Enhanced Activity of Bulky N-Heterocylic Carbenes in Nickel–NHC Catalyzed Kumada–Corriu Cross-Coupling of Aryl Tosylates

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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 nickel 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. 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). High-resolution mass spectra (HRMS) were measured on a 7T Bruker Daltonics FT-MS instrument (for HRMS). Melting points were measured on Melt EMP (laboratory devices). 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

All imidazolium salts,[1-5] nickel complex[6] and tosylates[7-10] used in this study were prepared by procedures reported in the literature. **IPr*·HCl**,[1] **IPr*^{OMe}·HCl**,[11] **IPaul·HCl**,[3] **BIAN-IPr·HCl**,[4] **BIAN-IPr^{CHPh2}·HCl**,[5] **[Ni(IPr*^{OMe})CpCl]**,[6] **1a**[7], **1b**[7], **1c**[7], **1d**[7], **1e**[7], **1f**[12], **1g**[13], **1h**[14], **1i**[15], **1j**[7], **1k**[7], **2a**[16], **2b**[17], **2c**[17], **2d**[18], **2e**[19], **2f**[20], **2g**[21], **2h**[21], **2i**[20], **2j**[22], **2k**[23], **2l**[24], **2m**[25], **2n**[24], **2o**[25], **2p**[24], **2q**[25], **2r**[26], **2s**[27], **2t**[28], **2u**[29], **2v**[30], **2x**[29], **2y**[31], **2z**[28], **2aa**[32], **2ab**[33] are known compounds. Spectroscopic data match those reported in the literature.

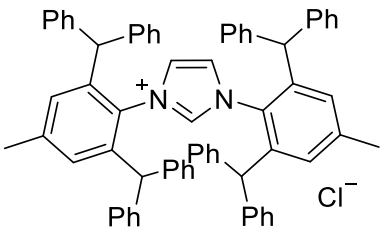
General Procedure for Nickel-Catalyzed C(sp^2)–C(sp^2) Cross-Coupling. An oven-dried vial equipped with a stir bar was charged with an aryl tosylate substrate (neat, typically, 0.25 mmol, 1.0 equiv), NHC ligand (neat, typically, 20 mol%) and NiF_2 (typically, 10 mol%), placed under a positive pressure of argon and subjected to three evacuation/backfilling cycles under vacuum. Tetrahydrofuran (0.19 M) was added with vigorous stirring at room temperature, the reaction mixture was warmed to 66 °C, a solution of Grignard reagent (typically, 3.0 equiv) was added dropwise with vigorous stirring and the reaction mixture was stirred for the indicated time at 66 °C. 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 20 mL), the organic layer was extracted with HCl (1.0 *N*, 2 x 5 mL), dried and concentrated. Note: for products containing basic nitrogen, NaOH (1.0 *N*) was used instead of HCl (1.0 *N*). 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).

Representative Procedure for Nickel-Catalyzed C(sp^2)–C(sp^2) Cross-Coupling. 1.0 g Scale. An oven-dried, two-necked flask (100 mL) equipped with a stir bar was charged with naphthalen-1-yl *p*-toluenesulfonate (1.00 g, 3.35 mmol, 1.0 equiv), IPr*^{OMe}·HCl (65.77 mg, 20 mol%) and NiF_2 (32.39 mg, 10 mol%). Tetrahydrofuran (10.05 mL, 0.19 M) was added with vigorous stirring at room temperature, the reaction mixture was heated to 66 °C, a solution of *p*-TolylMgBr (1.0 M in THF, 10.05 mL, 3.0 equiv) was added dropwise with vigorous stirring and the reaction mixture was stirred for 1 h at 66 °C. After the indicated time, the reaction mixture was cooled to room temperature, diluted with HCl (1.0 *N*, 10 mL) and Et_2O (1 x 100 mL), the organic layer was extracted with HCl (1.0 *N*, 2 x 15 mL), dried and concentrated. The sample was analyzed by

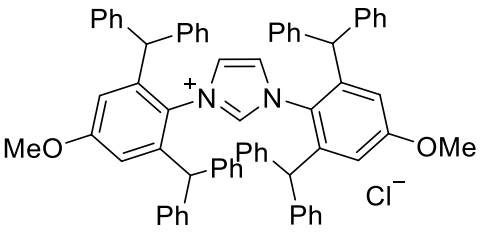
^{1}H NMR ($CDCl_3$, 400 MHz) and GC-MS to obtain conversion, yield and selectivity using internal standard and comparison with authentic samples. Characterization data are included in the section below.

Representative Procedure for Double Nickel-Catalyzed C(sp^2)–C(sp^2) Cross-Coupling. Anoven-dried vial equipped with a stir bar was charged with naphthalene-2,7-diyl bis(*p*-toluenesulfonate) (neat, 0.117 g, 0.25 mmol, 1.0 equiv), IPr*^{OMe}·HCl (49.08 mg, 20 mol%) and NiF_2 (10 mol%, 2.42 mg), placed under a positive pressure of argon and subjected to three evacuation/backfillingcycles under vacuum. Tetrahydrofuran (0.19 M), the reaction mixture was heated to 66 °C, a solution of *p*-TolylMgBr (1.0 M in THF, 1.0 mL, 4.0 equiv) was added dropwise with vigorous stirring and the reaction mixture was stirred for 21 h at 66 °C. After the indicated time, the reaction mixture was colled to room temperature, diluted with HCl (1.0 N, 1.0 mL) and Et_2O (1 x 20 mL), the organic layer was extracted with HCl (1.0 N, 2 x 5 mL) and NaOH (1.0 N, 2 x 5 mL), the organic layers were combined, dried and concentrated. A sample was analyzed by ^{1}H NMR ($CDCl_3$, 400 MHz) and/or GC-MS to obtain conversion, yield and selectivity using internal standard and comparison with authentic samples. Purification by chromatography on silica gel (EtOAc/hexanes) afforded the title product. Characterization data are included in the section below.

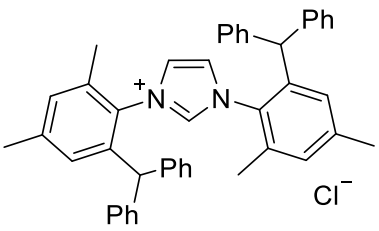
Characterization Data of Starting Materials



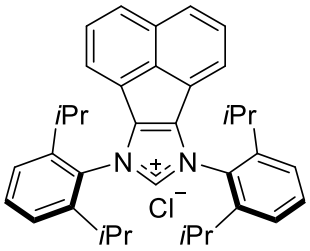
IPr*·HCl Yield 79%, (0.804 g). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 12.01 (s, 1H), 7.27 – 7.13 (m, 24H), 6.79 (d, *J* = 6.1 Hz, 12H), 5.54 (s, 2H), 5.20 (s, 4H), 2.20 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 143.05, 142.60, 141.90, 141.84, 140.66, 130.99, 130.13, 129.98, 129.35, 128.86, 128.77, 127.18, 127.09, 123.75, 51.52, 22.04.



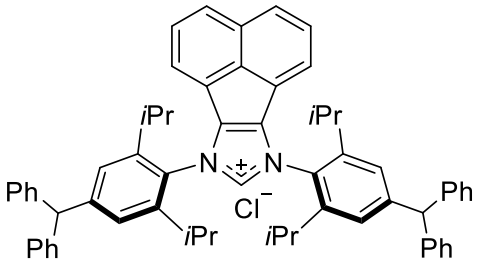
IPr*^{OMe}·HCl Yield 73% (1.138 g). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 11.96 (s, 1H), 7.27 – 7.26 (m, 8H), 7.20 – 7.14 (m, 26H), 6.82 (m, 8H), 6.47 (s, 4H), 5.48 (s, 2H), 5.21 (s, 4H), 3.52 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.05, 142.74, 142.43, 141.67, 130.11, 129.29, 128.90, 128.79, 127.25, 127.22, 125.22, 123.91, 115.82, 55.39, 51.74.



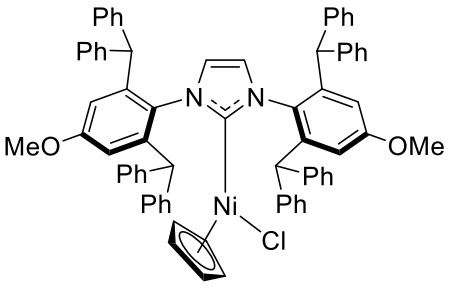
IPaul·HCl Yield 86% (3.120 g). White solid. The product is obtained as 2:1 mixture of rotamers A and B. **^{1}H NMR of rotamer A (400 MHz, $CDCl_3$)** δ 10.76 (s, 1H), 7.35 – 7.28 (m, 12H), 7.17 – 7.08 (m. 8H), 6.61(s, 2H), 6.59 (s, 2H), 5.47 (s, 2H), 2.26 (s, 6H), 2.11 (s, 6H). **NMR of rotamer B (400 MHz, $CDCl_3$)** δ 11.47 (s, 1H), 7.35– 7.28 (m, 12H), 7.17 – 7.08 (m. 8H), 6.67 (s, 2H), 6.51 (s, 2H), 5.32 (s, 2H), 2.26 (s, 6H), 2.16 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 142.59, 142.47, 141.89, 141.77, 141.43, 140.32, 139.88, 135.22, 135.13, 131.12, 130.88, 130.52, 129.96, 129.88, 129.83, 129.51, 129.46, 128.94, 128.74, 127.28, 127.18, 127.07, 127.03, 123.98, 123.70, 51.61, 51.53, 21.61, 18.23



BIAN-IPr·HCl Yield 87% (1.433 g). Yellow solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 11.24 (s, 1H), 8.04 (d, *J* = 8.2 Hz, 2H), 7.69 (t, *J* = 7.6 Hz, 2H), 7.60 (t, *J* = 7.6 Hz, 2H), 7.48 (d, *J* = 7.6 Hz, 4H), 7.26 (t, *J* = 6.0 Hz, 2H), 2.71 (bs, 4H), 1.37 (d, *J* = 2.8 Hz, 12H), 1.17 (d, *J* = 6.4 Hz, 12H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 145.04, 144.6, 137.70, 132.46, 130.80, 130.73, 130.24, 129.28, 128.50, 125.18, 123.20, 123.10, 29.57, 24.87, 23.76.

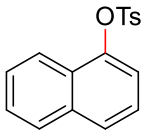


BIAN-IPr^{CHPh2}·HCl Yield 85% (0.425 g). Yellow solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 11.08 (s, 1H), 8.03 (d, *J* = 8.4 Hz, 2H), 7.62 (t, *J* = 7.7 Hz, 2H), 7.39-7.36 (m, 8H), 7.29 – 7.22 (m, 14H), 7.17 (s, 4H), 5.70 (s, 2H), 2.67 – 2.64 (m, 4H), 1.26 (d, *J* = 6.4 Hz, 12H), 1.02 (d, *J* = 6.7 Hz, 12H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 148.29, 144.77, 143.30, 137.78, 130.84, 130.68, 130.25, 129.71, 128.75, 128.51, 127.54, 126.83, 126.28, 123.34, 123.02, 57.05, 29.58, 24.70, 23.70.



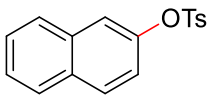
[Ni(IPr*^{OMe})CpCl] Yield 58% (0.319 g). Purple-pink powder. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.31 – 7.20 (m, 20H), 7.07 (s, 12H), 6.76 – 6.74 (m, 8H), 6.71 (s, 4H), 5.80 (s, 4H), 5.01 (s, 2H), 4.64 (s, 5H), 3.64 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 168.45, 159.16, 144.48, 144.10, 143.28, 132.20, 130.47, 129.40, 128.40, 126.72, 126.47, 125.39, 115.14, 93.05, 55.30, 51.47.

All tosylates reported in the manuscript have been described in the literature and prepared by the method reported previously.[7-10] ^{1}H NMR and ^{13}C NMR data are given for all starting materials for characterization purposes. *Note: In our experience aryl tosylates are routinely obtained in 57-98% yield on gram scale and purified by simple recrystallization or using flash chromatography.*



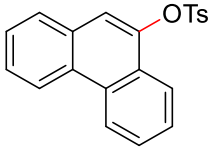
1a

Naphthalen-1-yl p-toluenesulfonate (**1a**). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.90 (d, *J* = 8.3 Hz, 1H), 7.81 – 7.76 (m, 3H), 7.73 (d, *J* = 8.2 Hz, 1H), 7.44 (dtd, *J* = 8.3, 6.8, 5.5 Hz, 2H), 7.36 (t, *J* = 7.9 Hz, 1H), 7.26 (d, *J* = 8.1 Hz, 2H), 7.19 (dd, *J* = 7.6, 1.0 Hz, 1H) 2.40 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 145.90, 145.58, 134.84, 132.86, 129.95, 128.64, 127.83, 127.43, 127.25, 126.86, 126.85, 125.26, 121.93, 118.56, 21.86.



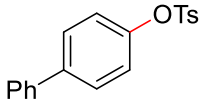
1b

Naphthalen-2-yl p-toluenesulfonate (**1b**). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 – 7.79 (m, 1H), 7.75 – 7.71 (m, 4H), 7.51 – 7.45 (m, 3H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.09 (dd, *J* = 9.0, 2.3 Hz, 1H), 2.42 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 147.31, 145.56, 133.55, 132.48, 132.00, 129.93, 129.90, 128.70, 128.02, 127.89, 127.00, 126.53, 121.31, 120.11, 21.87.



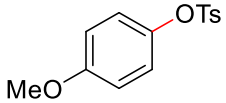
1c

Phenanthren-9-yl p-toluenesulfonate (**1c**). White solid**. ^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.62 (dd, *J* = 8.1, 5.1 Hz, 2H), 7.99 (d, *J* = 8.5 Hz, 1H), 7.80 (dd, *J* = 11.1, 8.8 Hz, 3H), 7,67 – 7.57 (m, 3H), 7.55 – 7.51 (m, 2H), 7.26 (d, *J* = 7.9 Hz, 2H), 2.40 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 145.64, 144.40, 132.92, 131.77, 131.16, 129.98, 129.33, 128.95, 128.69, 127.65, 127.38, 127.22, 127.12, 126.67, 122.82, 122.82, 122.71, 118.34, 21.87.



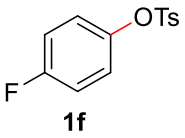
1d

Biphenyl-4-yl p-toluenesulfonate (**1d**). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.53 – 7.48 (m, 4H), 7.43 (t, *J* = 7.2 Hz, 2H), 7.37 – 7.32 (m, 3H), 2.46 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.15, 145.57, 140.34, 139.95, 132.55, 129.97, 129.04, 128.75, 128.42, 127.84, 127.25, 122.85, 21.93.



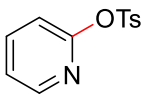
1e

4-Methoxyphenyl p-toluenesulfonate (**1e**). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 6.88 (d, *J* = 9.2 Hz, 2H), 6.76 (d, *J* = 9.2 Hz, 2H), 3.76 (s, 3H), 2.44 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 158.32, 145.42, 143.19, 132.41, 129.86, 128.73, 123.52, 114.59, 55.70, 21.88.



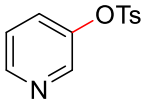
1f

4-Fluorophenyl p-toluenesulfonate (**1f**). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.69 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 6.99 – 6.92 (m, 4H), 2.45 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.17 (d, J^F = 246.6 Hz), 145.75, 145.56 (d, J^F = 3.0 Hz, 132.12, 129.99, 128.72, 124.21 (d, J^F = 8.8 Hz), 116.50 (d, J^F = 23.7 Hz), 21.91.



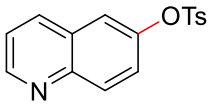
1g

Pyridin-2-yl p-toluenesulfonate (**1g**). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ8.25 (dd, *J* = 3.0, 1.9 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.78 – 7.74 (m, 1H) 7.34 (d, *J* = 8.5 Hz, 2H), 7.21 (ddd, *J* = 7.3, 4.9, 0.5 Hz, 1H), 7.09 (d, *J* = 8.1 Hz, 1H), 2.44 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 156.99, 148.39, 145.45, 140.23, 133.62, 129.80, 128.62, 122.77, 115.97, 21.80.



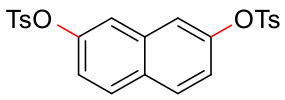
1h

Pyridin-3-yl p-toluenesulfonate (**1h**). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.50 (dd, *J* = 4.8, 1.3 Hz, 1H), 8.16 (d, *J* = 2.6 Hz, 1H), 7.70 (d, *J* = 8.3 Hz, 2H), 7.49 – 7.46 (m, 1H), 7.35 – 7.28 (m, 3H), 2.46 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 148.32, 146.59, 146.20, 144.09, 131.68, 130.42, 130.18, 128.64, 124.38, 21.89.



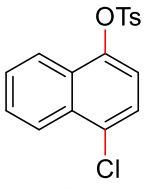
1i

Quinolin-6-yl p-toluenesulfonate (**1i**). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.92 (dd, *J* = 4.4, 1.5 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 8.01 (d, *J* = 9.1 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 2.3 Hz, 1H), 7.43 (dd, *J* = 8.8, 4.4 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.26 (dd, *J* = 9.2, 2.3 Hz, 1H), 2.45 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.04, 147.36, 146.74, 145.83, 136.18, 132.24, 131.54, 130.04, 128.66, 128.46, 124.78, 122.01, 120.13, 21.88.



1j

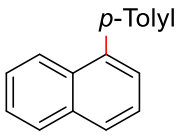
Naphthalene-2,7-diyl bis(p-toluenesulfonate) (**1j**). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.73 (dd, *J* = 8.6, 3.5 Hz, 6H), 7.38 (d, *J* = 2.2 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 4H), 7.12 (dd, *J* = 8.9, 2.3 Hz, 2H), 2.46 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 148.13, 145.81, 133.86, 132.41, 130.45, 130.06, 129.86, 128.65, 121.95, 120.05, 21.94.



1k

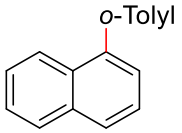
4-Chloronaphthalen-1-yl p-toluenesulfonate (**1k**). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.21 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 8.3 Hz, 2H), 7.59 (ddd, *J* = 8.3, 7.0, 1.1 Hz, 1H), 7.51 – 7.45 (m, 2H), 7.29 (d, *J* = 8.5 Hz, 2H) 7.13 (d, *J* = 8.2 Hz, 1H), 2.42 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 145.86, 144.80, 132.56, 132.02, 131.81, 130.76, 130.07, 128.68, 128.45, 128.02, 127.62, 125.45, 124.75, 122.47, 118.56, 21.90.

Characterization Data of Cross-Coupling Products



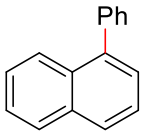
2a

1-(*p*-Tolyl)naphthalene (**2a**). Yeld 98% (53.48 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.90 (dd, *J* = 13.4, 7,8 Hz, 2H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.50 – 7.45 (m, 2H), 7.43 – 7.38 (m, 4H), 2.45 (m, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 140.40, 137.97, 137.09, 133.97, 131.87, 130.13, 129.15, 128.42, 127.61, 126.27, 126.10, 125.88, 125.58, 21.43.



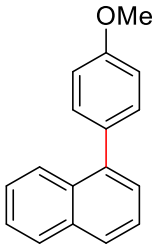
2b

1-(*o*-Tolyl)naphthalene (**2b**). Yeld 96% (52.39 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.88 (dd, *J* = 15.5, 8.2 Hz, 2H), 7.54 – 7.44 (m, 3H), 7.39 – 7.22 (m, 6H), 2.02 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 140.38, 139.94, 136.98, 133.67, 132.15, 130.54, 130.03, 128.38, 127.74, 127.60, 126.79, 126.27, 126.14, 125.89, 125.74, 125.56, 20.25.



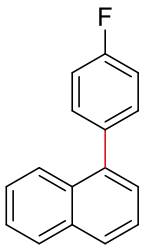
2c

1-Phenylnaphthalene (**2c**). Yeld 94% (48.00 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.88 (dd, *J* = 17.4, 8.8 Hz, 3H), 7.54 – 7.41 (m, 9H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 141.29, 138.72, 133.83, 132.77, 129.04, 128.59, 128.37, 127.82, 127.61, 127.53, 126.46, 126.11, 125.98, 125.77.



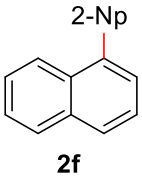
2d

1-(4-Methoxyphenyl)naphthalene (**2d**). Yeld 98% (57.40 mg). White solid**. ^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.93 – 7.87 (m, 2H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.51 – 7.38 (m, 6H), 7.03 – 7.00 (m, 2H), 3.86 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.08, 140.05, 133.99, 133.25, 131.96, 131.28, 128.42, 127.49, 127.08, 126.22, 126.09, 125.87, 125.58, 113.86, 55.50.



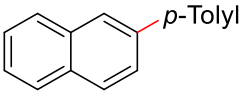
2e

1-(4-Fluorophenyl)naphthalene (**2e**). Yeld 98% (54.45 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.91 (d, *J* = 8.1 Hz, 1H), 7.85 (t, *J* = 8.4 Hz, 2H), 7.53 – 7.38 (m, 6H), 7.18 (t, *J* = 8.8 Hz, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.44 (d, J^F = 245.0 Hz), 139.32, 136.82 (d, J^F = 3.4 Hz) 133.95, 131.75 (d, J^F = 8.1 Hz) 131.5, 128.51, 127.98, 127.19, 126.34, 126.03, 125.94, 125.53, 115.37 (d, J^F = 21.2 Hz).



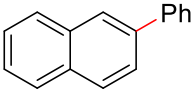
2f

1,2'-Binaphthalene (**2f**). Yeld 98% (62.31 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.96 – 7.88 (m, 7H), 7.63 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.57 – 7.48 (m, 5H), 7.42 (ddd, *J* = 8.2, 6.8, 1.4 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 140.32, 138.48, 133.98, 133.57, 132.73, 131.91, 128.91, 128.66, 128.50, 128.25, 127.93, 127.83, 127.42, 126.48, 126.29, 126.26, 126.22, 126.00, 125.60.



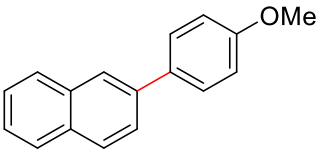
2g

2-(*p*-Tolyl)naphthalene (**2g**). Yeld 88% (48.03 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.02 (s, 1H), 7.91 – 7.84 (m, 3H), 7.74 (dd, *J* = 8.5, 1.7, 1H), 7.63 (d, *J* = 8.1 Hz, 2H), 7.51 – 7.45 (m, 2H), 7.30 (*J* = 8.1 Hz, 2H), 2.42 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 138.46, 138.21, 137.17, 133.70, 132.48, 129.60, 128.35, 128.14, 127.63, 127.25, 126.24, 125.78, 125.56, 125.43, 21.16.



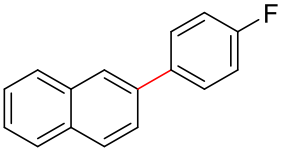
2h

2-Phenylnaphthalene (**2h**). Yeld 90% (45.96 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.04 (s, 1H), 7.92 – 7.85 (m, 3H), 7.76 – 7.71 (m, 3H), 7.52 – 7.45 (m, 4H), 7.38 (t, *J* = 7.2 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 141.14, 138.57, 133.68, 132.62, 128.89, 128.44, 128.22, 127.67, 127.46, 127.38, 126.31, 125.96, 125.83, 125.62.



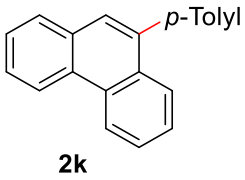
2i

2-(4-Methoxyphenyl)naphthalene (**2i**). Yeld 98% (57.40 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.99 (d, *J* = 1.4 Hz, 1H), 7.90 – 7.84 (m, 3H), 7.72 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.68 – 7.65 (m, 2H), 7.52 – 7.44 (m, 2H), 7.04 – 6.97 (m, 2H), 3.87 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.40, 138.31, 133.91, 133.79, 132.46, 128.61, 128.52, 128.22, 127.80, 126.41, 125.83, 125.62, 125.21, 114.48, 55.56.



