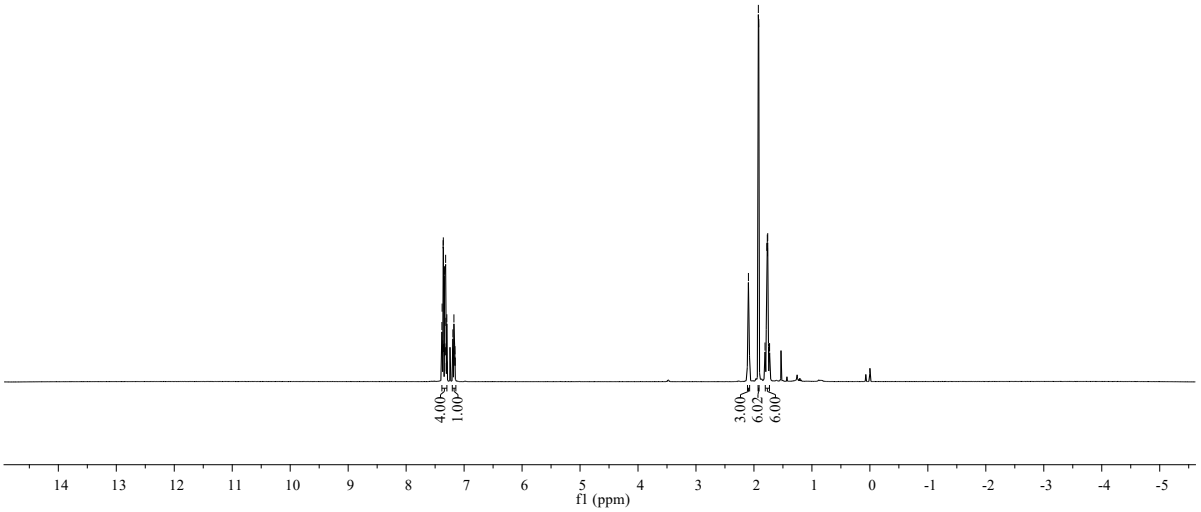

2aa
7.27
7.25
7.14
7.12
2.32
2.08
1.90
1.90
1.80
1.77
1.76
1.75
1.72
2.00
2.00
3.00
3.00
6.00
6.00
f1 (ppm)
148.64
135.07
128.98
124.90
43.44
37.01
35.99
29.17
21.06
f1 (ppm)