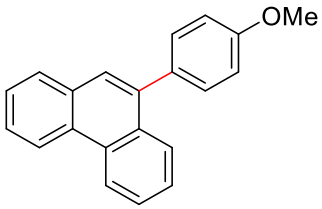
2j

2-(4-Fluorophenyl)naphthalene (**2j**). Yeld 81% (45.01 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7,98 (d, *J* = 1.5 Hz, 1H), 7.91 – 7.85 (m, 3H), 7.70 – 7.64 (m, 3H), 7.53 – 7.46 (m, 2H), 7.17(t, *J* = 8.7 Hz, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.70 (d, J^F = 245.8 Hz), 137.73, 137.41 (d, J^F = 3.2 Hz), 133.79, 132.69, 129.13 (d, J^F = 7.9Hz), 128.70, 128.30, 127.83, 126.59, 126.19, 125.82, 125.58, 116.91 (d, J^F = 21.5 Hz).



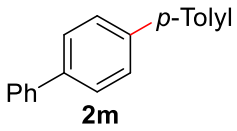
2k

9-(*p*-Tolyl)phenanthrene (**2k**). Yeld 98% (65.75 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.73 (dd, *J* = 22.0, 8.3 Hz, 2H), 7.91 (ddd, *J* = 26.5, 8.2, 1.2 Hz, 2H), 7.66 – 7.57 (m, 4H), 7.52 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 7.9 Hz, 2H), 2.47 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 138.90, 138.00, 137.23, 131.78, 131.41, 130.78, 130.11, 129.19, 128.79, 127.60, 127.14, 126.98, 126.65, 126.61, 126.56, 123.05, 122.69, 21.47.



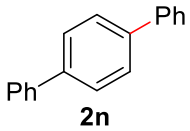
2l

9-(4-Methoxyphenyl)phenanthrene (**2l**). Yeld 98% (69.68 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.73 (dd, *J* = 22.4, 8.2 Hz, 2H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.87 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.67 – 7.61 (m, 4H), 7.55 – 7.51 (m, 1H), 7.49 – 7.45 (m, 2H), 7.04 (d, *J* = 8.7 Hz, 2H), 3.89 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.17, 138.55, 133.27, 131.80, 131.54, 131.29, 130.80, 130.00, 128.74, 127.62, 127.10, 126.98, 126.62, 126.56, 123.06, 122.68, 113.91, 55.55.



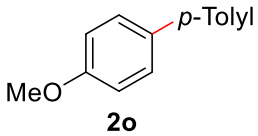
2m

4-Methyl-1-1':4'-1''-terphenyl (**2m**). Yeld 92% (56.20 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.66-7.63 (m, 6H), 7.54 (d, *J* = 8.1 Hz, 2H), 7.49 – 7.44 (m, 2H), 7.35 (t, *J* = 7.4, 1H), 7.27 (d, *J* = 7.8 Hz, 2H), 2.41 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 140.93, 140.22, 139.99, 137.97, 137.34, 129.73, 128.98, 127.64, 127.47, 127.21, 127.06, 21.32.



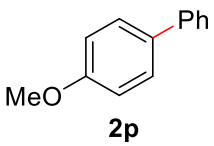
2n

1,1':4',1''-Terphenyl (**2n**). Yeld 98% (56.43 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.68 (s, 4H), 7.67 – 7.63 (m, 4H), 7.48 – 7.44 (m, 4H), 7.39 – 7.34 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 140.87, 140.29, 129.00, 127.69, 127.53, 127.24.



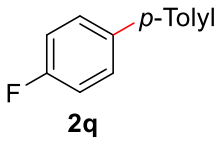
2o

4-Methoxy-4'-methyl-1-1'-biphenyl (**2o**). Yeld 77% (38.17 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.50 (d, *J* = 8.8 Hz, 2H), 7.44 (d, *J* = 8.1 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 6.95 (d, *J* = 8.8 Hz, 2H), 3.83 (s, 3H), 2.37 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.07, 138.11, 136.51, 133.88, 129.61, 128.11, 126.74, 114.30, 55.48, 21.23.



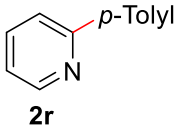
2p

4-Methoxy-1,1'-biphenyl (**2p**). Yeld 77% (35.47 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.55 – 7.50 (m, 4H), 7.42 – 7.38 (m, 2H), 7.31 – 7.27 (m, 1H), 6.98 – 6.94 (m, 2H), 3.83 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.28, 140.98, 133.92, 128.90, 128.33, 126.91, 126.83, 114.35, 55.51.



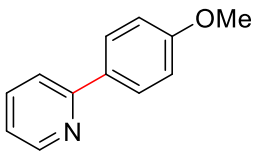
2q

4-Fluoro-4'-methyl-1,1'-biphenyl (**2q**). Yeld 93% (43.30 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** 7.53 – 7.50 (m, 2H), 7.43 (d, *J* = 8.2 Hz, 2H), 7.25 – 7.23 (m, 2H), 7.12 – 7.07 (m, 2H), 2.39 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.45 (d, J^F = 128.0 Hz), 137.55, 137.43 (d, J^F = 3.2 Hz), 137.21, 129.71, 128.63 (d, J^F = 8.0 Hz), 127.02, 115.72 (d, J^F = 21.3 Hz), 21.26.



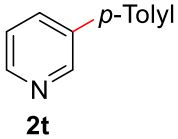
2r

2-(*p*-Tolyl)pyridine (**2r**). Yeld 65% (27.50 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.67 (d, *J* = 4.6 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 2H), 7.75 – 7.69 (m, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.19 (ddd, *J* = 6.6, 4.8, 2.1 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.62, 149.76, 139.10, 136.84, 136.77, 129.65, 126.92, 121.96, 120.42, 21.45.



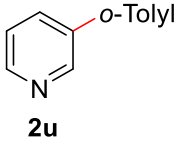
2s

2-(4-methoxyphenyl)pyridine (**2s**). Yeld 72% (33.37 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.64 – 8.62 (m, 1H), 7.93 (d, *J* = 9.0 Hz, 2H), 7.71 – 7.63 (m, 2H), 7.16 – 7.13 (m, 1H), 6.98 (d, *J* = 8.9 Hz, 2H), 3.84 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.60, 157.28, 149.72, 136.85, 132.19, 128.33, 121.59, 119.99, 114.27, 55.53.



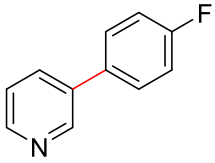
2t

3-(*p*-Tolyl)pyridine (**2t**). Yeld 67% (28.35 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.84 (d, *J* = 1.8 Hz, 1H), 8.57 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.86 (ddd, *J* = 7.9, 2.2, 1.8 Hz, 1H), 7.49 (*J* = 8.2 Hz, 2H), 7.35 (ddd, *J* = 7.9, 4.8, 0.7 Hz, 1H), 7.29 (d, *J* = 7.9 Hz, 2H), 2.41 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 148.38, 138.21, 136.72, 135.10, 134.31, 129.97, 127.15, 123.69, 21.34.



2u

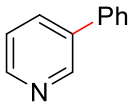
3-(*o*-Tolyl)pyridine (**2u**). Yeld 56% (23.69 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.60 (dd, *J* = 4.9, 1.7 Hz, 2H), 7.67 – 7.64 (m, 1H), 7.37 – 7.33 (m, 1H), 7.32 – 7.26 (m, 3H), 7.23 – 7.21 (m, 1H), 2.28 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 150.13, 148.30, 138.24, 137.57, 136.61, 135.74, 130.72, 130.02, 128.26, 126.23, 123.16, 20.53.



2v

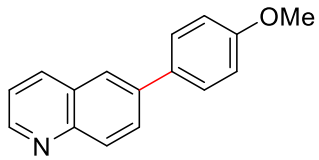
3-(4-Fluorophenyl)pyridine (**2v**). Yeld 89% (38.53 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.83 (s, 1H), 8.55 (d, *J* = 4.1, 1H), 7.86 (dt, *J* = 7.9, 2.0 Hz, 1H), 7.53 – 7.50 (m, 2H), 7.32 (dd, *J* = 7.9, 4.8 Hz, 1H), 7.17 – 7.07 (m, 2H). **^{13}C NMR (100**

MHz, $CDCl_3$) δ 163.18 (d, J^F = 247.3 Hz),148.80, 148.45, 135.98, 134.50, 134.23 (d, J^F = 3.0 Hz, 129.10 (d, J^F = 8.2 Hz), 123.84, 116.35 (d, J^F = 21.5 Hz).



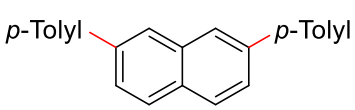
2x

3-Phenylpyridine (**2x**). Yeld 50% (19.40 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.86 (d, *J* = 1.7 Hz, 1H), 8.60 (d, *J* = 3.8 Hz, 1H), 7.88 (ddd, *J* = 7.9, 2.3, 1.7 Hz, 1H), 7.60 – 7.57 (m, 2H), 7.51 – 7.47 (m, 2H), 7.42 (ddd, *J* = 7.3, 3.8, 1.3 Hz, 1H), 7.37 (dd, 7.9, 4.9 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 148.68, 148.54, 138.03, 136.82, 134.54, 129.27, 128.28, 127.35, 123.74.



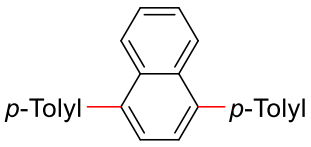
2y

6-(4-Methoxyphenyl)quinoline (**2y**). Yeld 55% (32.35 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.89 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.17 (ddd, *J* = 16.0, 8.3, 0.9 Hz, 2H), 7.97 – 7.95 (m, 2H), 7.66 (d, *J* = 8.7 Hz, 2H), 7.41 (d, *J* = 8.4, 4.2 Hz, 1H), 7.04 (d, *J* = 8.7 Hz, 2H), 3.88 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.69, 150.28, 147.58, 139.08, 136.29, 132.93, 129.97, 129.24, 128.68, 124.82, 121.61, 114.59, 55.58.



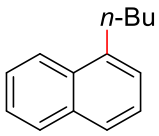
2z

2,7-Di-*p*-tolylnaphthalene (**2z**). Yeld 86% (66.31 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.06 (s, 2H), 7.91 (d, *J* = 8.6 Hz, 2H), 7.72 (dd, *J* = 8.5, 1.7 Hz, 2H), 7.64 (d, *J* = 8.0 Hz, 4H), 7.30 (d, *J* = 7.8 Hz, 4H), 2.43 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 139.03, 138.38, 137.39, 134.17, 131.70, 129.78, 128.26, 127.42, 125.84, 125.69, 21.34.



2aa

1,4-Di-*p*-tolylnaphthalene (**2aa**). Yeld 98% (75.56 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.99 – 7.97 (m, 2H), 7.45 – 7.40 (m, 8H), 7.32 (d, *J* = 7.8 Hz, 4H), 2.47 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 139.78, 138.07, 137.11, 132.17, 130.21, 129.18, 126.61, 125.89, 21.46.



2ab

1-Butylnaphthalene (**2ab**). Yeld 64% (29.49 mg). White solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.10 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.9 Hz, 1H), 7.76 (d, J = 8.1 Hz, 1H), 7.57 – 7.49 (m, 2H), 7.46 – 7.43 (m, 1H), 7.37 (d, *J* = 6.7 Hz, 1H), 3.13 (t, *J* = 7.8 Hz, 2H), 1.83 – 1.75 (m, 2H), 1.56 – 1.47 (m, 2H), 1.03 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 139.17, 134.04, 132.07, 128.91, 126.55, 126.03, 125.78, 125.71, 125.52, 124.09, 33.20, 33.01, 23.07, 14.21.

Reference

1. G. Berthon-Gelloz, M. A. Siegler, A. L. Spek, B. Tinant, J. N. H. Reek, E. I. Marko, *Dalton Trans*., 2010, **39**, 1444.
2. S. Meiries, K. Speck, D. B. Cordes, A. M. Z. Slawin, S. P. Nolan, *Organometallics*, 2013, **32**, 330.
3. P. Shaw, A. R Kennedy, D. J. Nelson, *Dalton Trans.*, 2016, **45**, 11772.
4. K. V. Vasudevan, R. R. Butorac, C. D. Abernethy, A. H. Cowley, *Dalton Trans.*, 2010, **39**, 7401.
5. L. Q. Hu, R. L. Deng, Y. F Li, C. J. Zeng, D. S.Shen, F. S. Liu, *Organometallics*, 2018, **37**, 214.
6. A. R. Martin, Y. Makida, S. Meiries,A. M. Z. Slawin, S. P. Nolan, *Organometallics*, 2013, **32**, 6265.
7. A. Piontek, W. Ochędzan-Siodłak, E. Bisz, M. Szostak, *Adv. Synth. Catal.*, 2019, **361**, 2329.
8. T. Ogata, J. F. Hartwig, *J. Am. Chem. Soc.*, 2008, **42**, 13848.
9. T. Agrawal, S. P. Cook, *Org. Lett.*, 2013, **15**, 96.
10. X. Lei, A. Jalla, M. A. A. Shama, J. M. Staffoed, B. Cao, *Synthesis*, 2015, **47**, 2578.
11. Q. Cao, J. L. Howard, E. Wheatley, D. L. Browne, *Angew. Chem. Int. Ed.*, 2018, **57**, 11339.
12. T. Ankner, G. Hilmersson, *Org. Lett.*, 2009, **11**, 503.
13. T. M. Gogsig, A. T. Lindhardt, M. Dekhane, J. Grouleff, T. Skrydstrup, *Chem. Eur. J.*, 2009, **15**, 5950.
14. J. I. Kuroda, K. Inamoto, K. Hiroya, T. Doi, *Eur. Org. Chem.*, 2009, 2251.
15. N. Murai, M. Miyano, M. Yonaga, K. Tanaka, *Org. Lett.*, 2012, **14**, 2818.
16. J. L. Tao, Z. X. Wang, *Eur. J. Org. Chem.*, 2015, 6534.
17. Z. Zhou, G. Cao, N. Liu, *Chem. Lett.*, 2019, **48**, 547.
18. Y. Y. Chua, H. A. Doung, *Chem. Commun.*, 2016, **52**, 1466.
19. K. Chen, W. Chen, X. Yi, W. Chen, M. Liu, H. Wu, *Chem. Commun.*, 2019, **55**, 9287.
20. Z. K. Yang, D. Y. Wang, H. Minami, H. Ogawa, T. Ozaki, T. Saito, K. Miyamoto, C. Wang, M. Uchiyama, *Chem. Eur. J.*, 2016, **22**, 15693.
21. Z. C. Cao, Q. Y. Luo, Z. J. Shi, *Org. Lett.*, 2016, **18**, 5978.
22. H. Zhou, J. Li, H. Yang, C. Xia, G. Jiang, *Org. Lett.*, 2015, **17**, 4628.
23. T. Xiao, X. Dong, Y. Tang, L. Zhou, *Adv. Synth. Catal.*, 2012, **354**, 3195.
24. X. Yi, K. Chen, J. Guo, W. Chen, W. Chen, *Adv. Synth. Catal.*, 2020, **362**, 4373.
25. T. Agrawal, S. P. Cook, *Org. Lett.*, 2014, **16**, 5080.
26. M. J. Iglesias, A. Prieto, M. C. Nicasio, *Org. Lett.*, 2012, **14**, 4318.
27. V. P. Reddy, R. Qiu, T. Iwasaki, N. Kambe, *Org. Lett.*, 2013, **15**, 1290.
28. R. Ambre, H. Yang, W. C. Chen, G. P.A. Yap, T. Jurca, T. G. Ong, *Eur. J. Inorg. Chem.*, 2019, **30**, 3511.

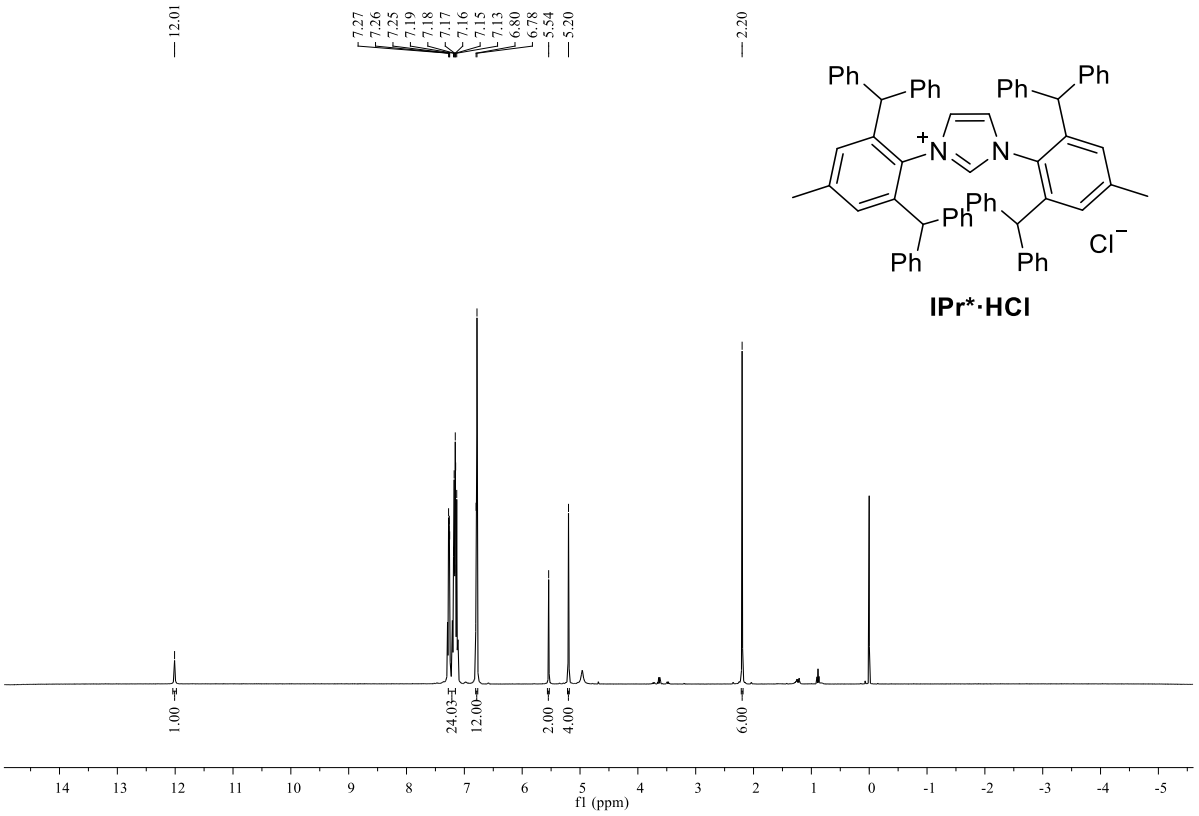
29. A. Cervantes-Reyes, A. C. Smith, G. M. Chinigo, D. C. Blakemore, M. Szostak, *Org. Lett.*, 2022, **24**, 1678.

30. X. Yang, S. Yang, L. Xiang, X. Pang, B. Chen, G. Huang, R. Yan, *Adv. Synth. Catal.*, 2015, **357**, 3732.

31. S. Karthik, T. Gandhi, *New J. Chem.*, 2018, **42**, 15811.

32. L. G. Xie, Z. X. Wang, *Chem. Eur. J.*, 2011, **17**, 4972.

33. Z. Li, L. Liu, H. M. Sun, Q. Shen, Y. Zhang, *Dalton Trans.*, 2016, **44**, 17739.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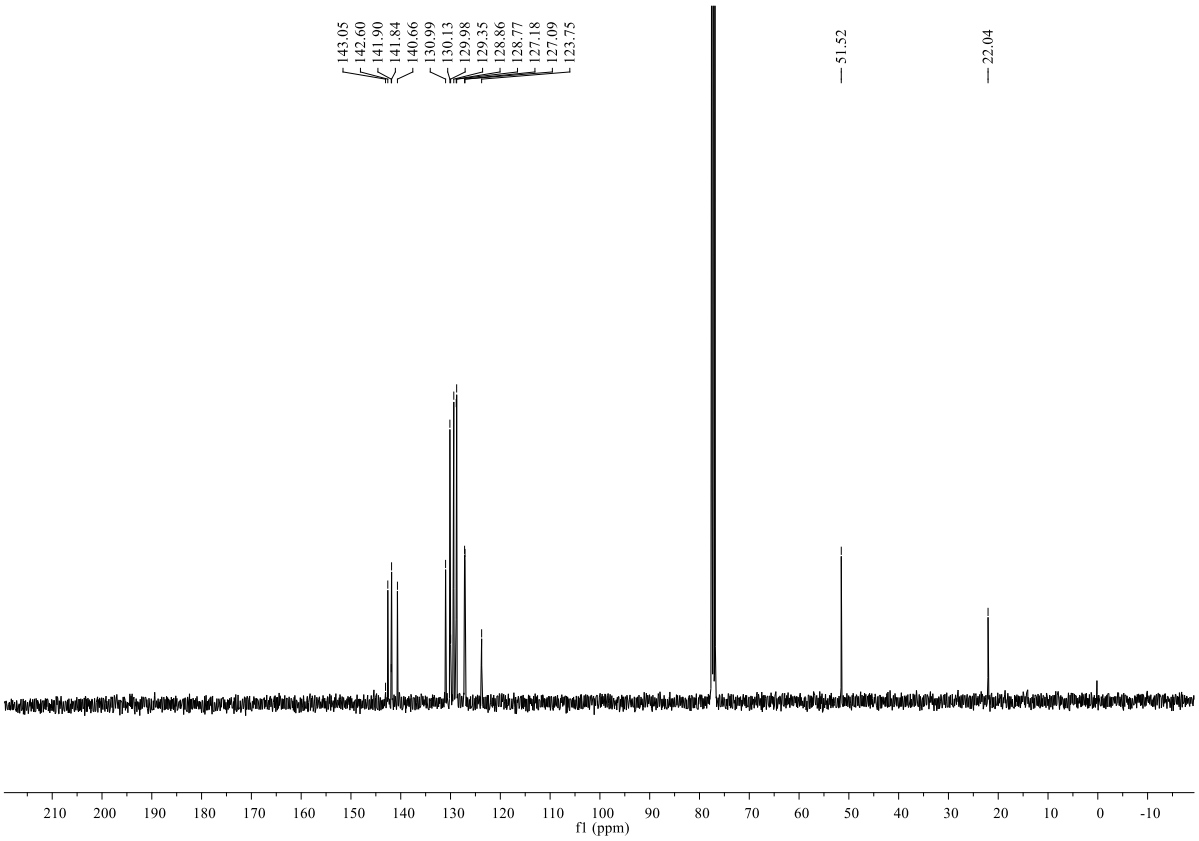
2.00
4.00
6.00
f1 (ppm)

IPr*·HCl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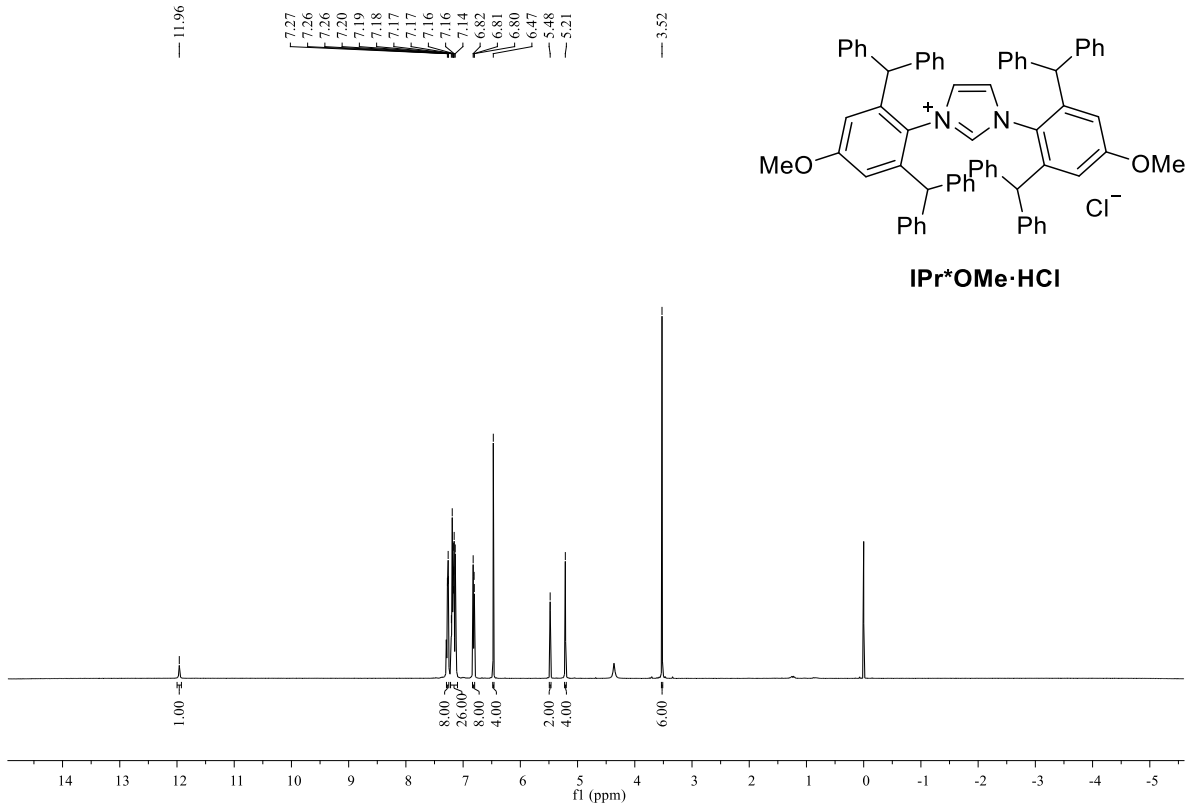
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6.00
f1 (ppm)

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Ph
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N
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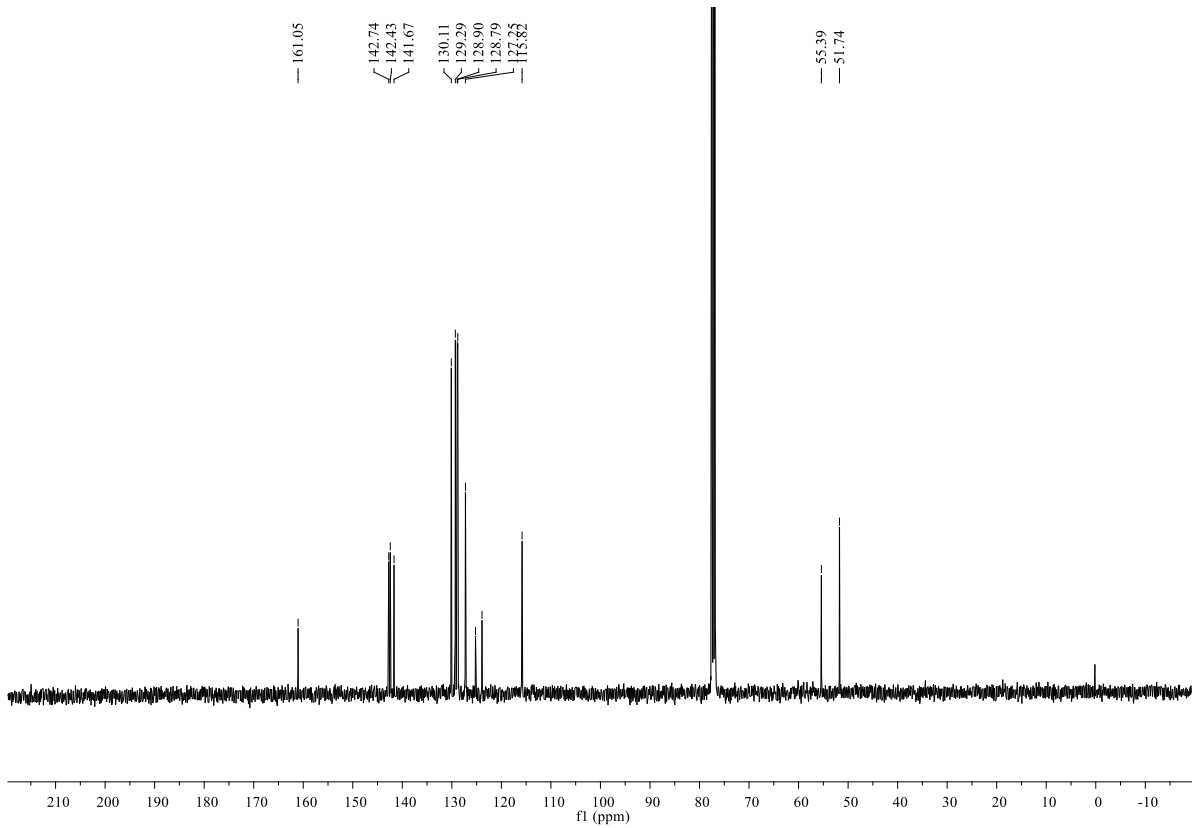
OMe
Ph
Ph
Ph
Ph
Cl⁻

IPr*OMe·HCl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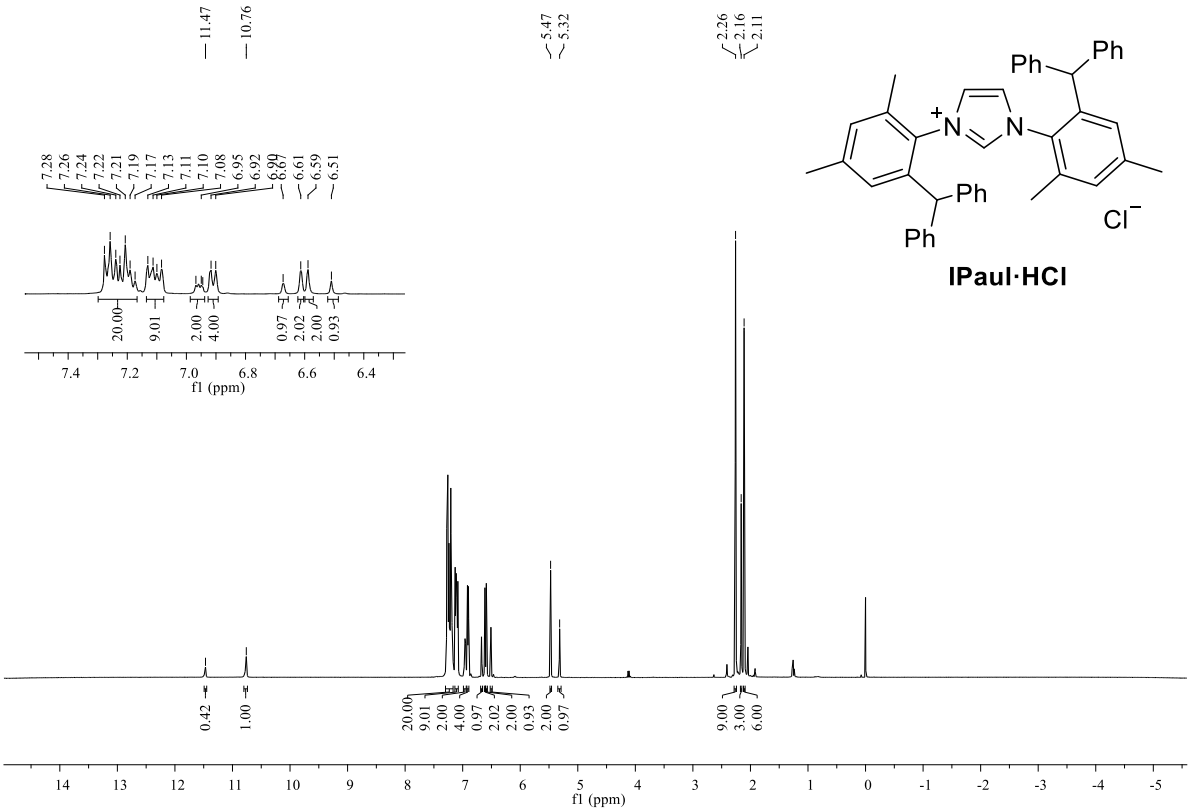
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Ph
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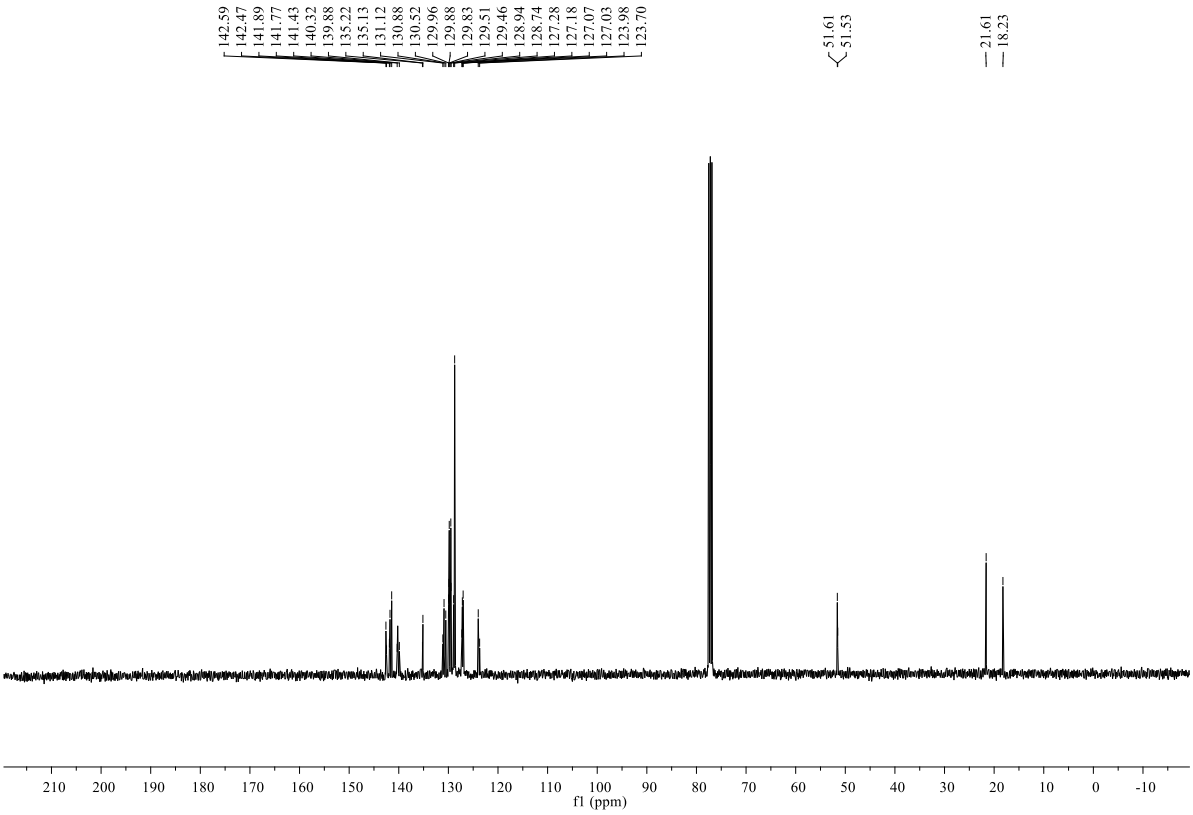
Cl⁻
IPaul·HCl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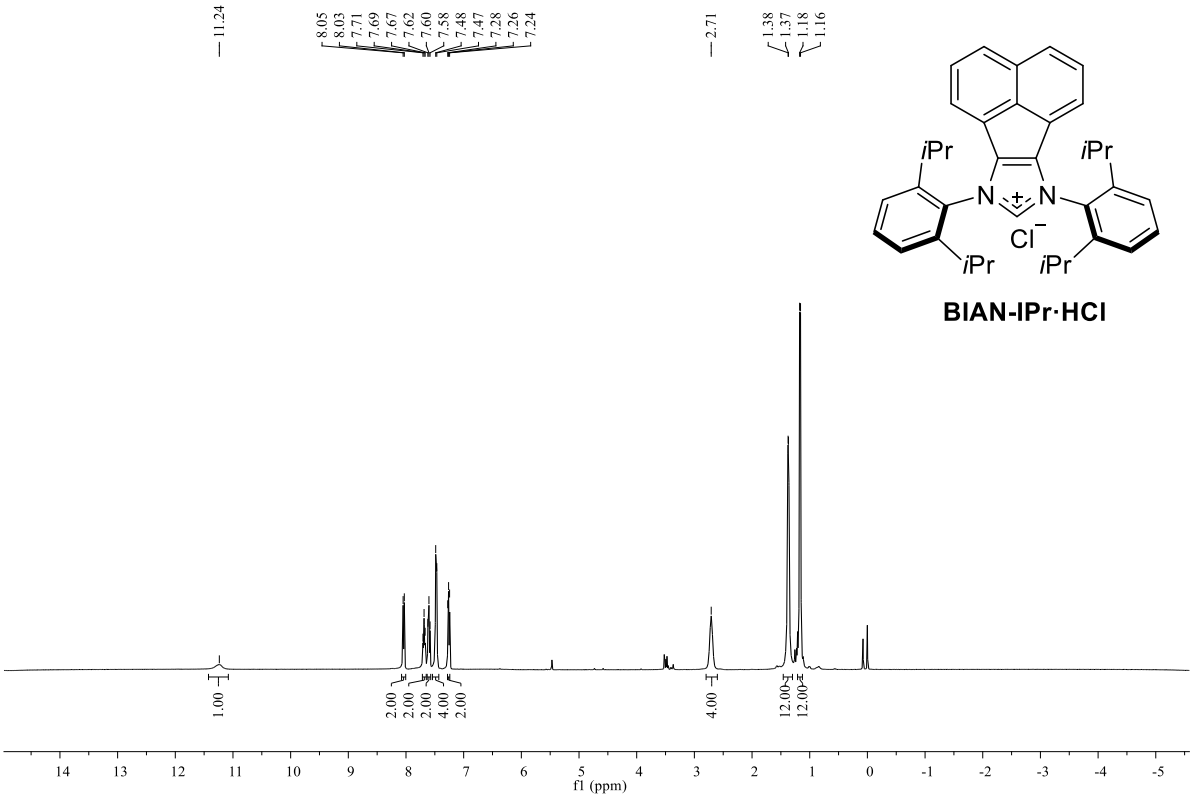
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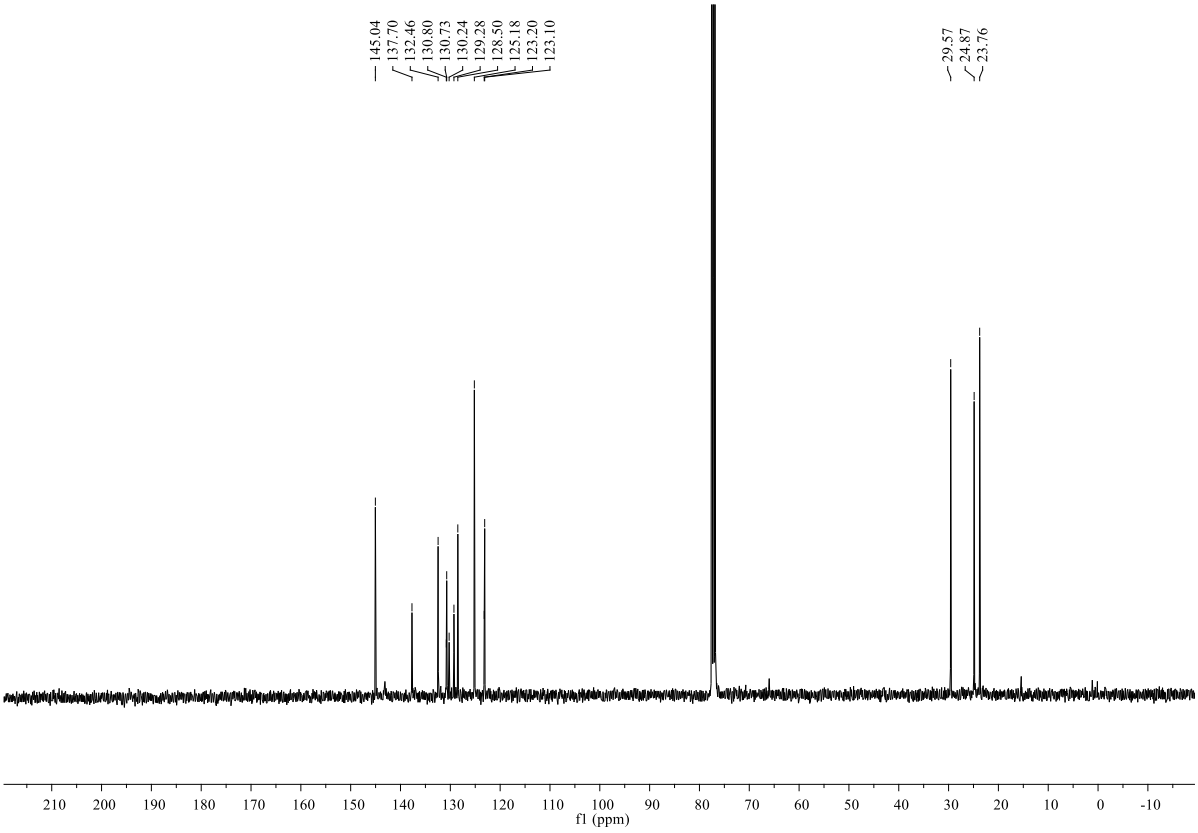
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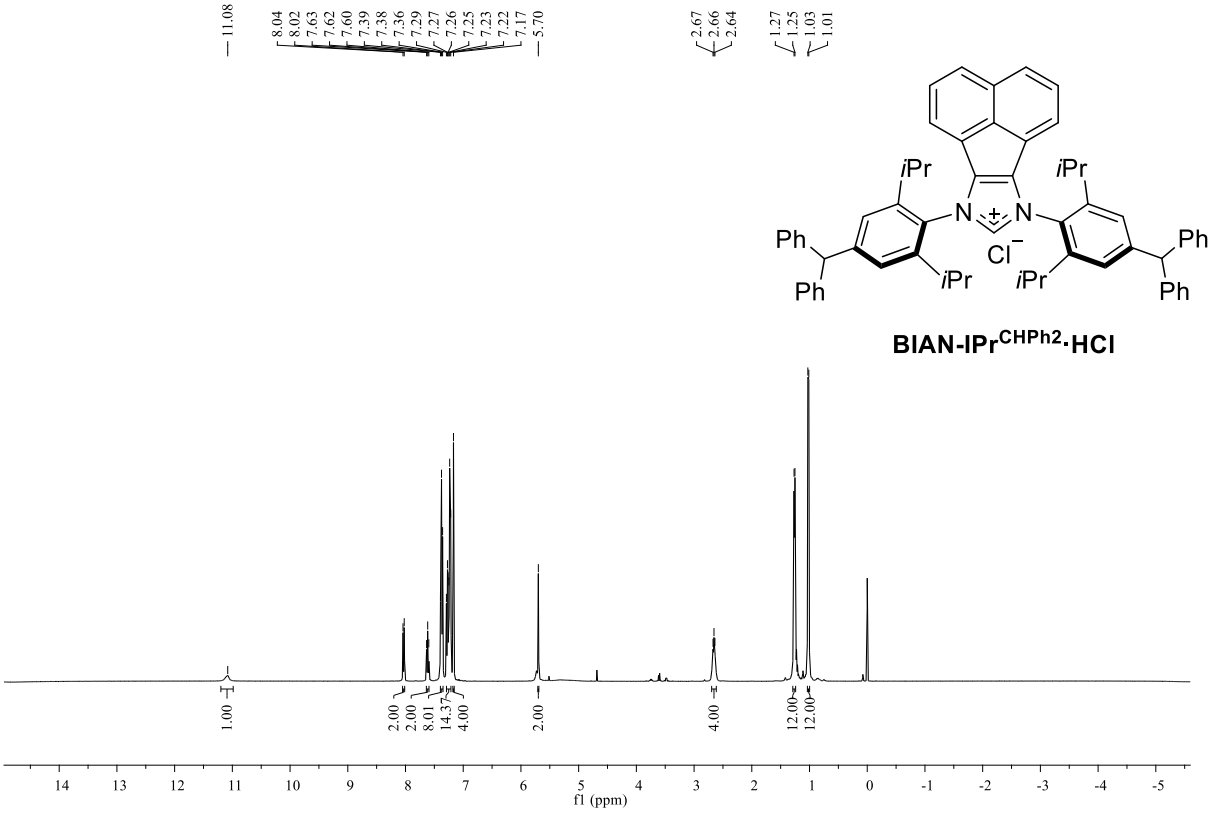

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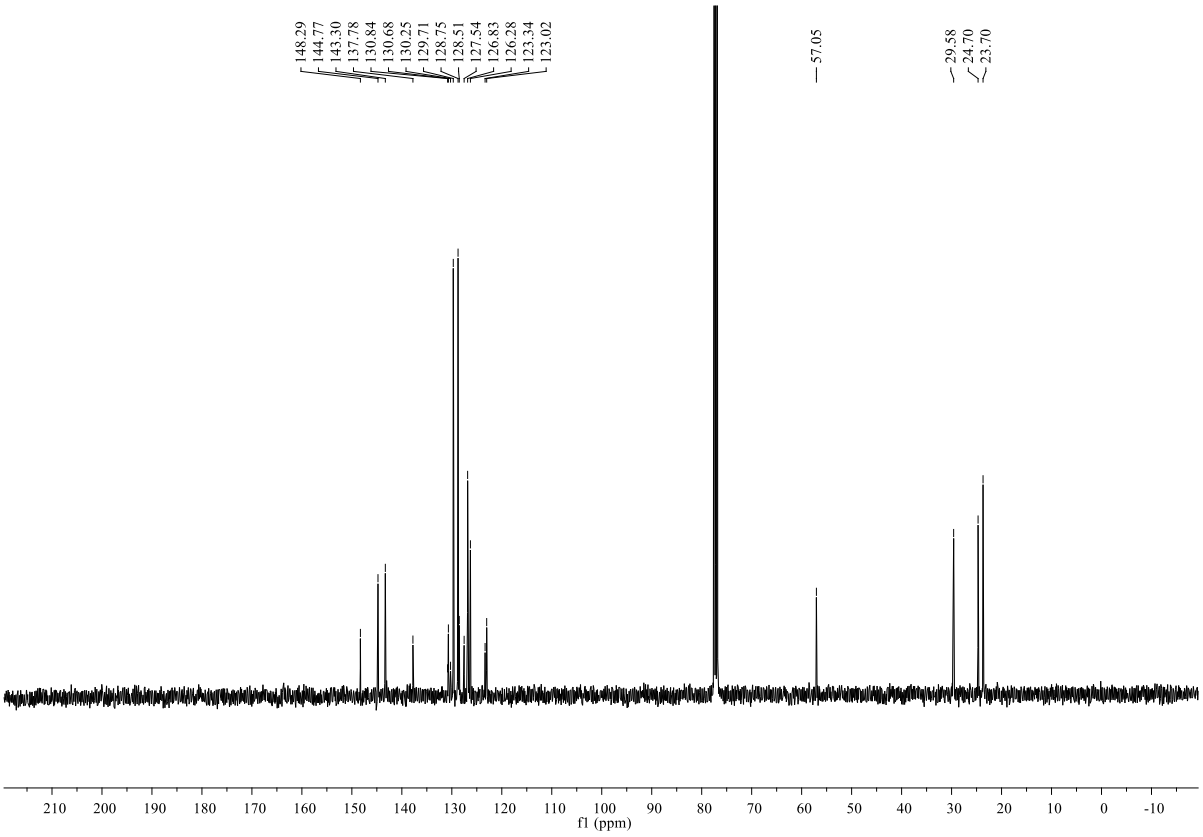