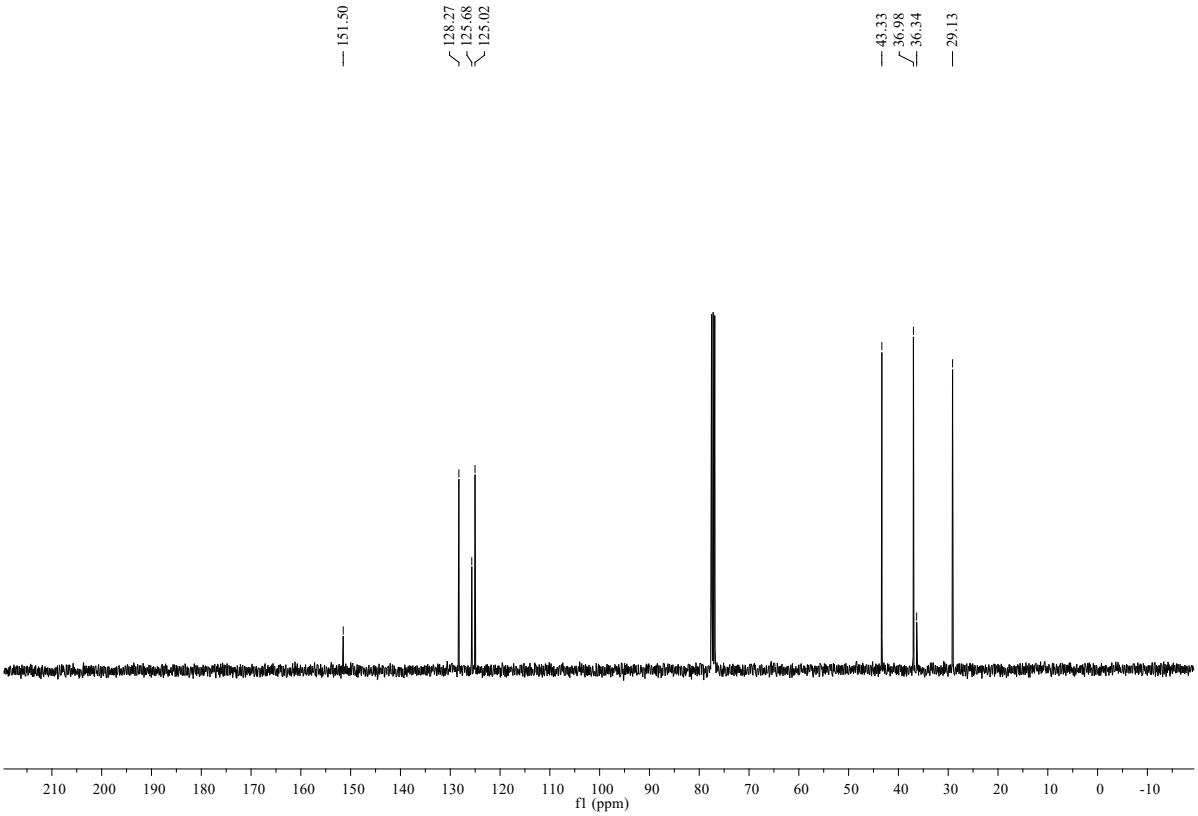

OMe
2ab
7.29
7.27
6.87
6.85
3.79
2.08
1.89
1.88
1.80
1.77
1.76
1.76
1.75
1.73
1.72
2.00
2.00
3.00
3.00
6.00
6.00
f1 (ppm)
157.48
143.88
125.96
113.54
55.38
43.55
36.97
35.70
29.15
f1 (ppm)

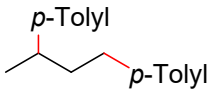

7.32
7.32
7.31
7.31
7.31
7.30
7.29
7.29
7.02
7.01
7.00
6.99
6.99
6.99
6.98
6.98
6.97
6.96
6.95
2.09
1.89
1.88
1.80
1.77
1.75
1.72
F
2ac
2.00
2.00
3.00
6.00
6.00
f1 (ppm)
162.24
159.82
147.24
147.22
126.53
126.45
114.91
114.71
43.51
36.88
36.01
29.10
f1 (ppm)


7.38
7.38
7.37
7.37
7.36
7.36
7.35
7.34
7.34
7.33
7.32
7.32
7.31
7.31
7.30
7.30
7.29
7.20
7.19
7.19
7.18
7.18
7.17
7.16
7.16
7.15
2.10
1.92
1.92
1.81
1.78
1.77
1.77
1.76
1.74
1.73
1.73

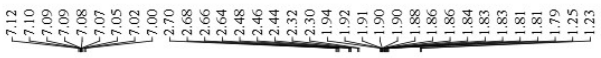
2ad


4.00
1.00
3.00
6.02
6.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5
f1 (ppm)


151.50
128.27
125.68
125.02
43.33
36.98
36.34
29.13
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