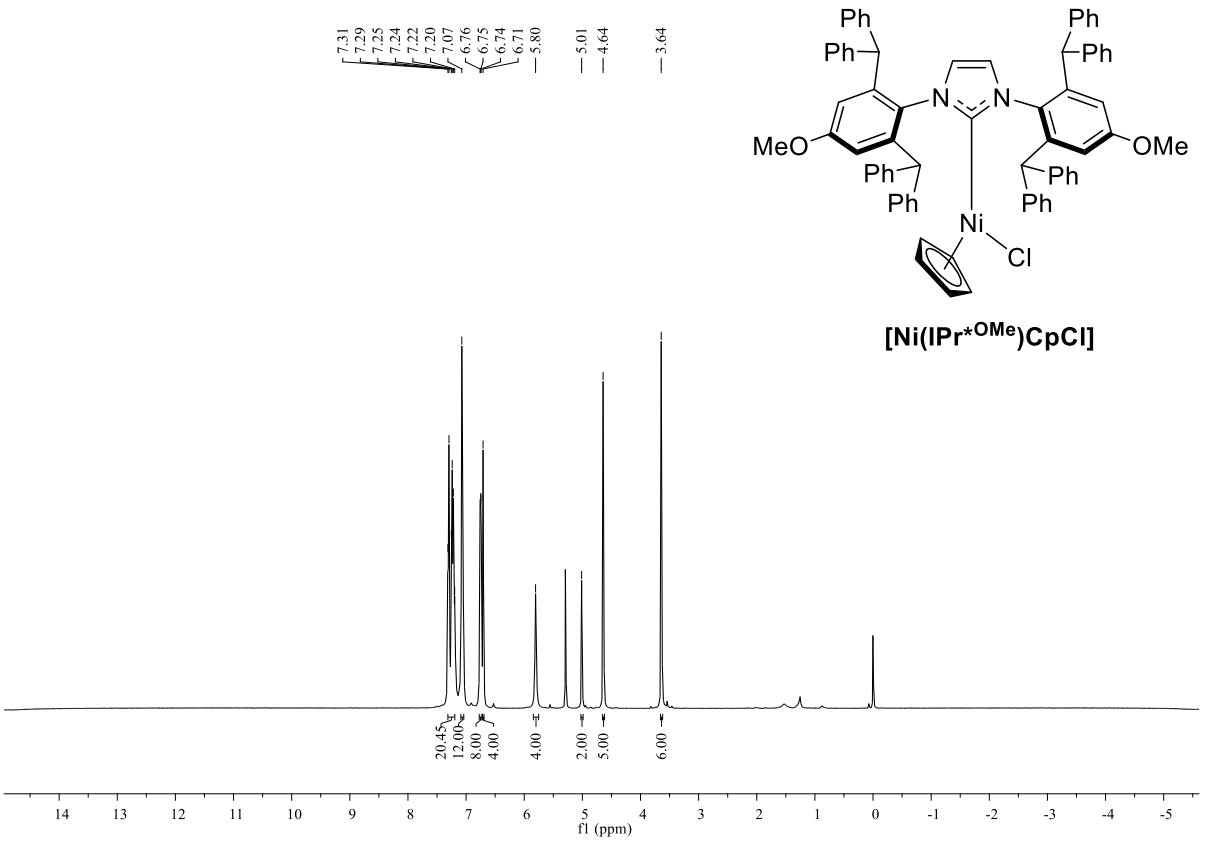

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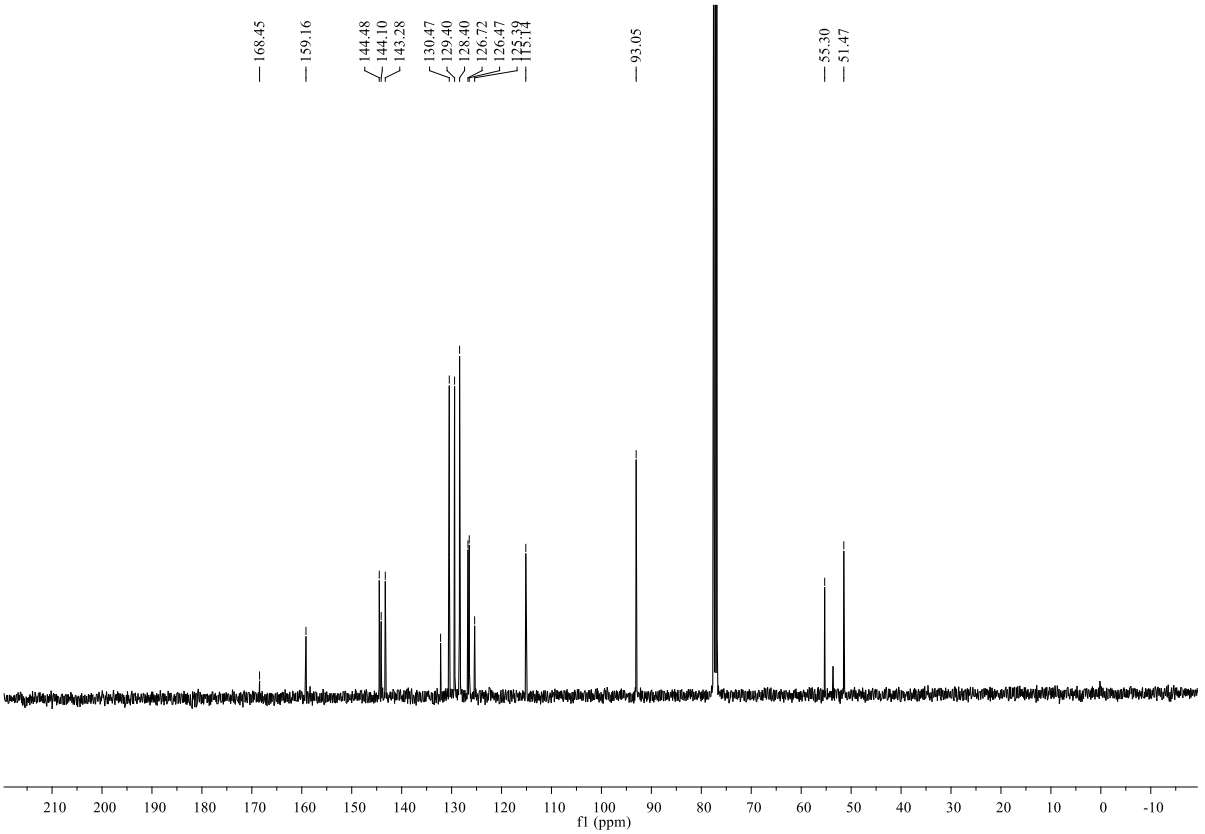

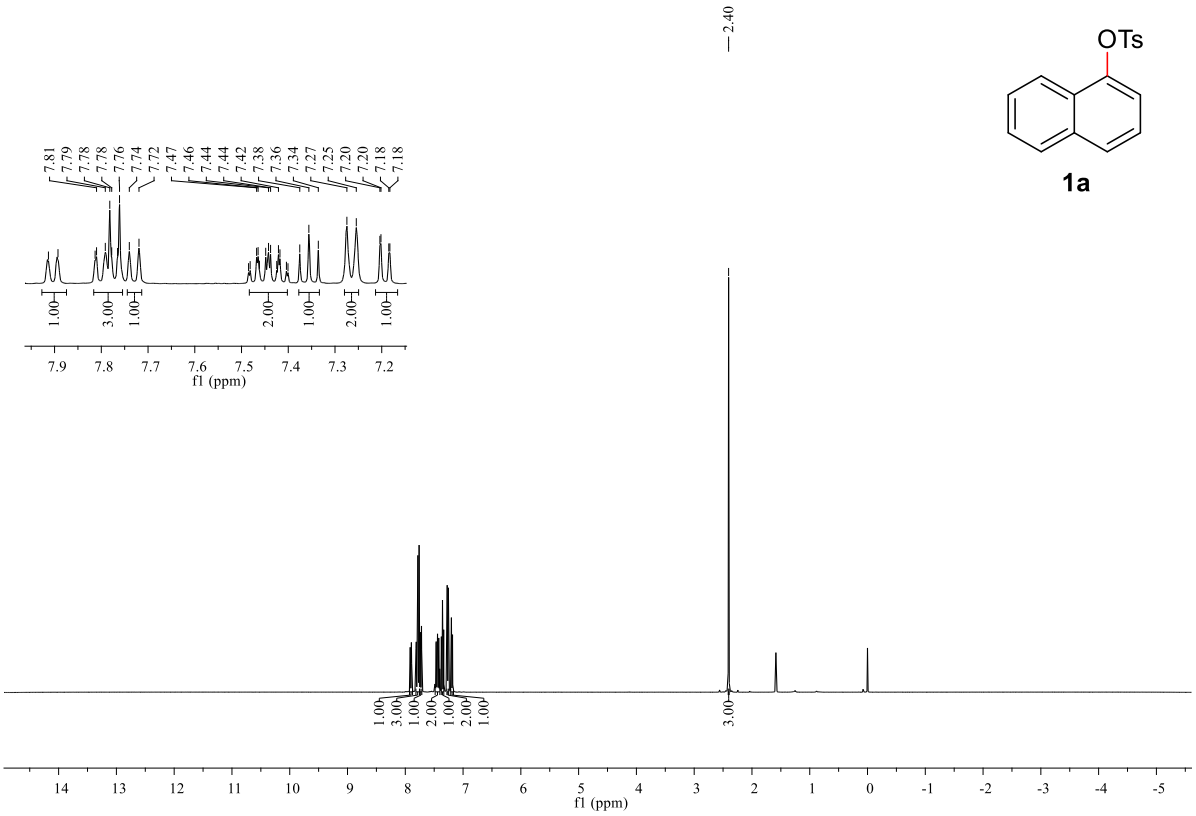
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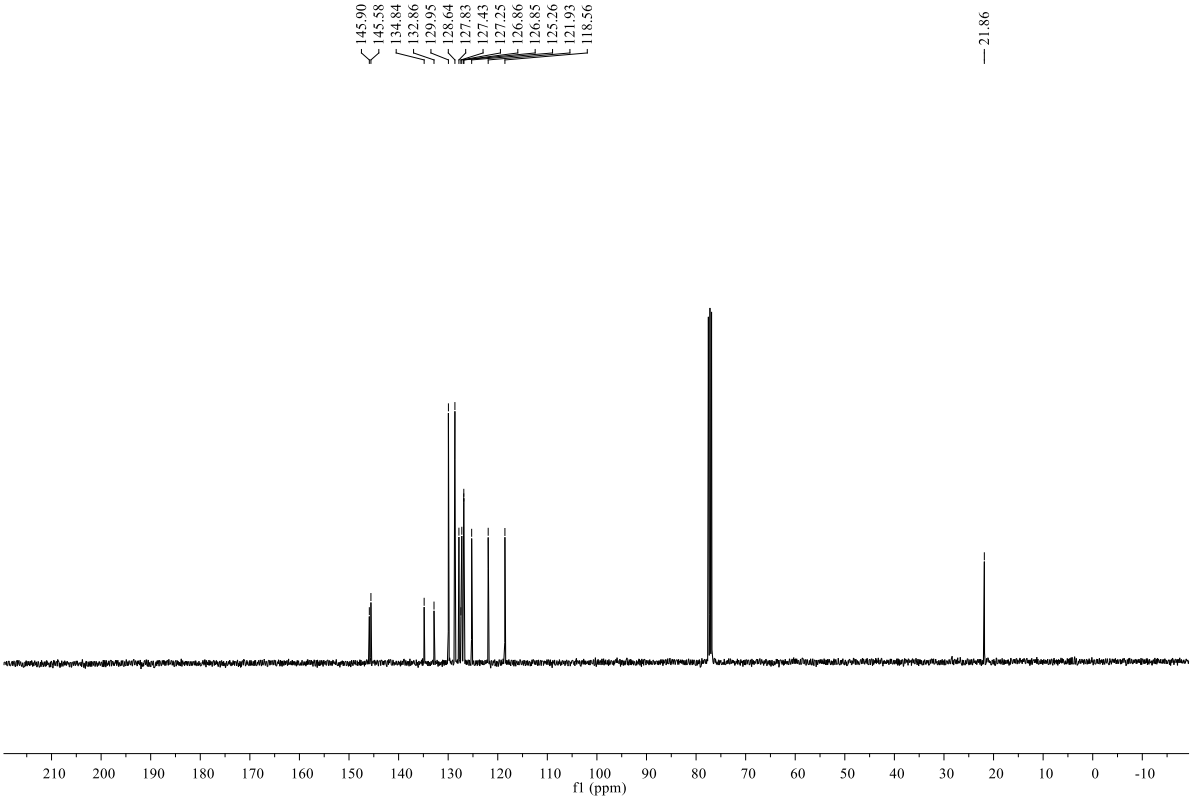
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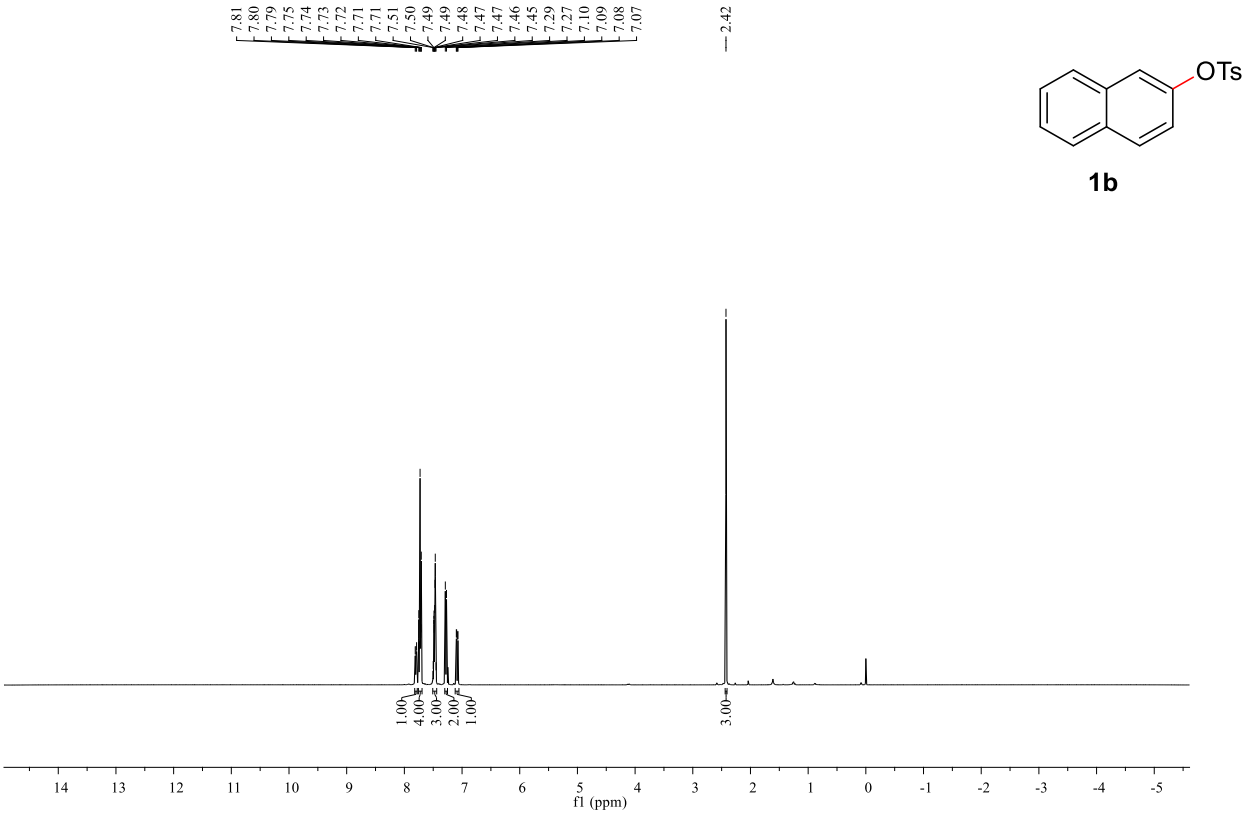
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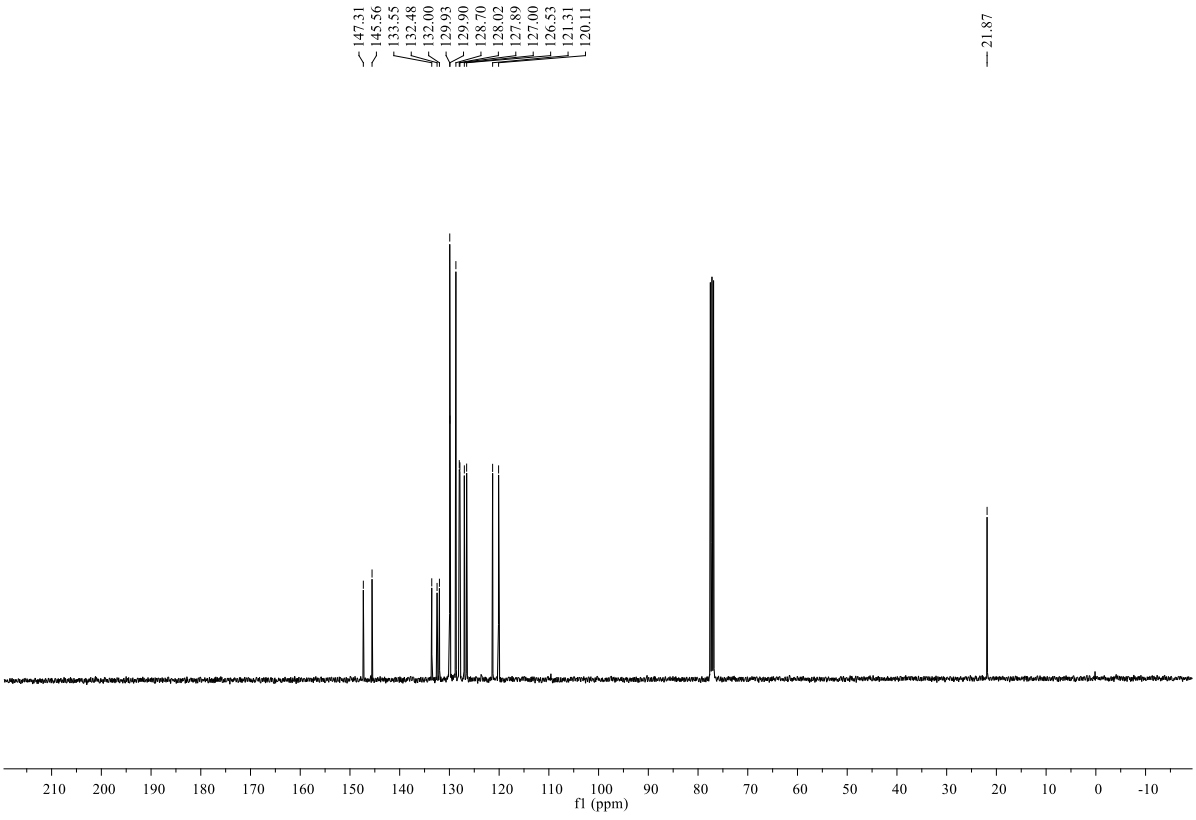
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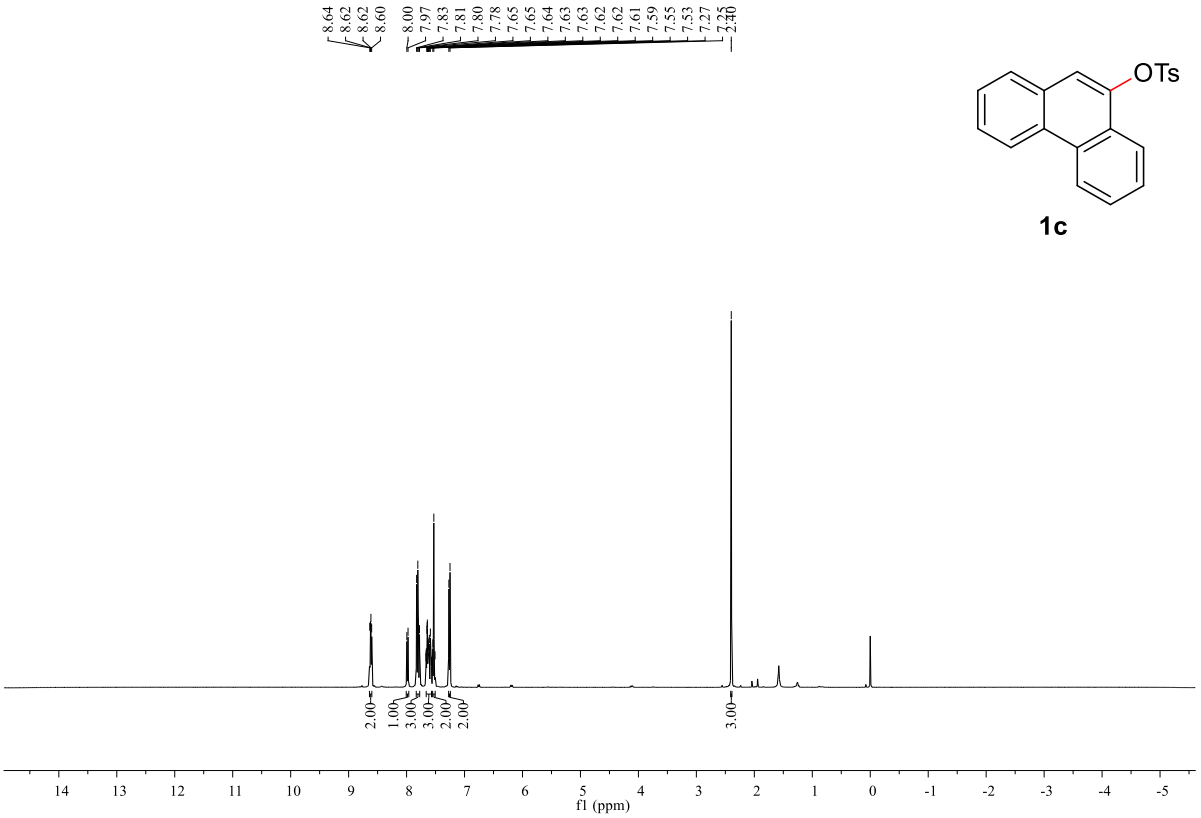
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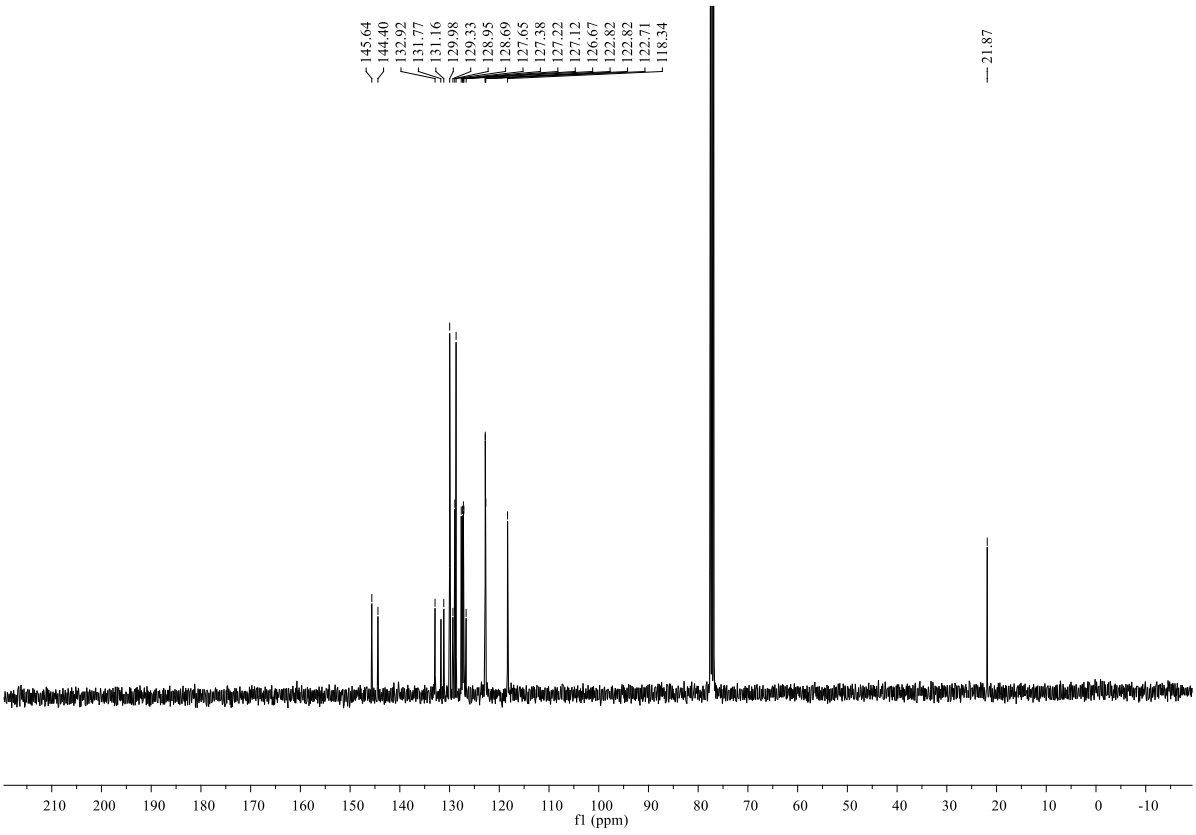
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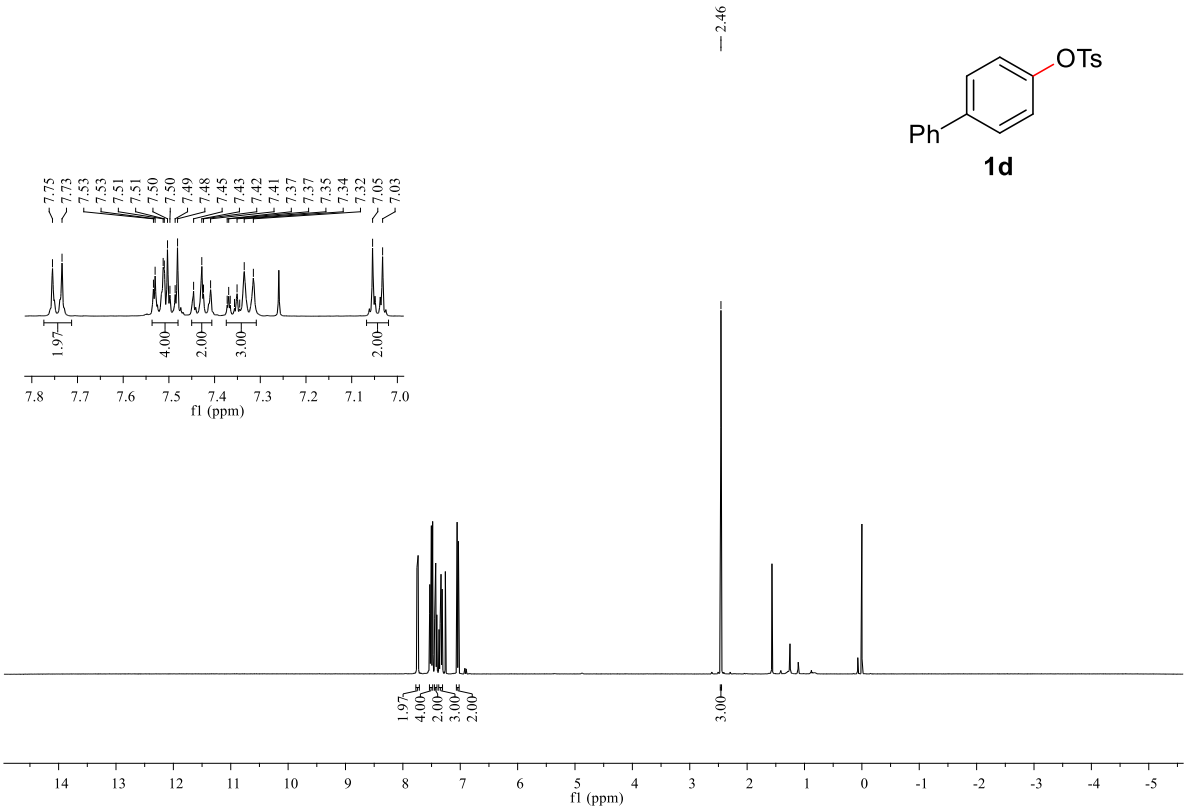
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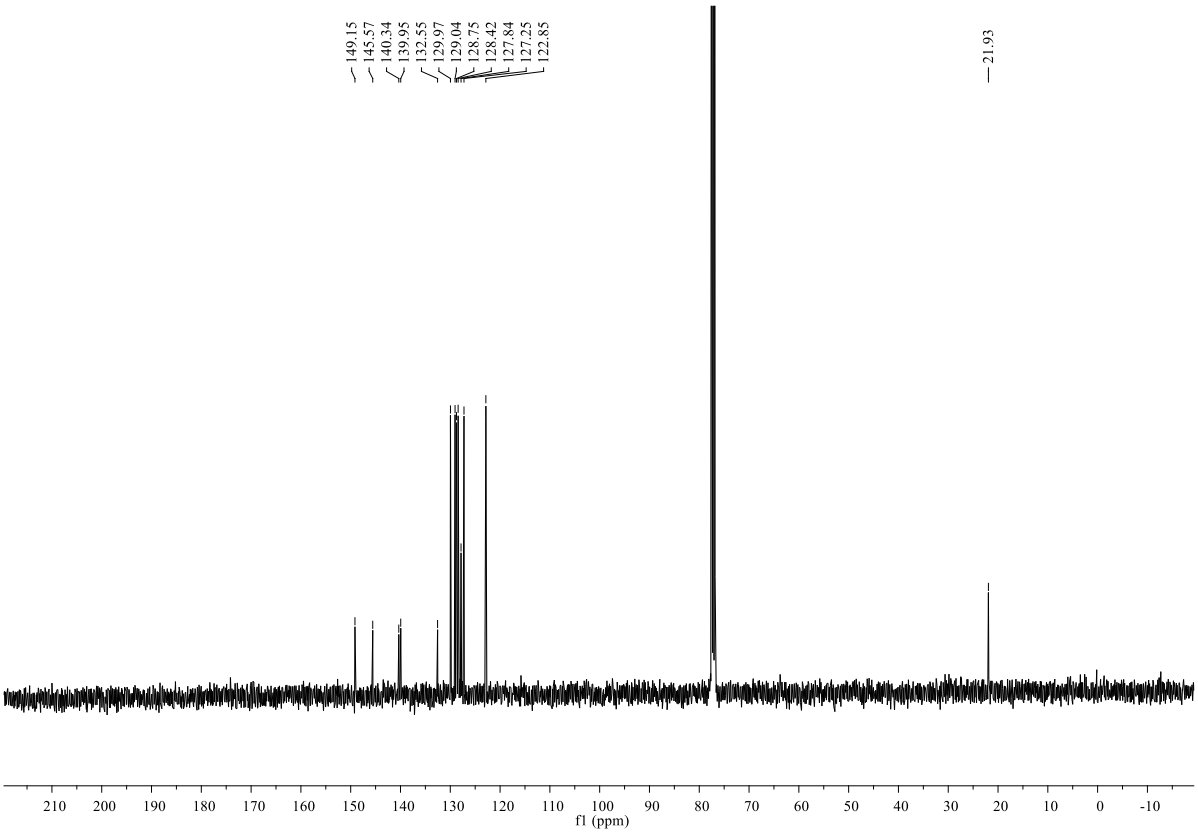
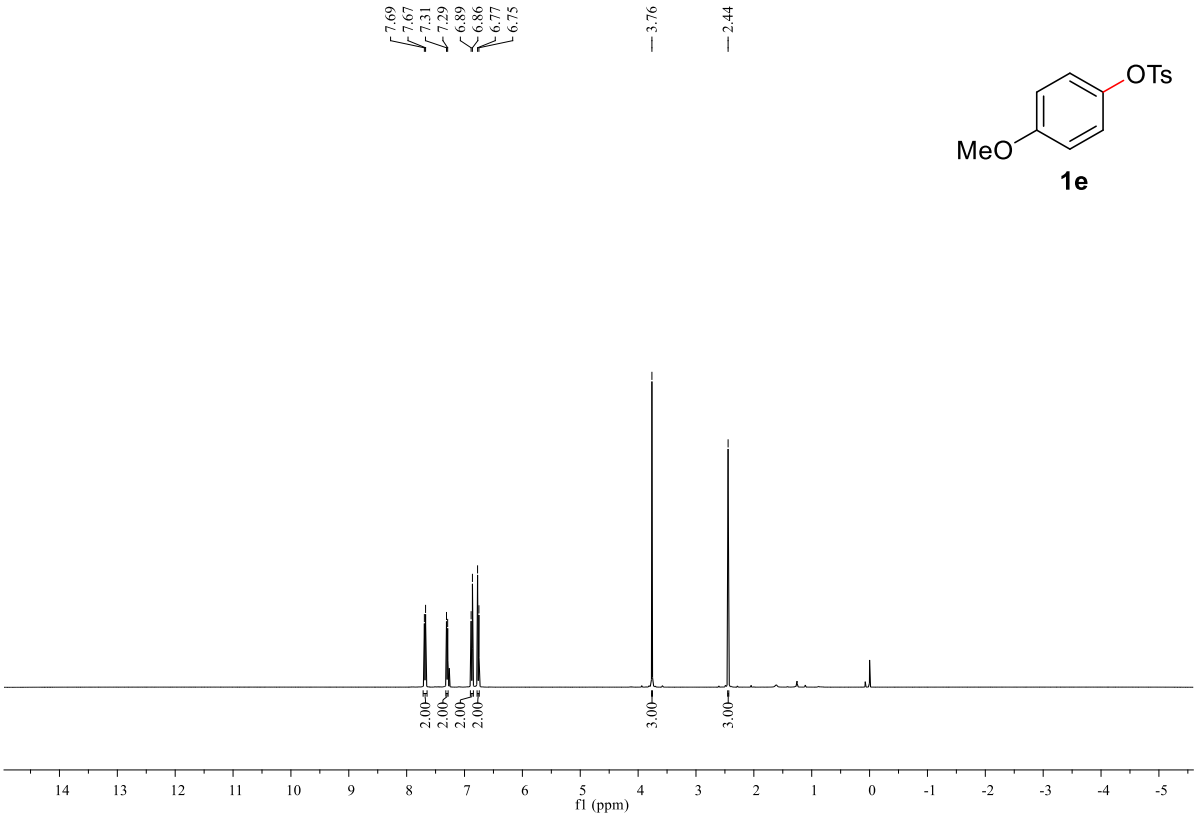
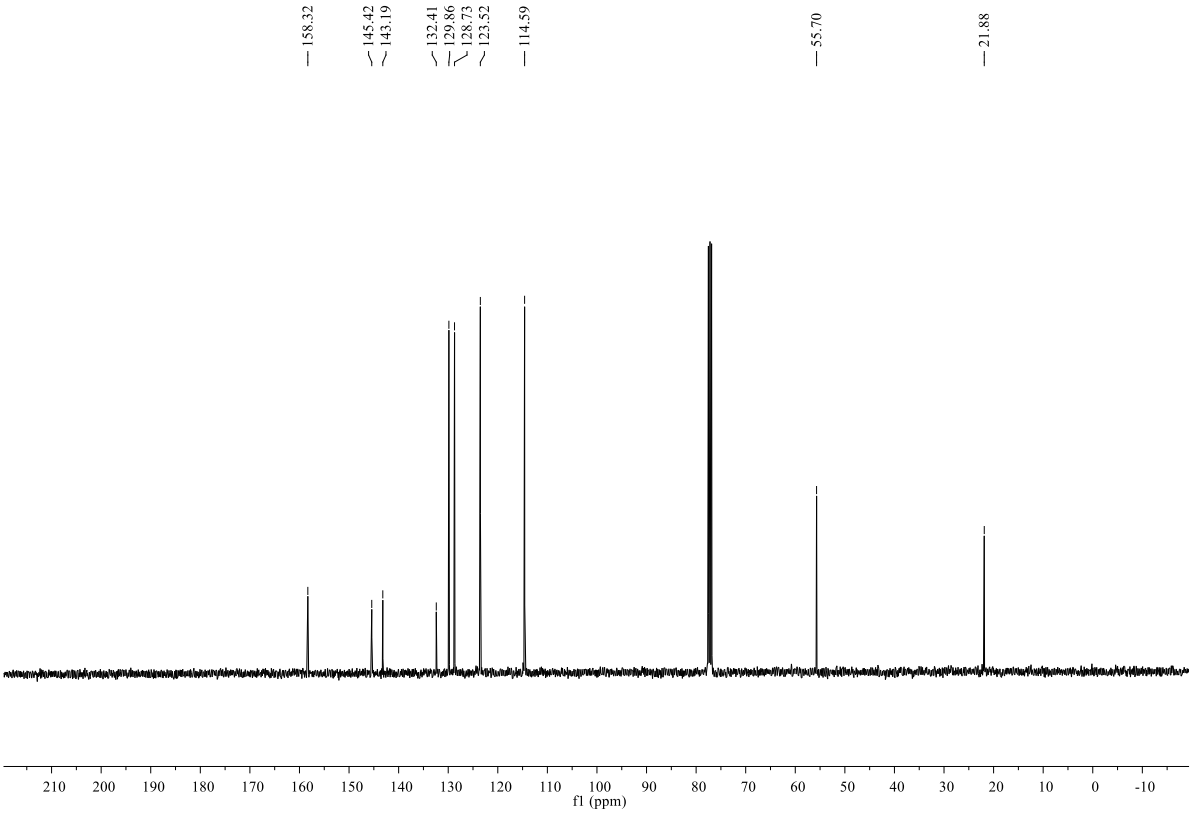
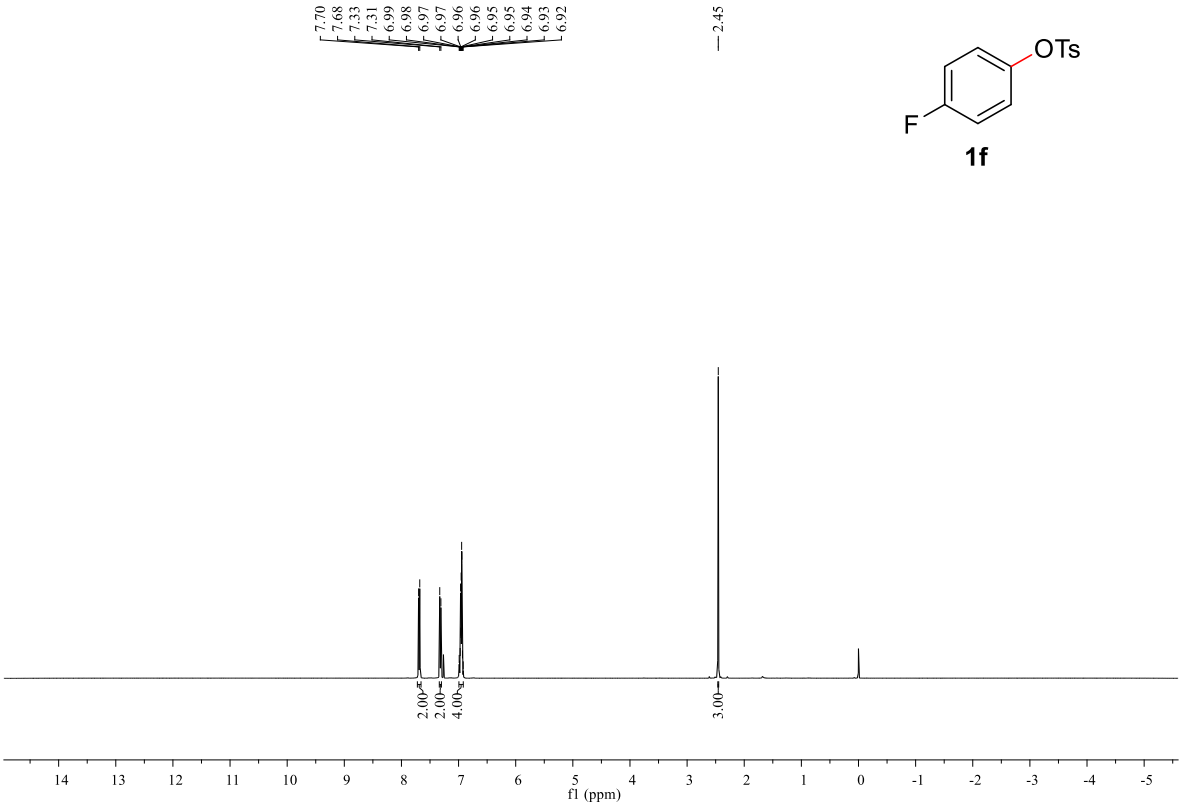
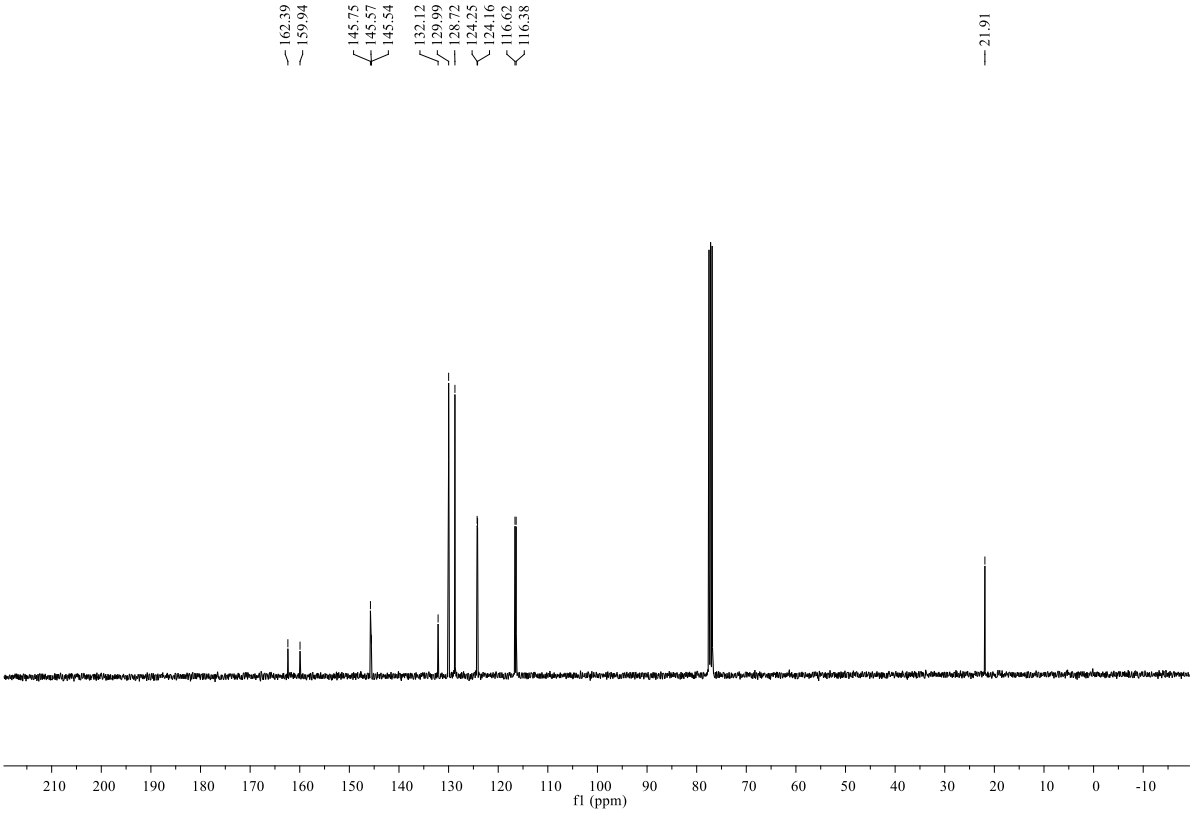
3.00
2.00
f1 (ppm)

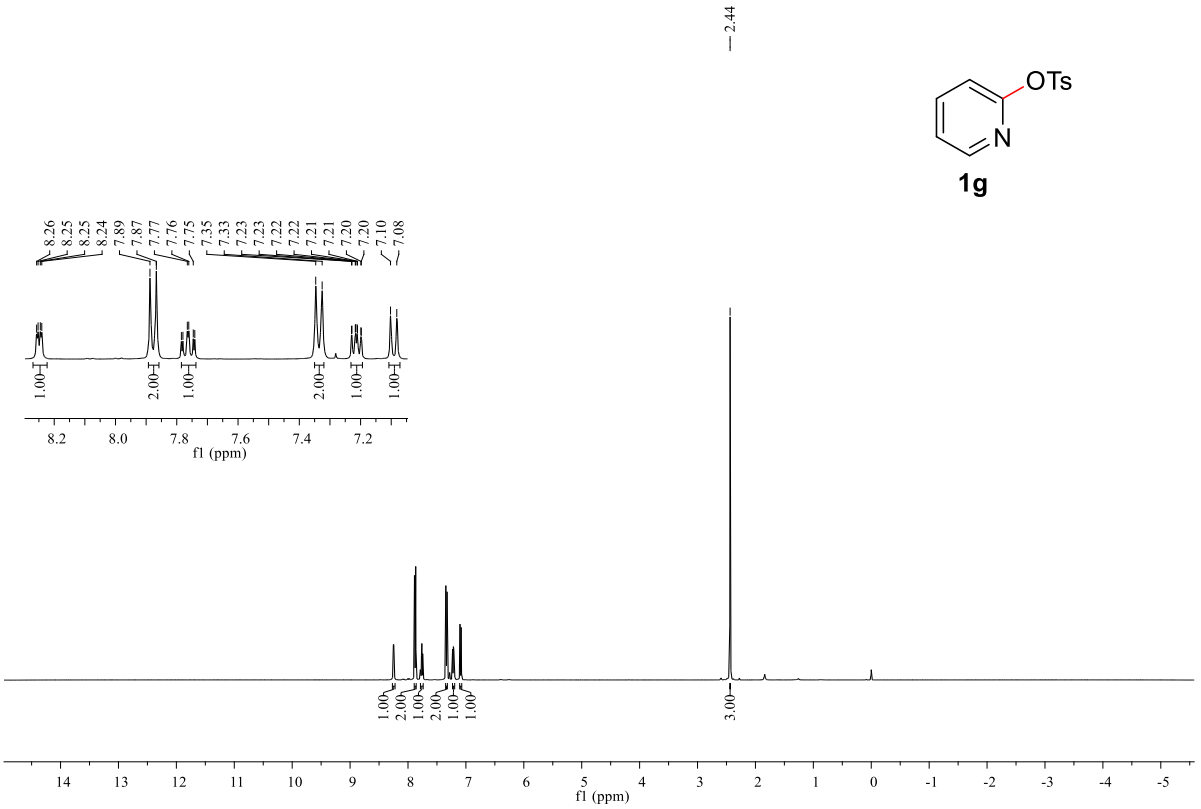

149.15
145.57
140.34
139.95
132.55
129.97
129.04
128.75
128.42
127.84
127.25
122.85
21.93
f1 (ppm)

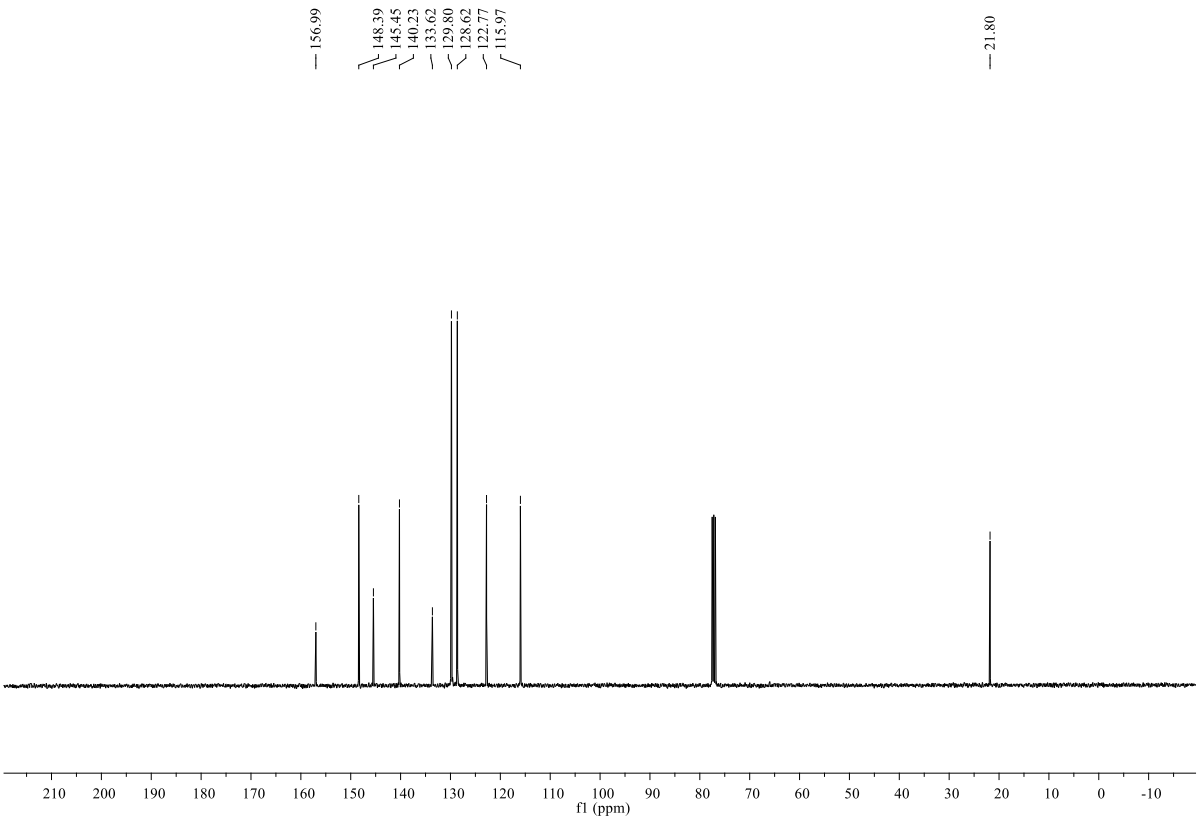

7.69
7.67
7.31
7.29
6.89
6.86
6.77
6.75
3.76
2.44
OTs
MeO
1e
2.00
2.00
2.00
2.00
3.00
3.00
f1 (ppm)