p-Tolyl
p-Tolyl

2ae


7.12
7.10
7.09
7.09
7.08
7.07
7.05
7.02
7.00
2.70
2.68
2.66
2.64
2.48
2.46
2.44
2.32
2.30
1.94
1.92
1.91
1.90
1.90
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1.86
1.86
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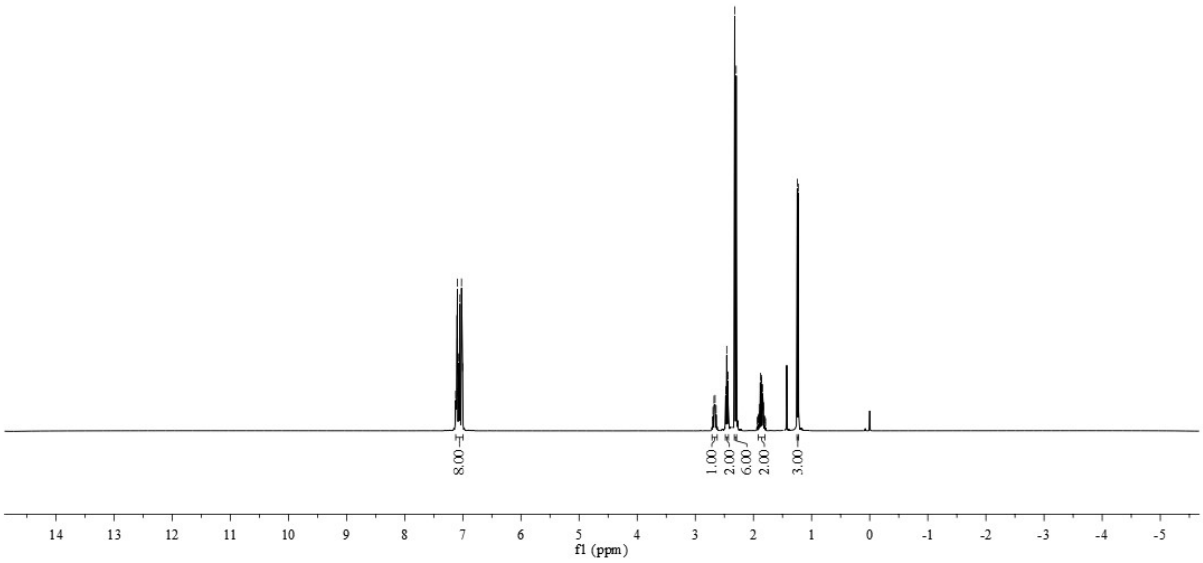
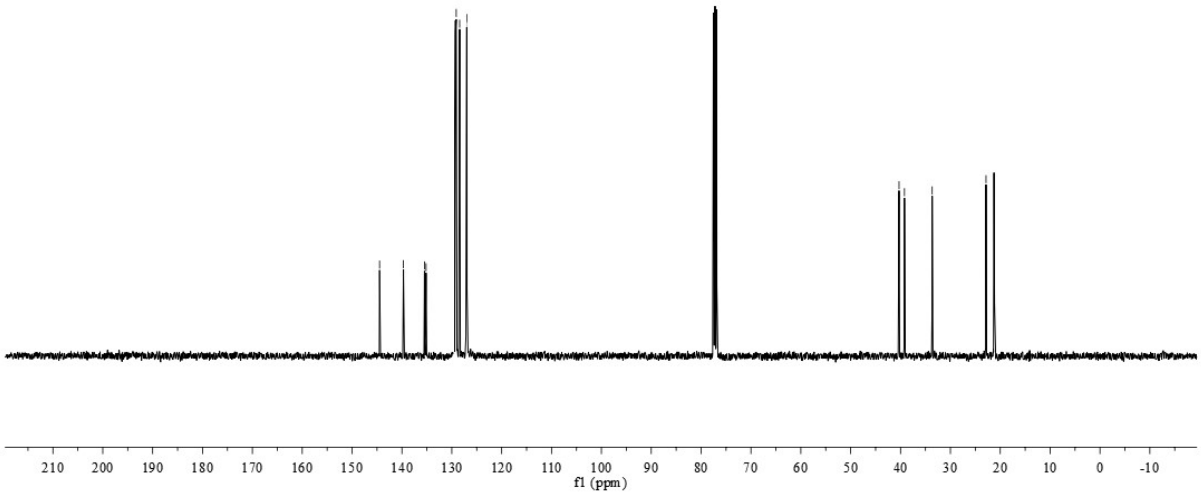
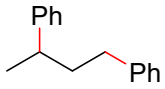
1.83
1.83
1.81
1.81
1.79
1.25
1.23