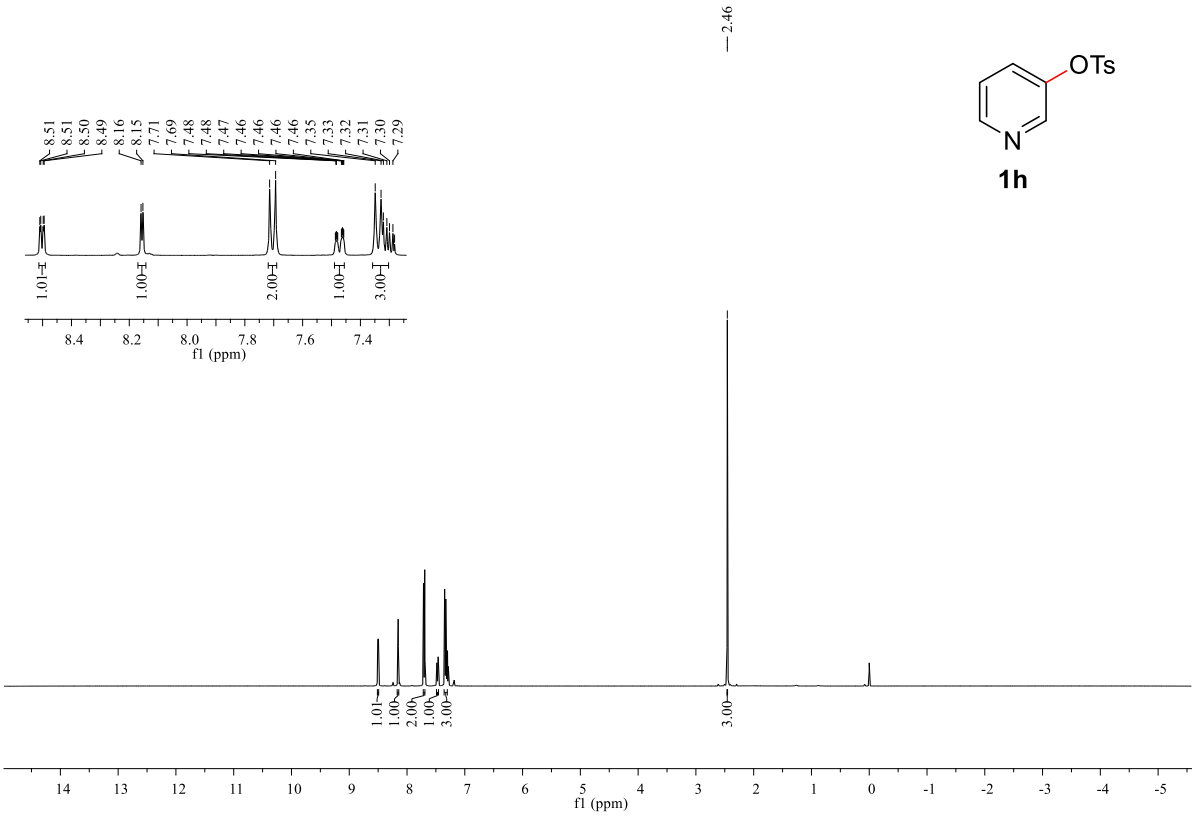

158.32
145.42
143.19
132.41
129.86
128.73
123.52
114.59
55.70
21.88
f1 (ppm)

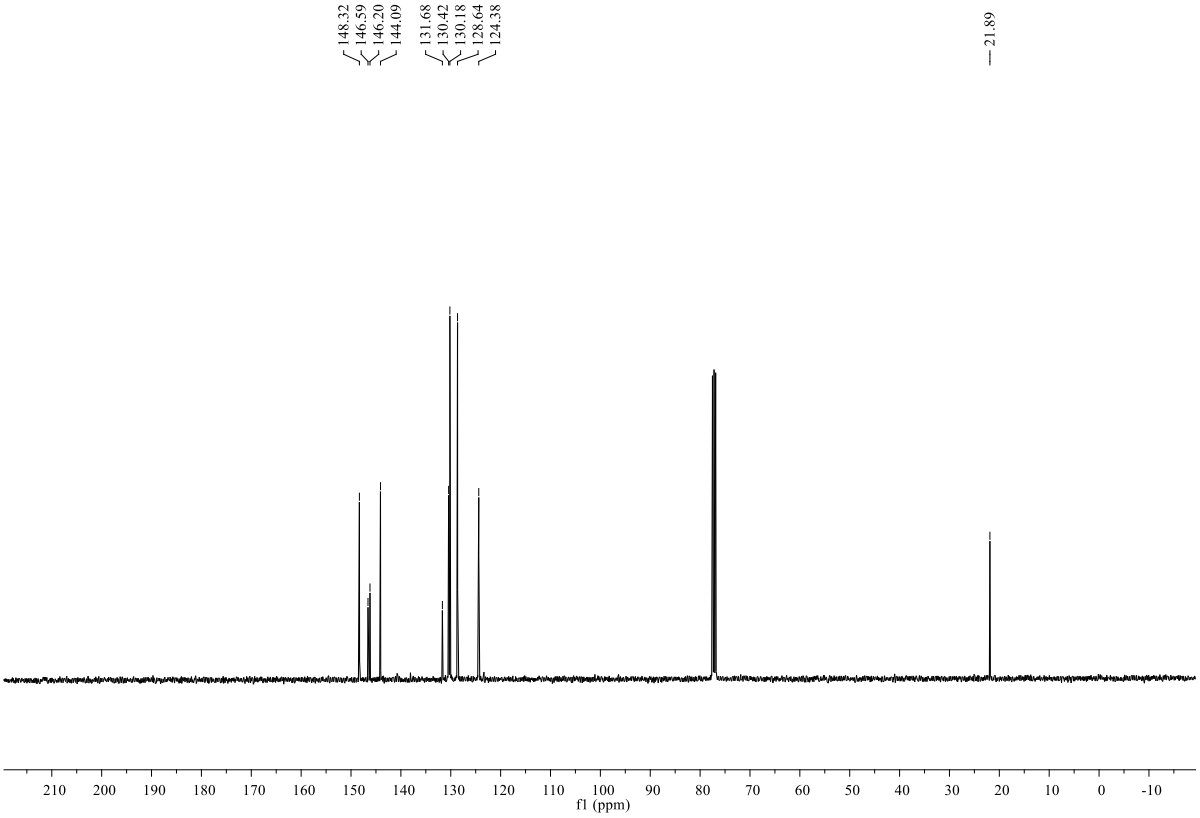

7.70
7.68
7.33
7.31
6.99
6.98
6.97
6.97
6.96
6.96
6.95
6.95
6.94
6.93
6.92
2.45
OTs
F
1f
2.00
2.00
4.00
3.00
f1 (ppm)

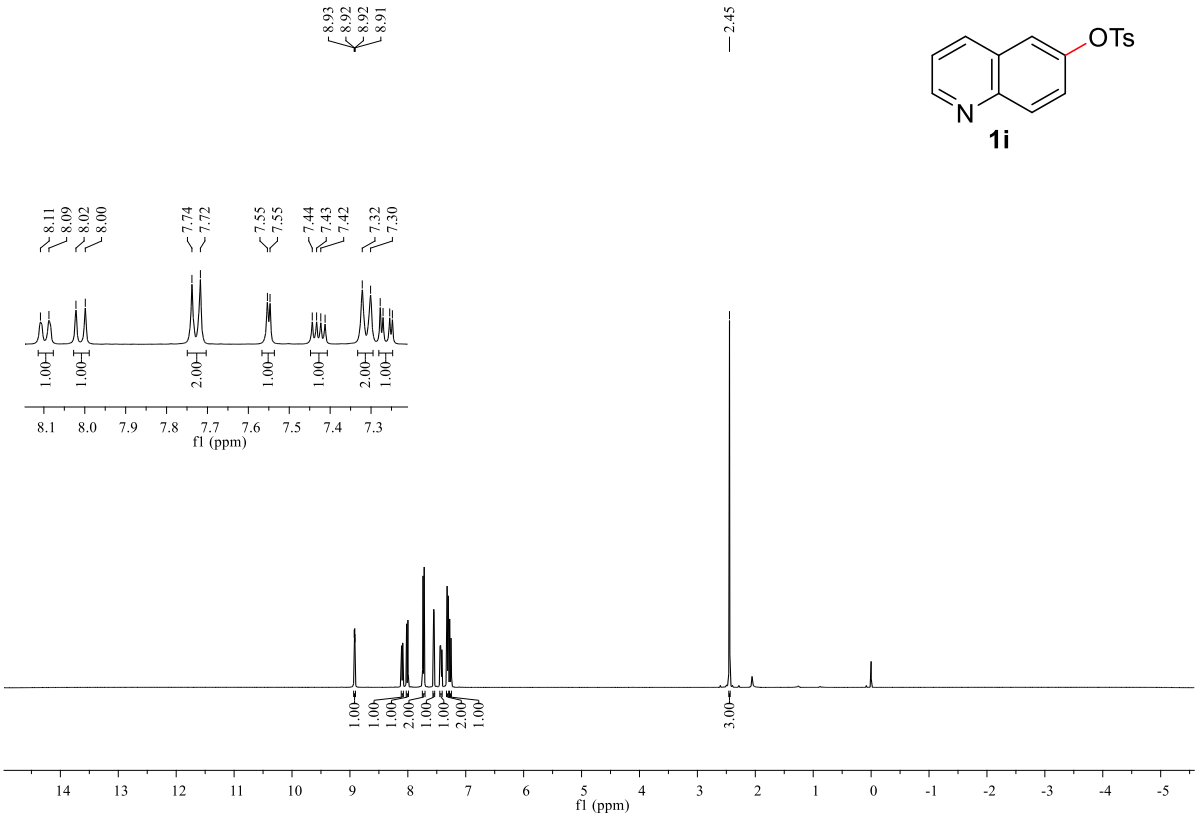

162.39
159.94
145.75
145.57
145.54
132.12
129.99
128.72
124.25
124.16
116.62
116.38
21.91
f1 (ppm)

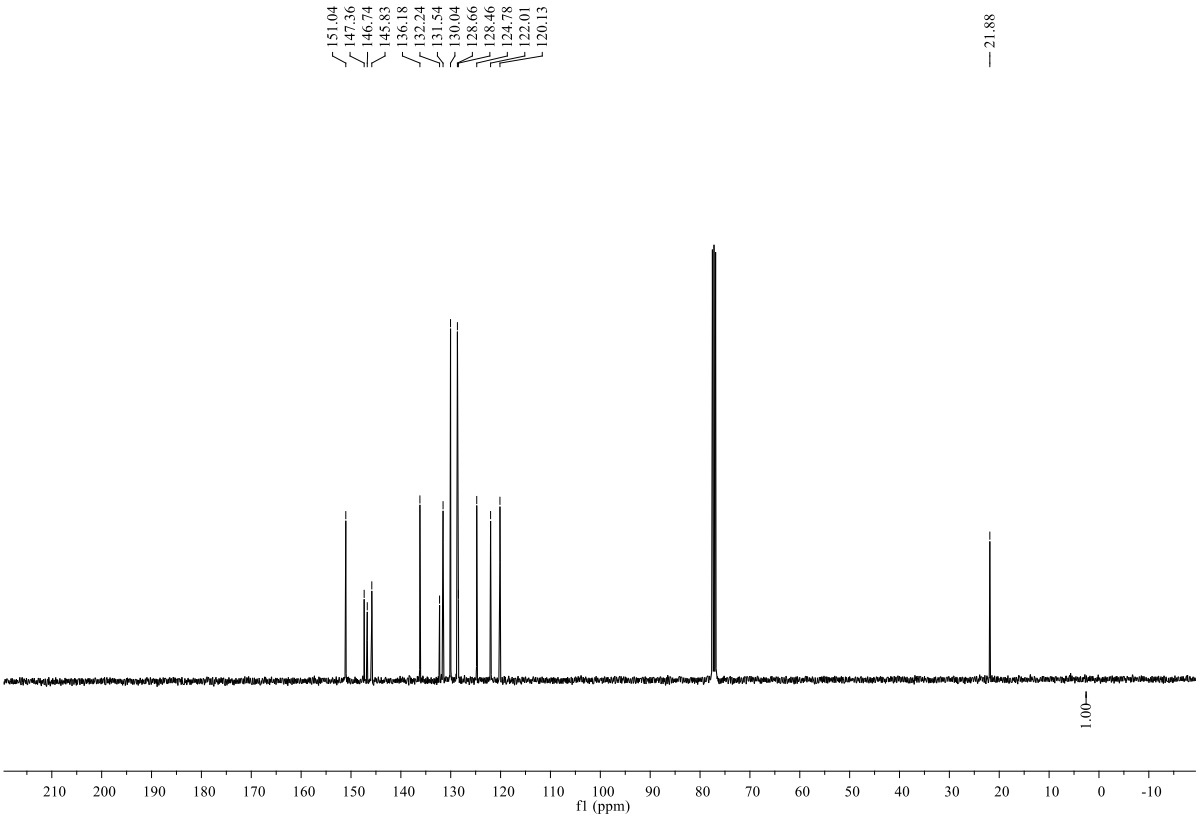

2.44
OTs
N
1g
8.26
8.25
8.25
8.24
7.89
7.87
7.77
7.76
7.75
7.35
7.33
7.23
7.23
7.22
7.22
7.21
7.21
7.20
7.20
7.10
7.08
1.00
2.00
1.00
2.00
1.00
1.00
8.2
8.0
7.8
7.6
7.4
7.2
f1 (ppm)
1.00
2.00
1.00
2.00
1.00
1.00
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)

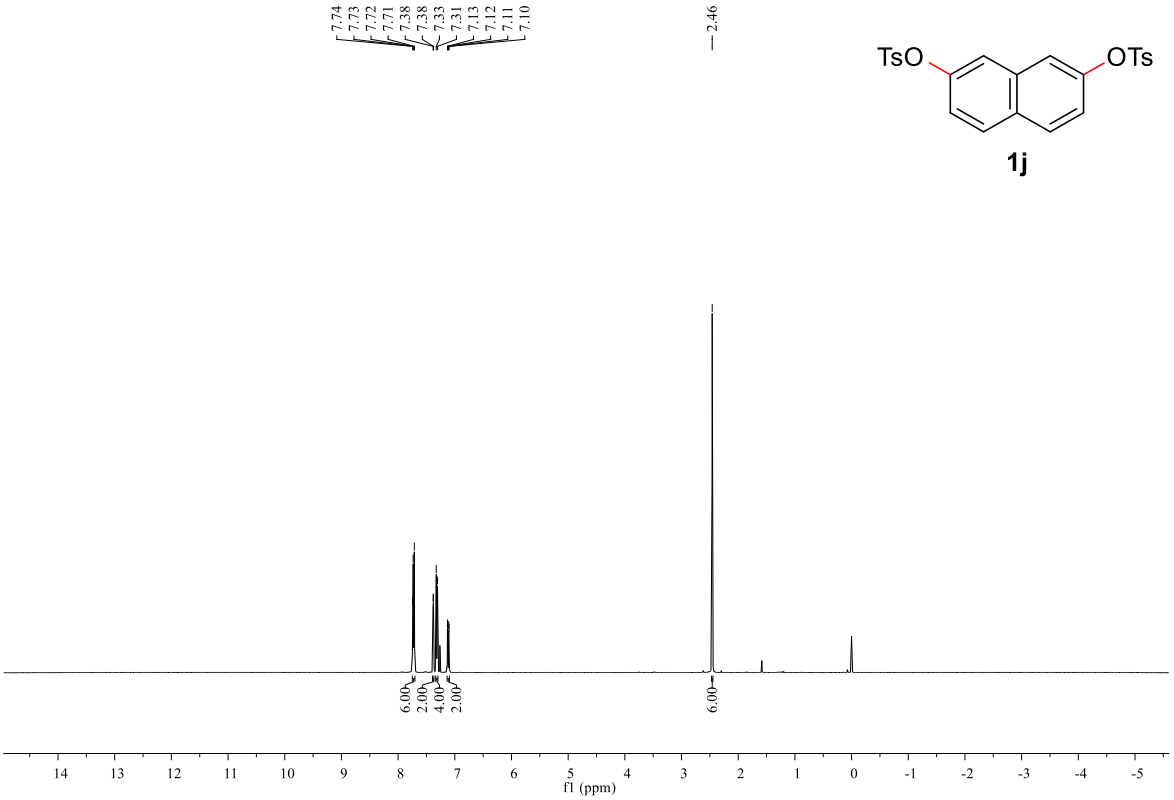

156.99
148.39
145.45
140.23
133.62
129.80
128.62
122.77
115.97
21.80
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

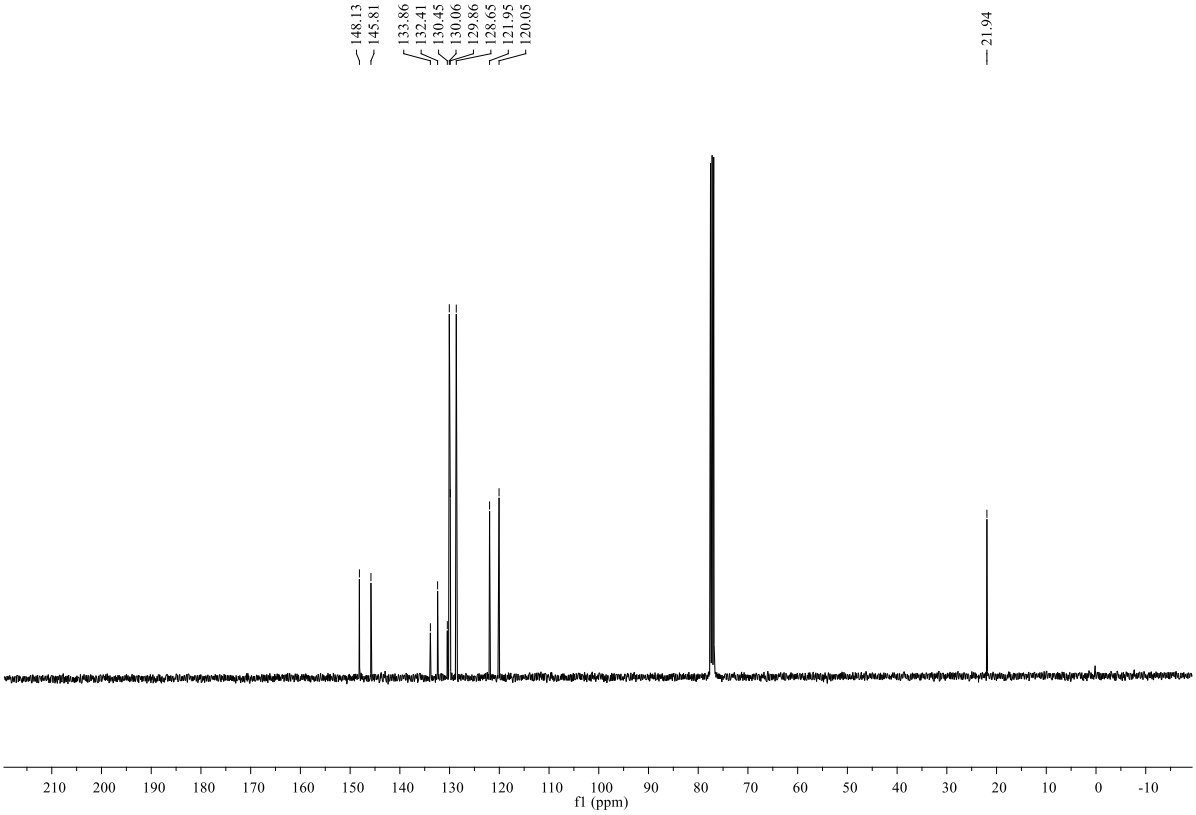

2.46
OTs
N
1h
8.51
8.51
8.50
8.49
8.16
8.15
7.71
7.69
7.48
7.48
7.47
7.46
7.46
7.46
7.46
7.35
7.33
7.32
7.31
7.30
7.29
1.01
1.00
2.00
1.00
3.00
8.4
8.2
8.0
7.8
7.6
7.4
f1 (ppm)
1.01
1.00
2.00
1.00
3.00
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)

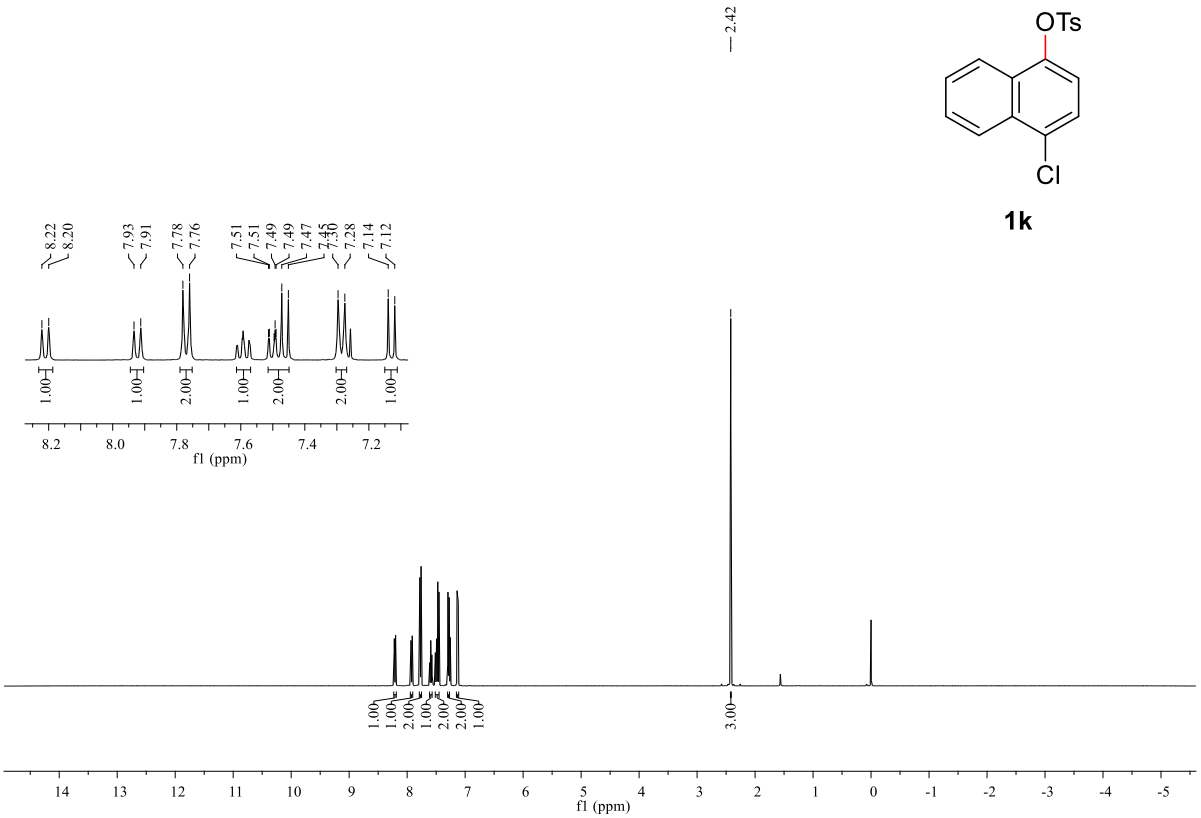

148.32
146.59
146.20
144.09
131.68
130.42
130.18
128.64
124.38
21.89
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