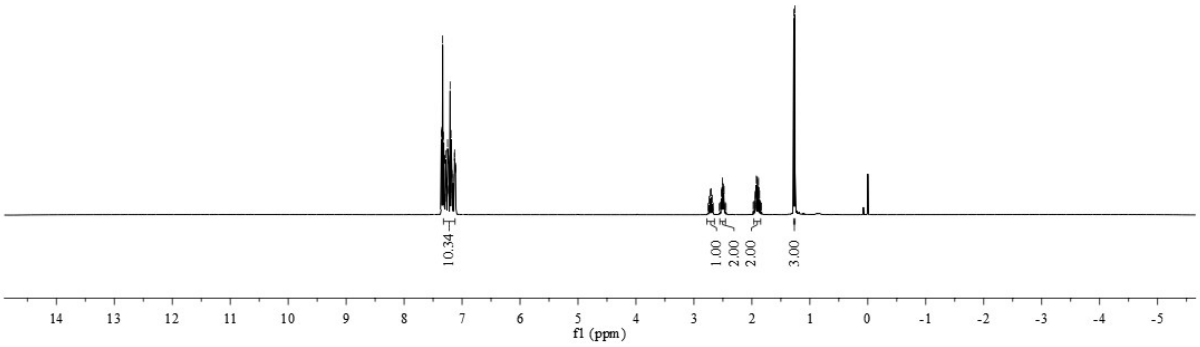

8.00
1.00
2.00
6.00
2.00
3.00
f1 (ppm)

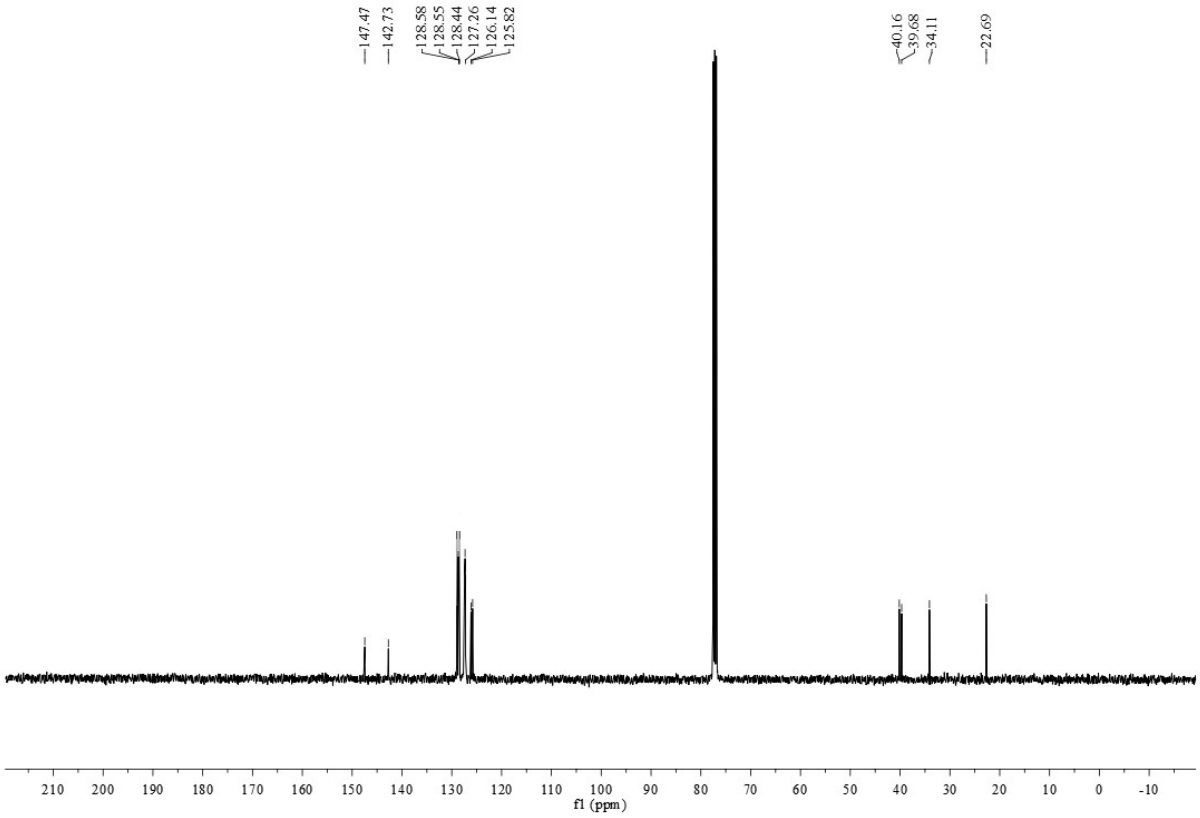

144.49
139.70
135.48
135.16
129.25
129.11
128.43
127.12
40.30
39.21
33.65
22.85
21.19
21.17