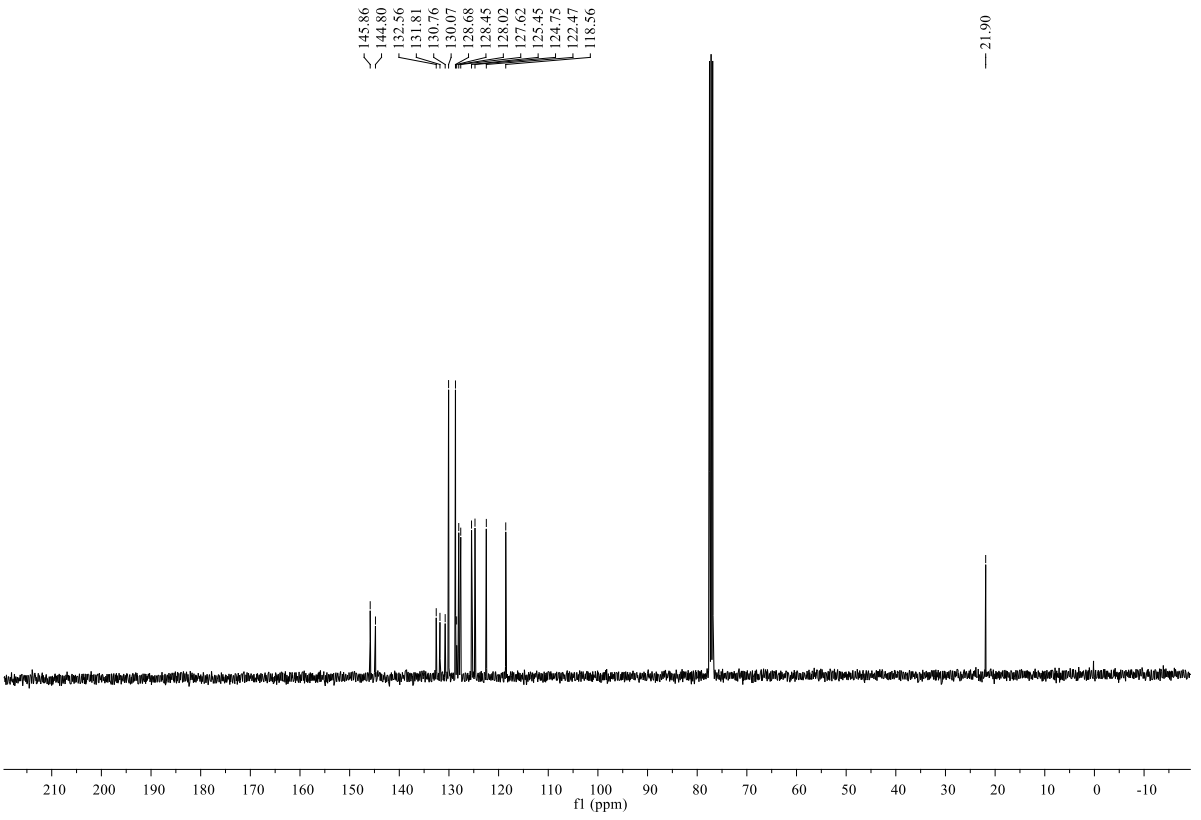

8.93
8.92
8.92
8.91
2.45
OTs
N
1i
8.11
8.09
8.02
8.00
7.74
7.72
7.55
7.55
7.44
7.43
7.42
7.32
7.30
1.00
1.00
2.00
1.00
1.00
2.00
1.00
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3
f1 (ppm)
1.00
1.00
1.00
2.00
1.00
1.00
2.00
1.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5
f1 (ppm)

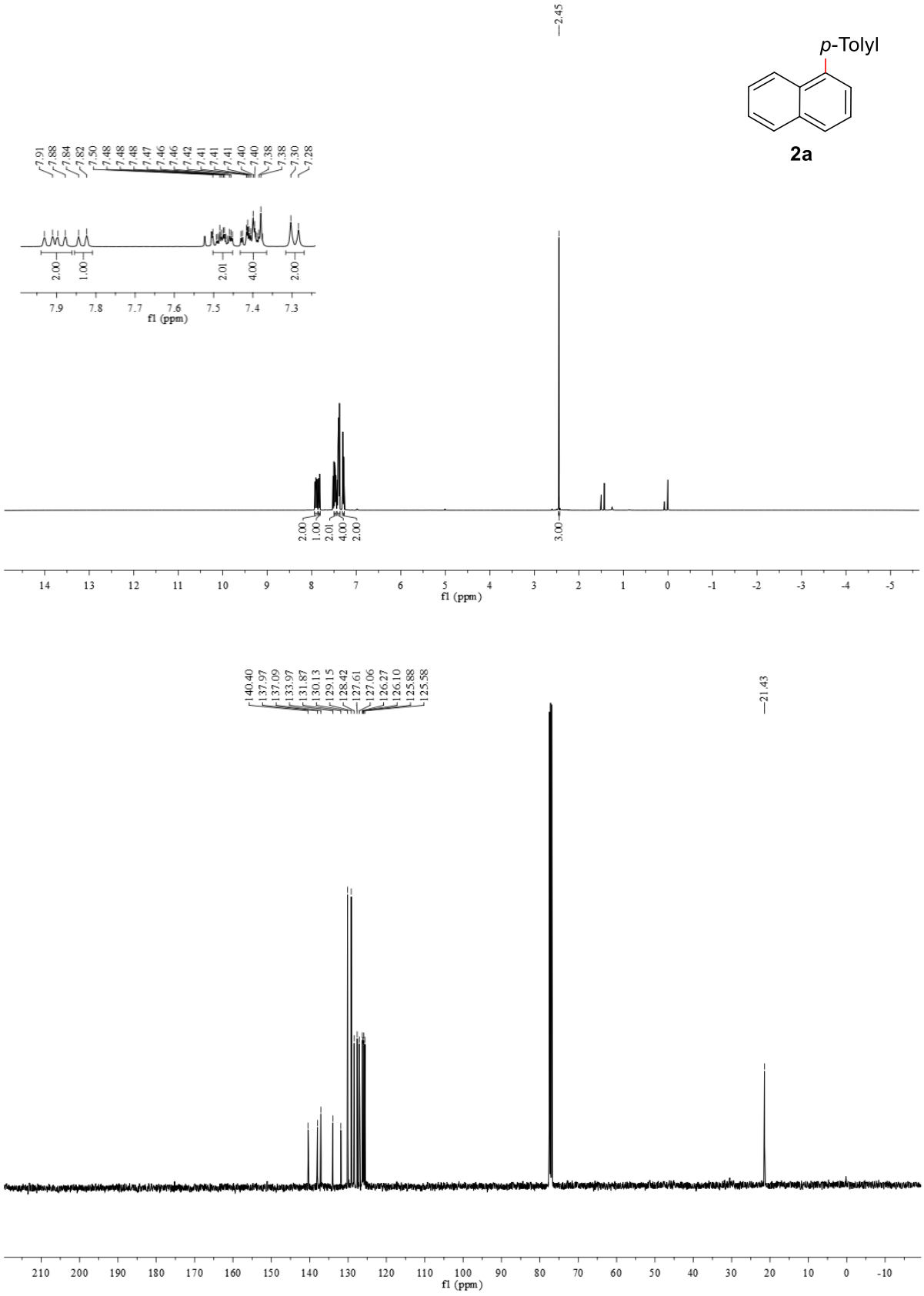

151.04
147.36
146.74
145.83
136.18
132.24
131.54
130.04
128.66
128.46
124.78
122.01
120.13
21.88
1.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

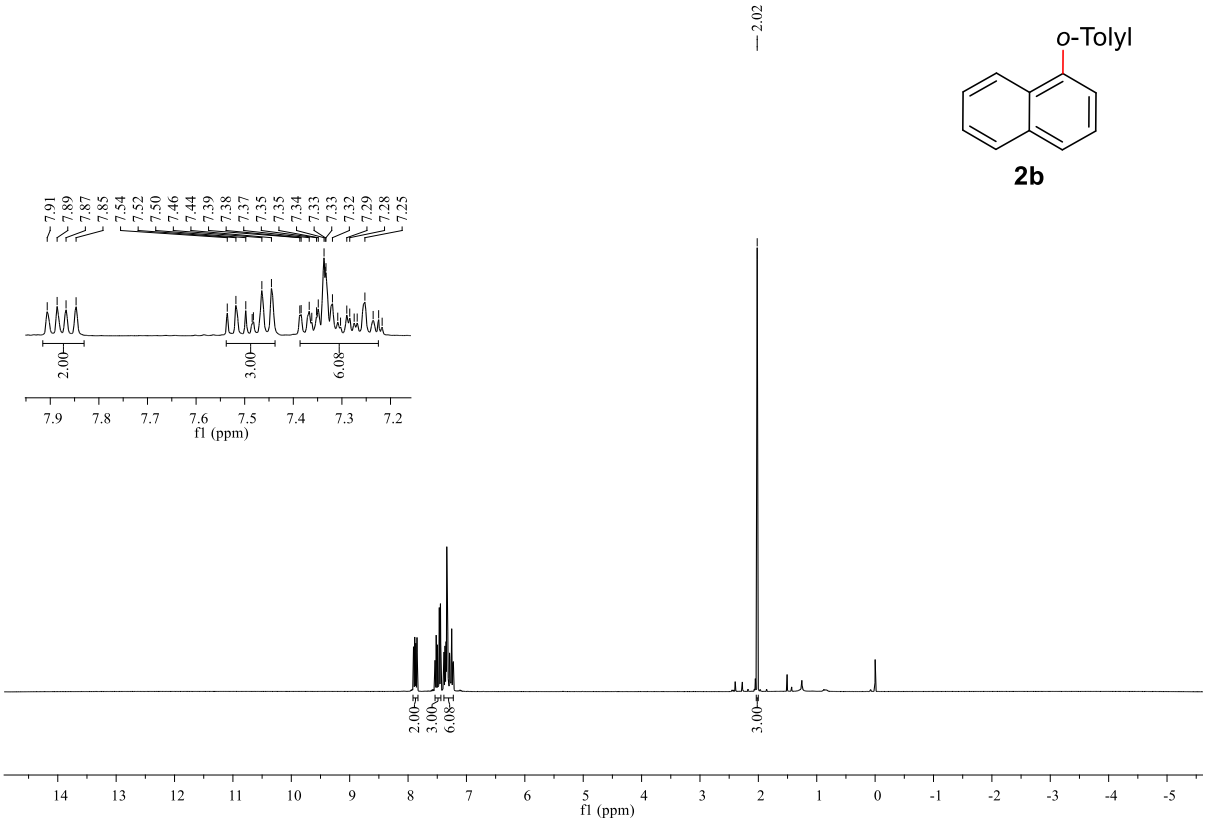

7.74
7.73
7.72
7.71
7.38
7.33
7.31
7.13
7.12
7.11
7.10
2.46
TsO
OTs
1j
6.00
2.00
4.00
2.00
6.00
f1 (ppm)

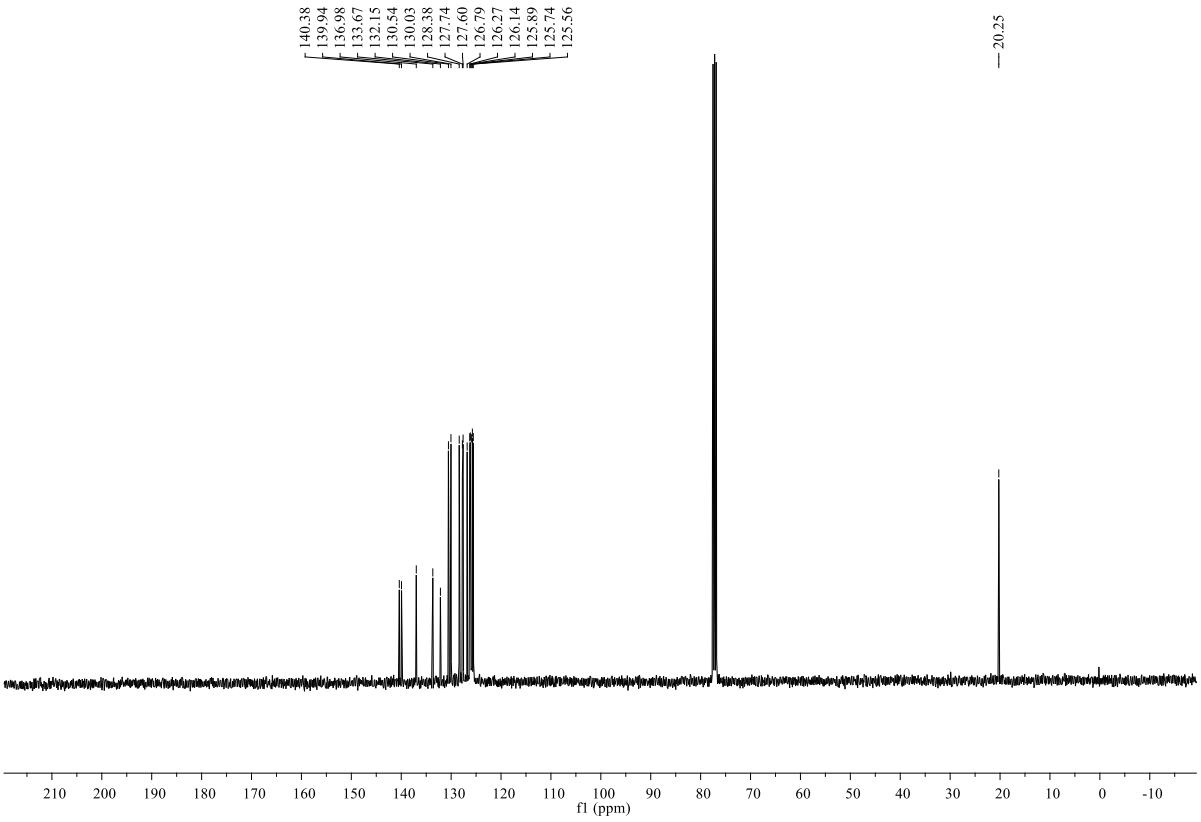

148.13
145.81
133.86
132.41
130.45
130.06
129.86
128.65
121.95
120.05
21.94
f1 (ppm)

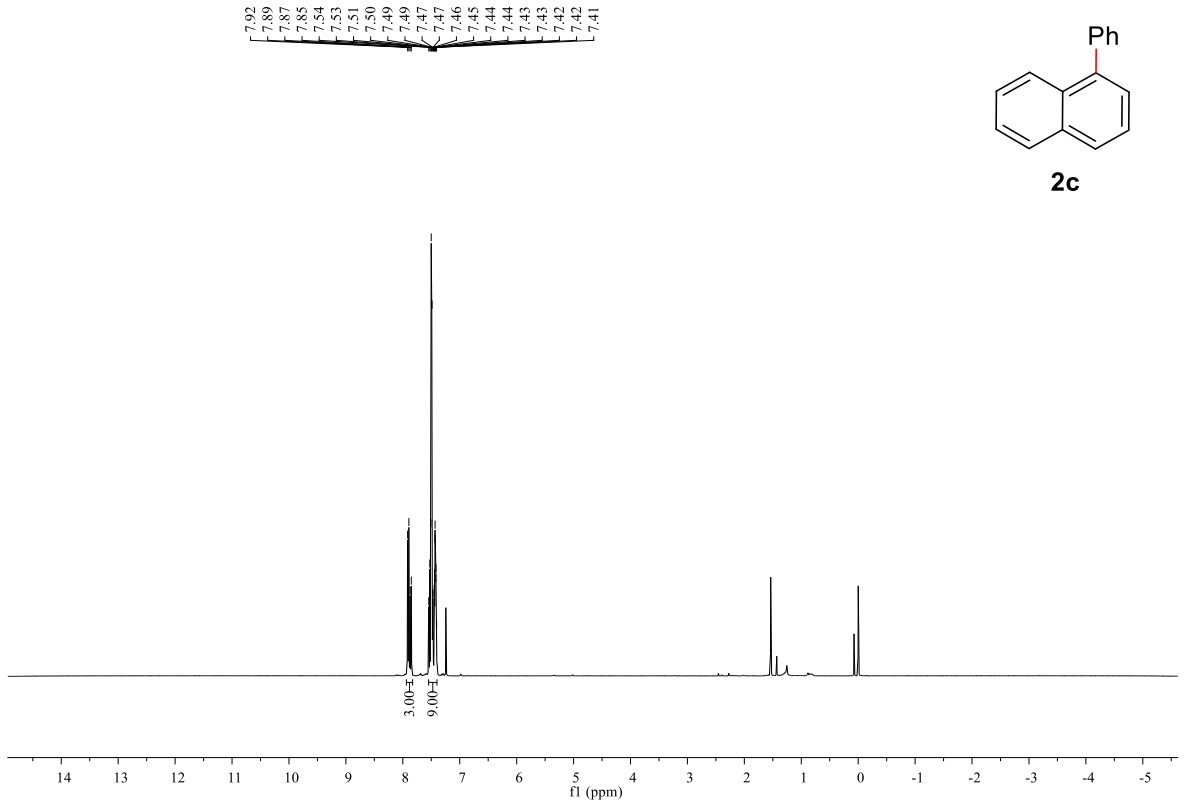

OTs
Cl
1k
2.42
8.22
8.20
7.93
7.91
7.78
7.76
7.51
7.51
7.49
7.49
7.47
7.45
7.30
7.28
7.14
7.12
1.00
1.00
2.00
1.00
2.00
2.00
1.00
3.00
f1 (ppm)

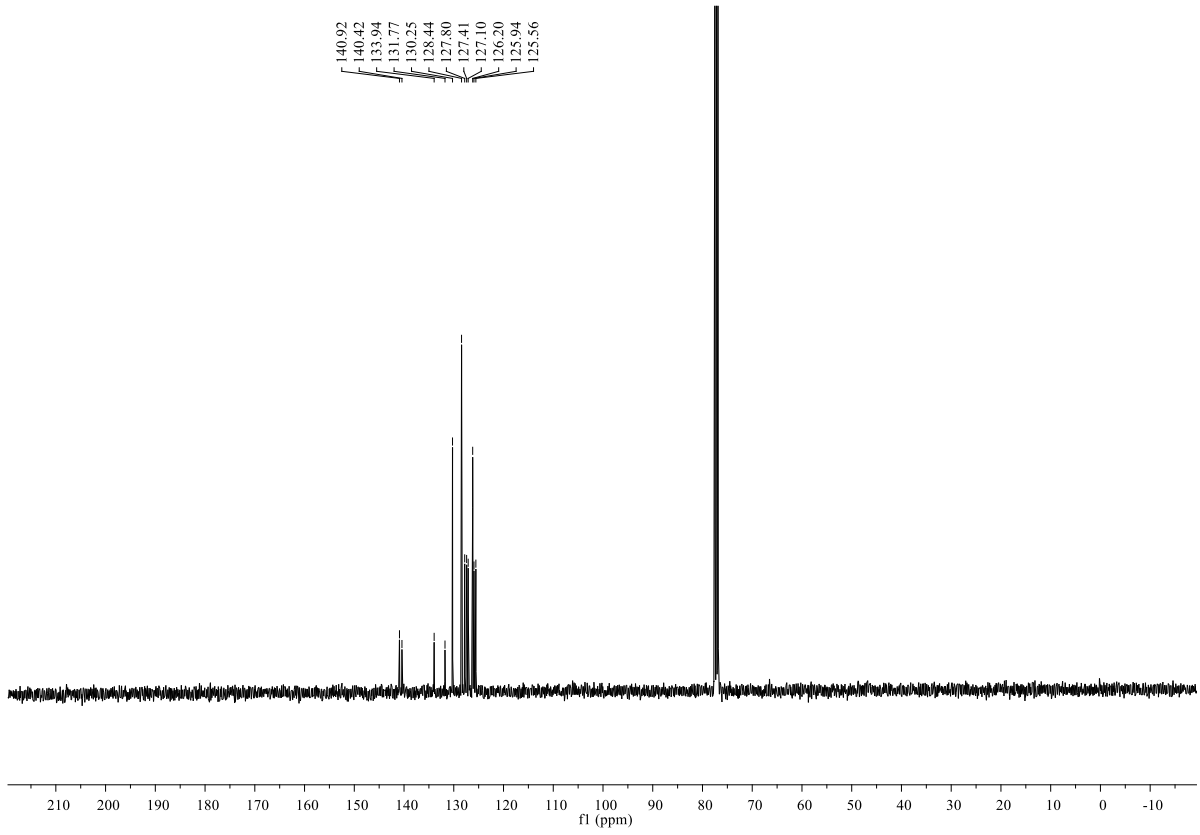

145.86
144.80
132.56
131.81
130.76
130.07
128.68
128.45
128.02
127.62
125.45
124.75
122.47
118.56
21.90
f1 (ppm)

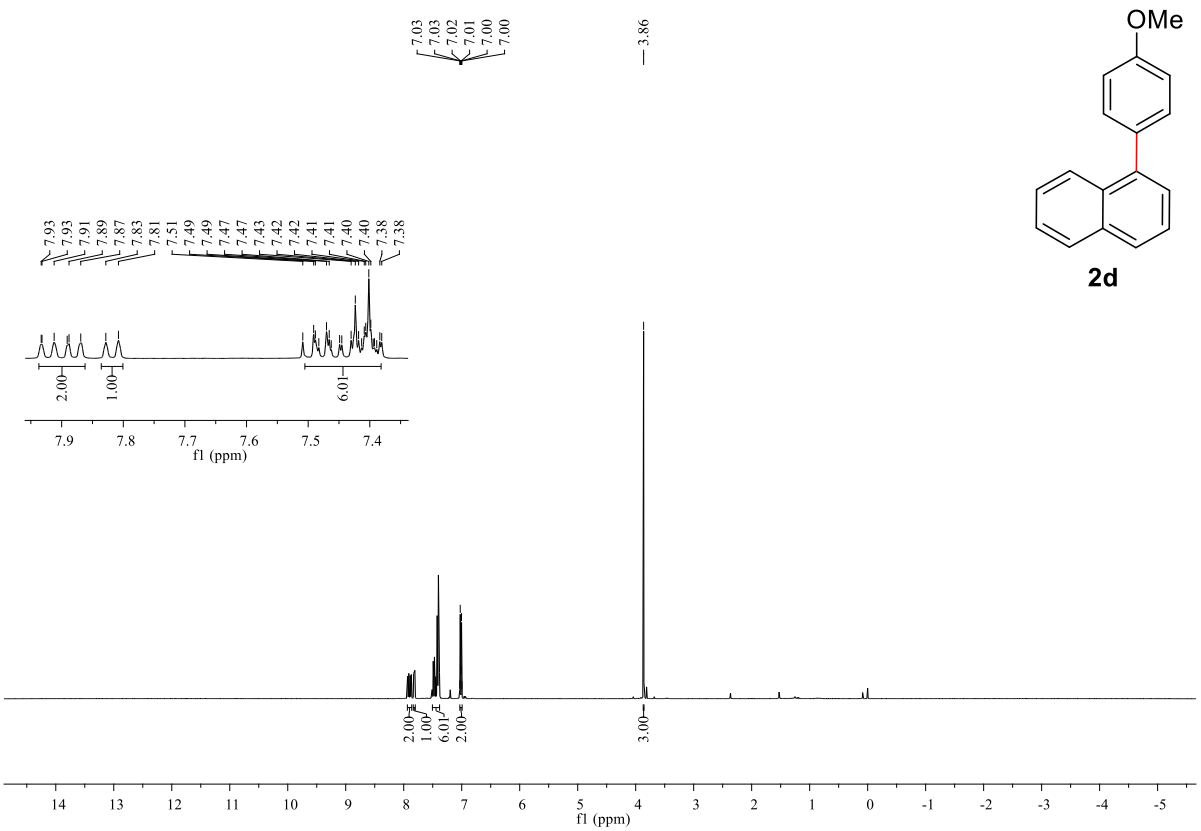

2.45
p-Tolyl
2a
7.91
7.88
7.84
7.82
7.50
7.48
7.48
7.48
7.47
7.46
7.46
7.42
7.41
7.41
7.41
7.40
7.40
7.38
7.38
7.30
7.28
2.00
1.00
2.01
4.00
2.00
7.9
7.8
7.7
7.6
7.5
7.4
7.3
f1 (ppm)
2.00
1.00
2.01
4.00
2.00
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)
140.40
137.97
137.09
133.97
131.87
130.13
129.15
128.42
127.61
127.06
126.27
126.10
125.88
125.58
21.43
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