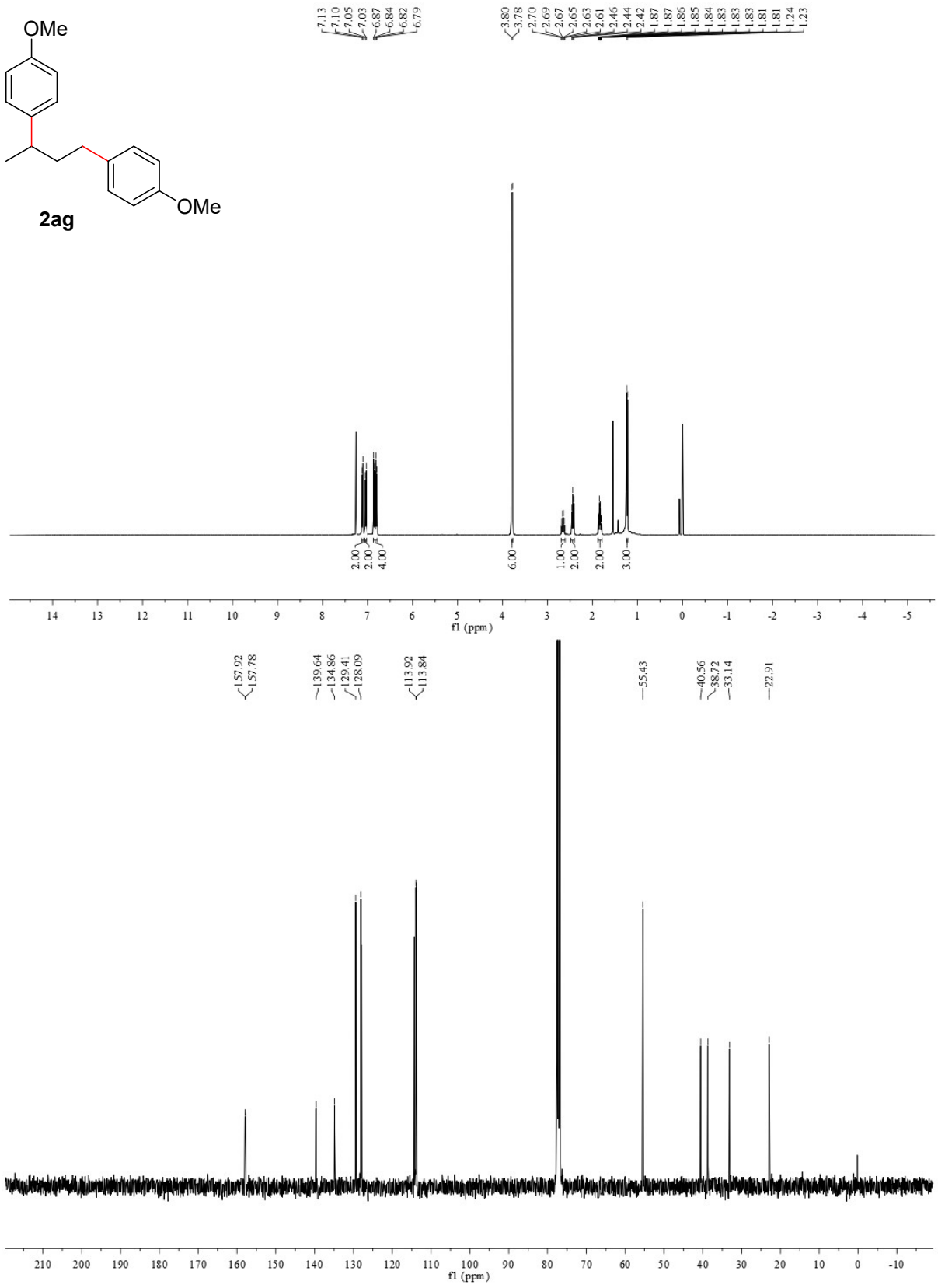

f1 (ppm)

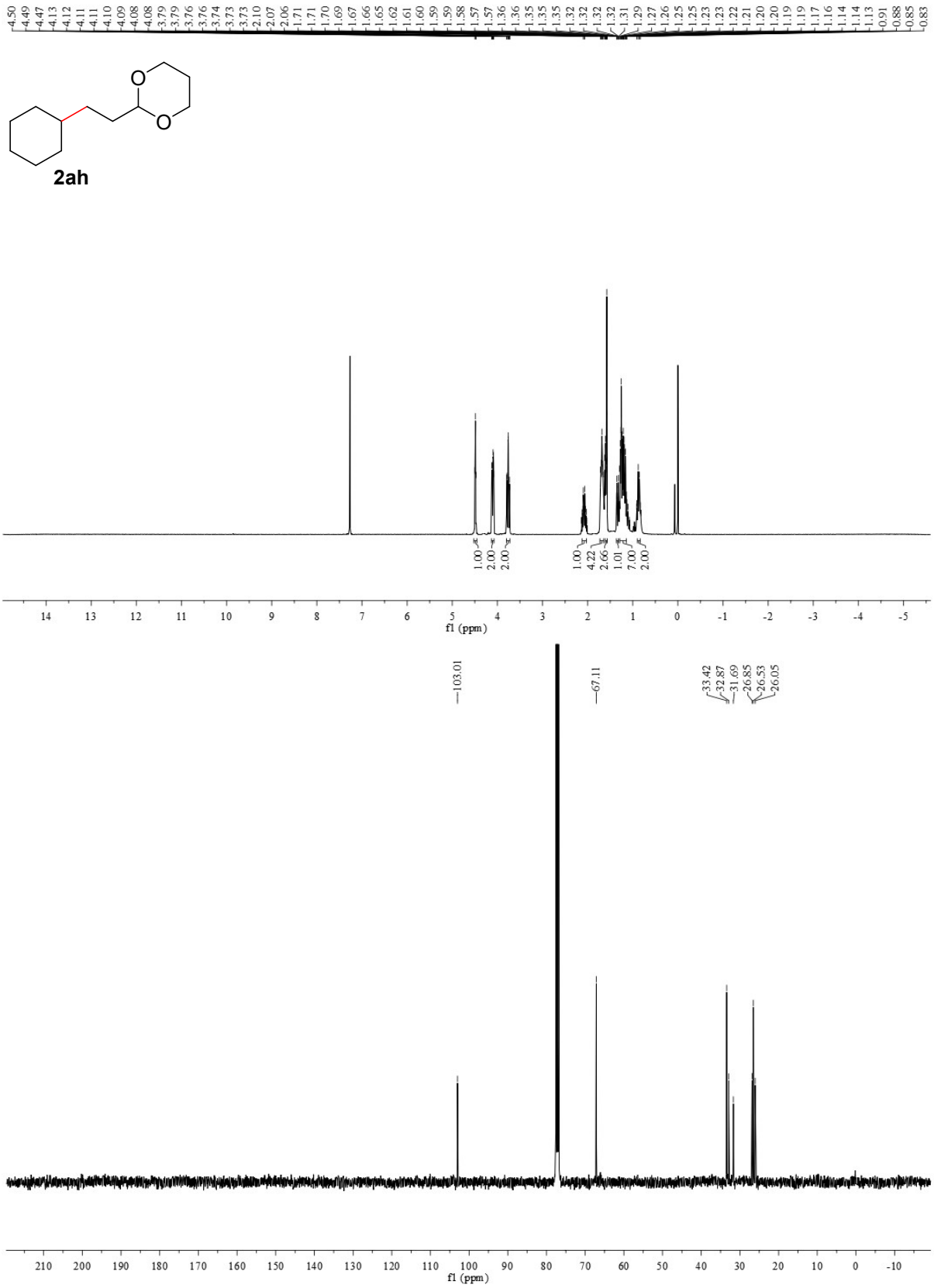

Ph
Ph

2af


10.34
1.00
2.00
2.00
3.00
f1 (ppm)


147.47
142.73
128.58
128.55
128.44
127.26
126.14
125.82
40.16
39.68
34.11
22.69
f1 (ppm)


OMe
OMe
2ag
7.13
7.10
7.05
7.03
6.87
6.84
6.82
6.79
3.80
3.78
2.70
2.69
2.67
2.65
2.63
2.61
2.46
2.44
2.42
1.87
1.87
1.86
1.85
1.84
1.83
1.83
1.83
1.81
1.81
1.24
1.23
2.00
2.00
4.00
6.00
1.00
2.00
2.00
3.00
f1 (ppm)
157.92
157.78
139.64
134.86
129.41
128.09
113.92
113.84
55.43
40.56
38.72
33.14
22.91
f1 (ppm)


4.50 4.49 4.47 4.13 4.12 4.11 4.11 4.10 4.09 4.08 4.08 3.79 3.79 3.76 3.76 3.74 3.73 3.73 2.10 2.07 2.06 1.71 1.71 1.70 1.69 1.67 1.66 1.65 1.62 1.61 1.60 1.59 1.59 1.58 1.57 1.57 1.36 1.36 1.35 1.35 1.35 1.32 1.32 1.32 1.31 1.29 1.27 1.26 1.25 1.25 1.23 1.23 1.22 1.21 1.20 1.20 1.19 1.19 1.17 1.16 1.14 1.14 1.13 0.91 0.88 0.85 0.83
O
O
2ah
1.00 2.00 2.00 1.00 4.22 2.66 1.01 7.00 2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5
f1 (ppm)
103.01 67.11 33.42 32.87 31.69 26.85 26.53 26.05
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

IBzH

Energy: -1229.298479 au

Sum of electronic and thermal Energies: -1228.824357 au

Geometry:

N	-1.06151300	0.08941200	0.17453600
C	0.00000000	0.00000000	1.03202100
C	-0.67435000	0.05840000	-1.16356100
H	-1.36826100	0.12881200	-1.98355500
C	-2.44508200	0.18170200	0.66540100
H	-2.31930700	0.45229200	1.71615400
C	-3.58253300	3.71561900	-0.21076700
H	-3.40693400	4.72281400	0.15062700
C	-2.96370300	2.63742400	0.41623800
H	-2.29967300	2.80957900	1.25720900
C	-3.18235700	1.32876800	-0.02850600
C	-4.03740200	1.12174700	-1.11395400
H	-4.23483500	0.11324700	-1.45912400
C	-4.65454900	2.20072400	-1.74724900
H	-5.31599800	2.02344300	-2.58812000
C	-4.42972300	3.49976600	-1.29759200
H	-4.91451000	4.33766500	-1.78595400
C	-3.19227600	-1.15114800	0.63382000
C	-2.67047900	-2.30418600	0.04639400
H	-1.69516600	-2.27909400	-0.42271800
C	-3.38994000	-3.50110500	0.06844800
H	-2.96771100	-4.38647200	-0.39407300
C	-4.63561800	-3.56285500	0.68487500
H	-5.19164300	-4.49339300	0.70434600
C	-5.16015700	-2.41743600	1.28543500
H	-6.12578900	-2.45439000	1.77753200
C	-4.44453800	-1.22510000	1.25828100

H	-4.86230100	-0.33960200	1.72633500
N	1.06151300	-0.08941200	0.17453600
C	0.67434900	-0.05840000	-1.16356100
H	1.36826000	-0.12881300	-1.98355600
C	2.44508200	-0.18170200	0.66540000
H	2.31930800	-0.45229300	1.71615300
C	3.58253400	-3.71561800	-0.21077100
H	3.40693500	-4.72281400	0.15062200
C	2.96370300	-2.63742400	0.41623500
H	2.29967300	-2.80958000	1.25720600
C	3.18235800	-1.32876800	-0.02850800
C	4.03740300	-1.12174600	-1.11395600
H	4.23483600	-0.11324600	-1.45912500
C	4.65454900	-2.20072300	-1.74725200
H	5.31599800	-2.02344100	-2.58812200
C	4.42972300	-3.49976500	-1.29759500
H	4.91451000	-4.33766400	-1.78595800
C	3.19227600	1.15114800	0.63382000
C	2.67047900	2.30418500	0.04639400
H	1.69516600	2.27909300	-0.42271900
C	3.38994000	3.50110500	0.06844800
H	2.96771100	4.38647200	-0.39407300
C	4.63561700	3.56285400	0.68487600
H	5.19164300	4.49339200	0.70434700
C	5.16015600	2.41743600	1.28543600
H	6.12578800	2.45439000	1.77753300
C	4.44453800	1.22509900	1.25828200
H	4.86230000	0.33960200	1.72633600