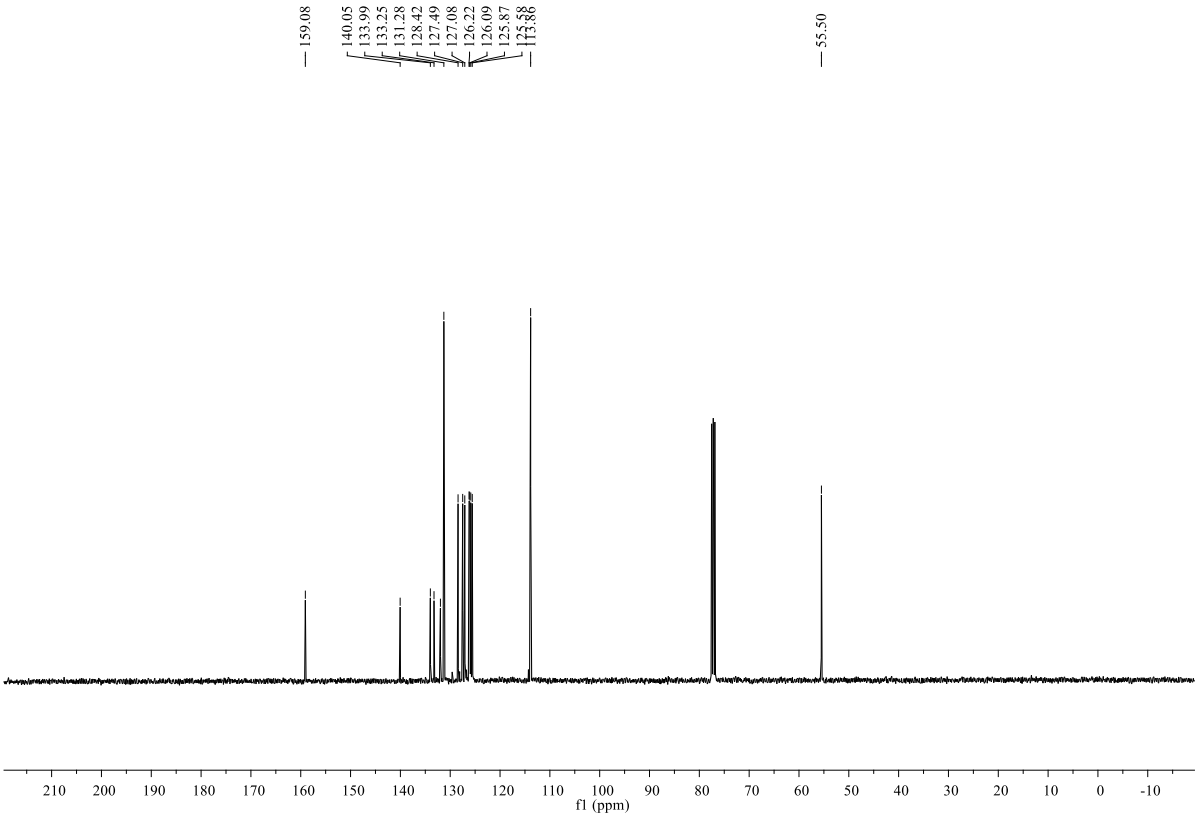

o-Tolyl
2b
2.02
7.91
7.89
7.87
7.85
7.54
7.52
7.50
7.46
7.44
7.39
7.38
7.37
7.35
7.35
7.34
7.33
7.33
7.32
7.29
7.28
7.25
2.00
3.00
6.08
f1 (ppm)
3.00

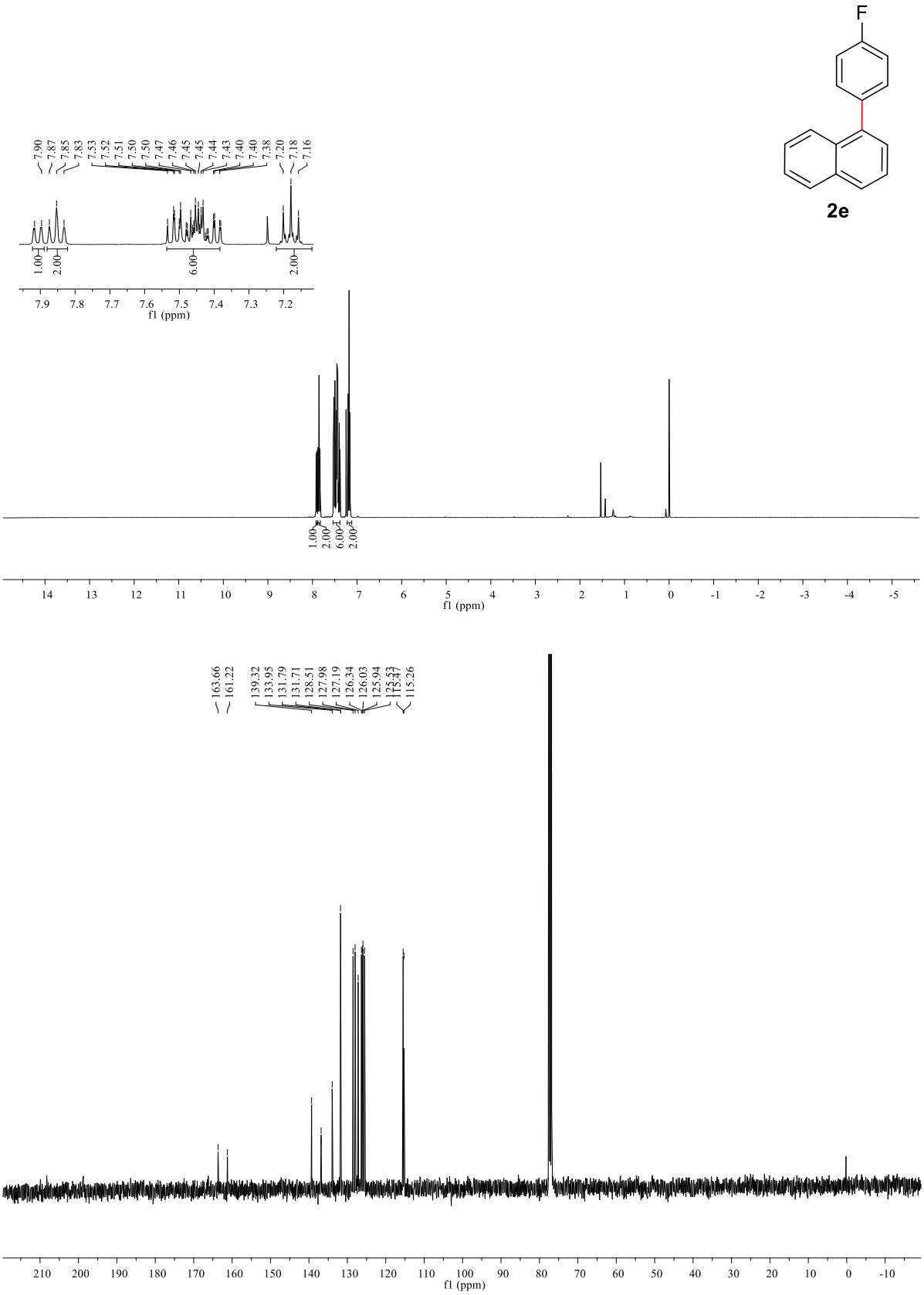

140.38
139.94
136.98
133.67
132.15
130.54
130.03
128.38
127.74
127.60
126.79
126.27
126.14
125.89
125.74
125.56
20.25
f1 (ppm)

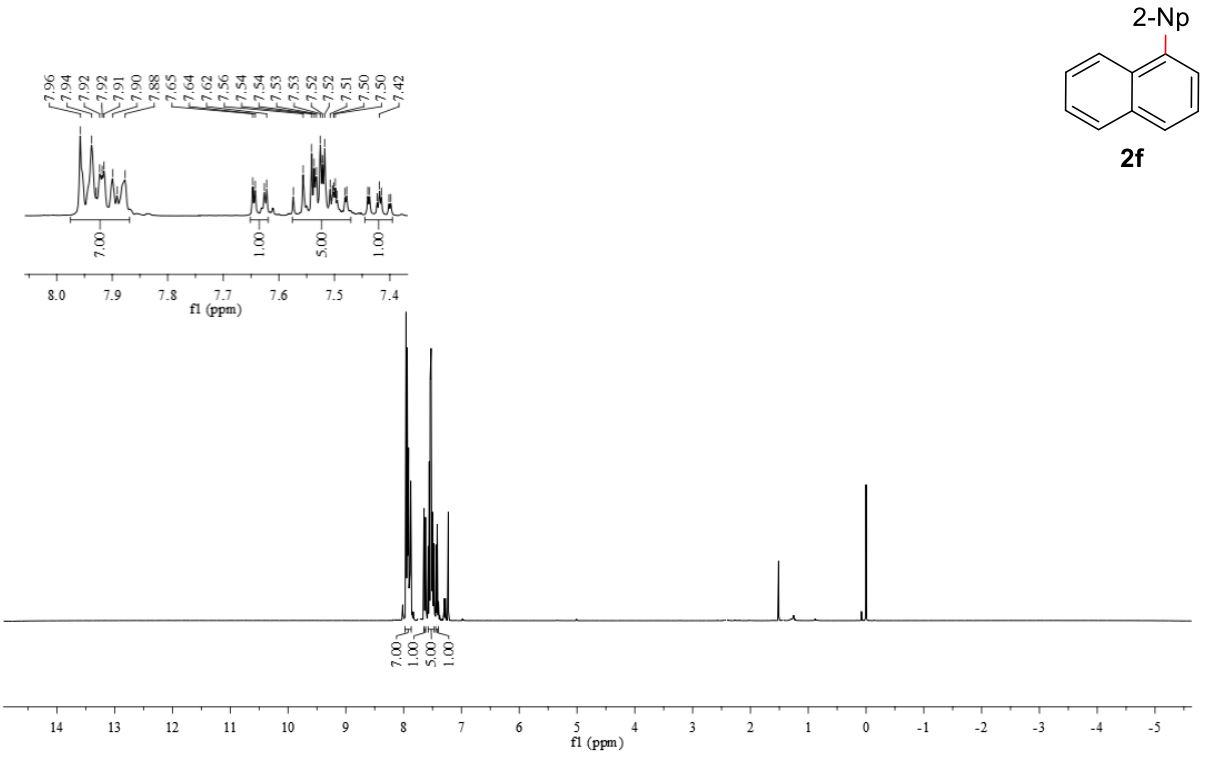

7.92
7.89
7.87
7.85
7.54
7.53
7.51
7.50
7.49
7.49
7.47
7.47
7.46
7.45
7.44
7.44
7.43
7.43
7.42
7.42
7.41
Ph
2c
3.00
9.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5
f1 (ppm)

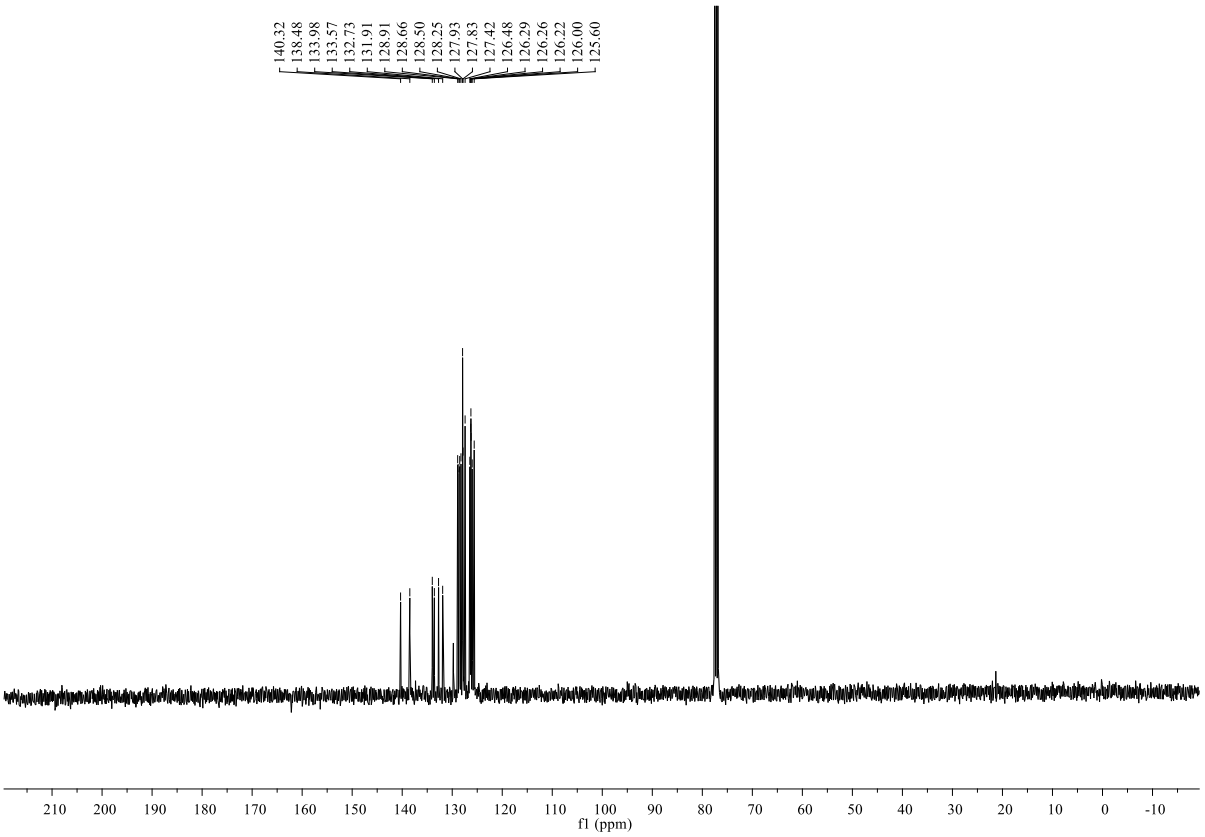

140.92
140.42
133.94
131.77
130.25
128.44
127.80
127.41
127.10
126.20
125.94
125.56
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

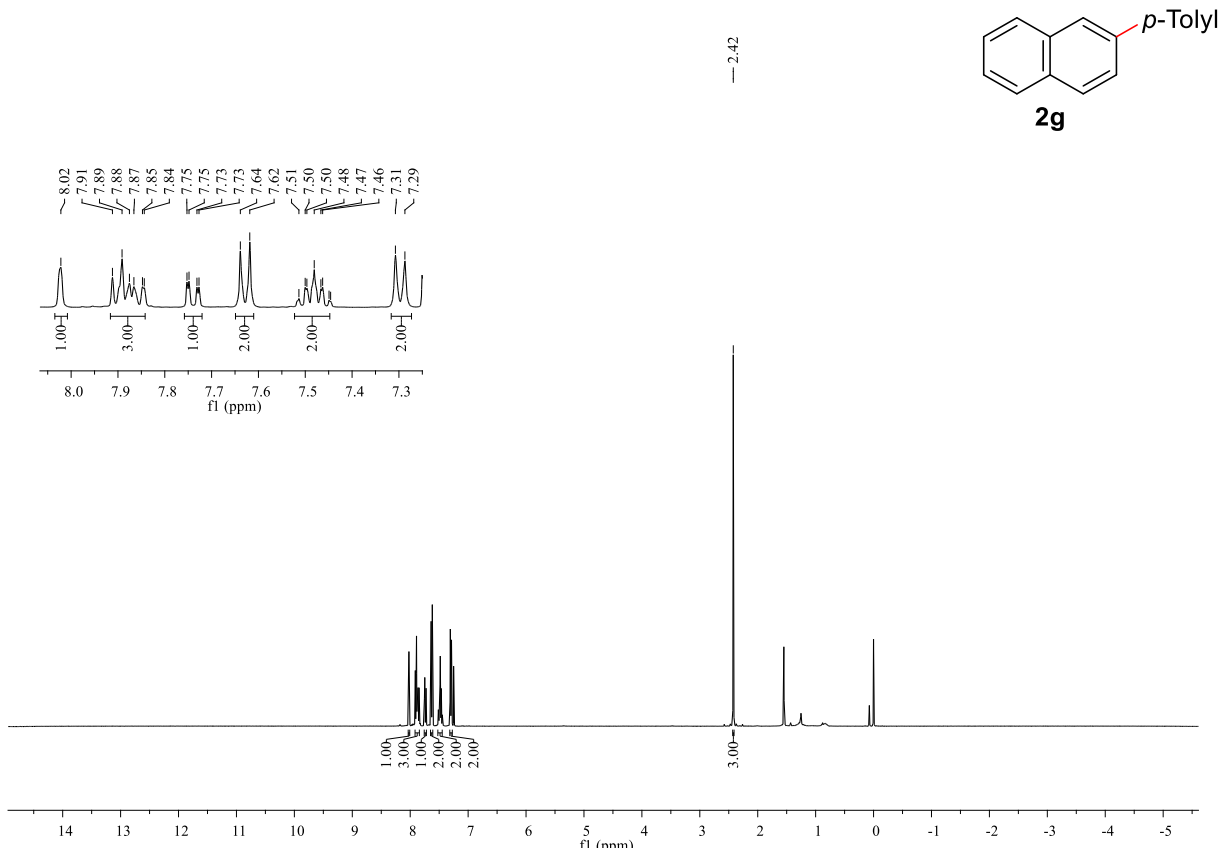

7.03
7.03
7.02
7.01
7.00
7.00
3.86
OMe
2d
7.93
7.93
7.91
7.89
7.87
7.83
7.81
7.51
7.49
7.49
7.47
7.47
7.43
7.42
7.42
7.41
7.41
7.40
7.40
7.38
7.38
2.00
1.00
6.01
7.9
7.8
7.7
7.6
7.5
7.4
f1 (ppm)
2.00
1.00
6.01
2.00
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)

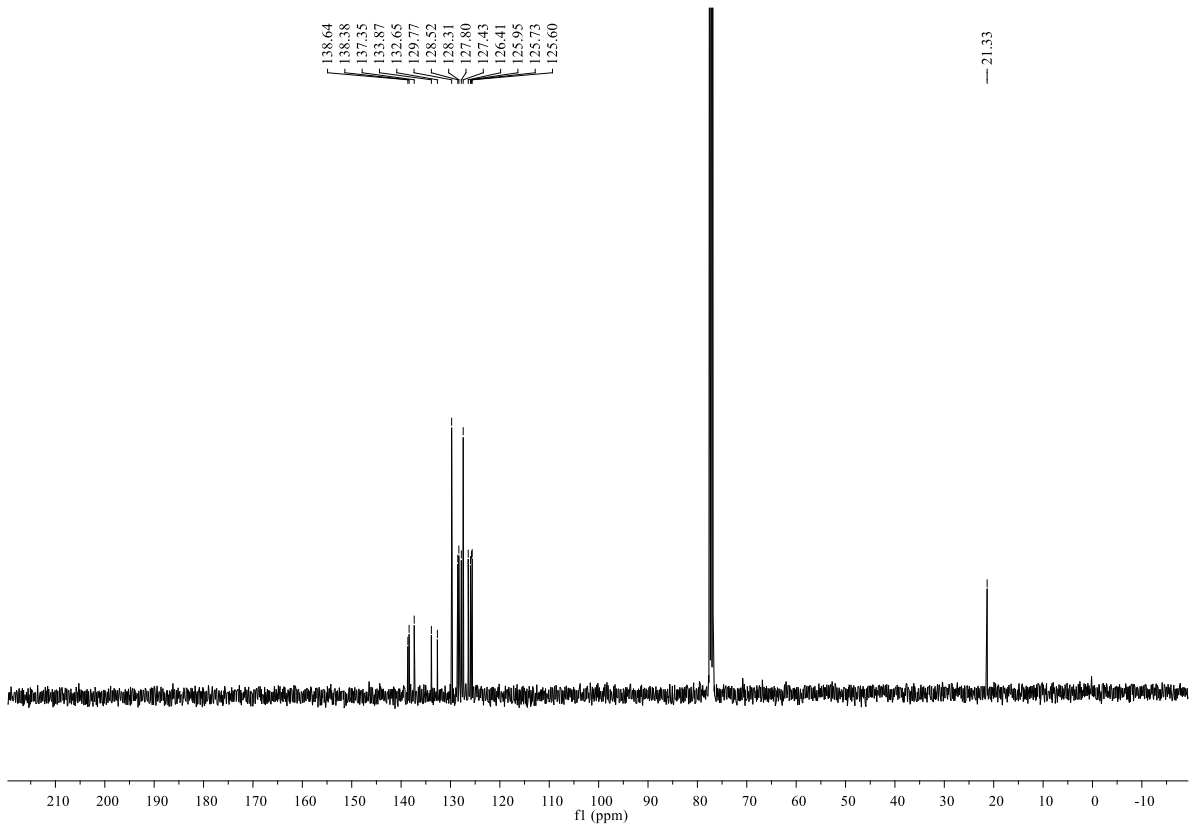

159.08
140.05
133.99
133.25
131.28
128.42
127.49
127.08
126.22
126.09
125.87
123.58
113.86
55.50
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

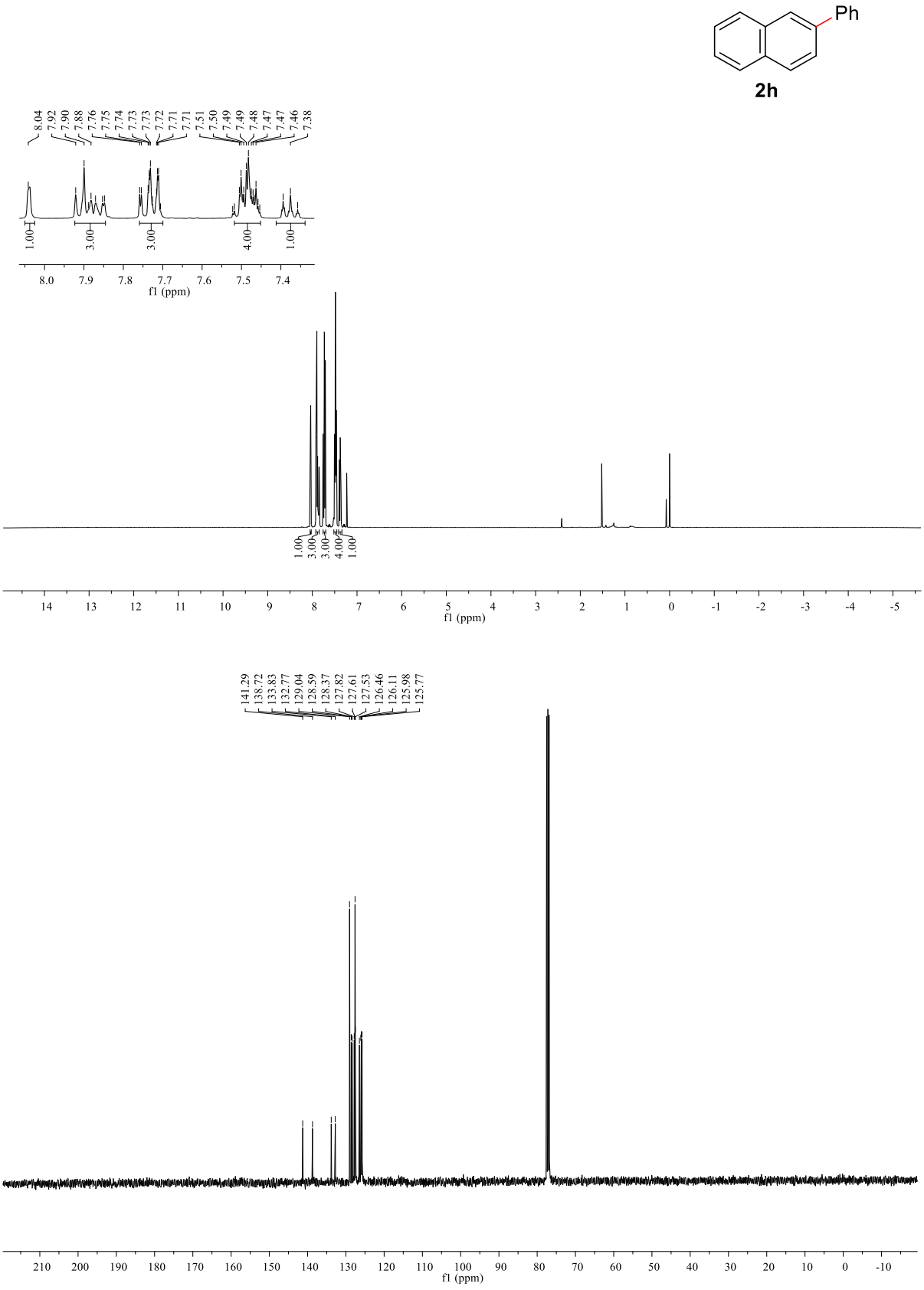

F
2e
7.90
7.87
7.85
7.83
7.53
7.52
7.51
7.50
7.50
7.47
7.46
7.45
7.45
7.44
7.43
7.40
7.40
7.38
7.20
7.18
7.16
1.00
2.00
6.00
2.00
f1 (ppm)
163.66
161.22
139.32
133.95
131.79
131.71
128.51
127.98
127.19
126.34
126.03
125.94
115.47
115.26

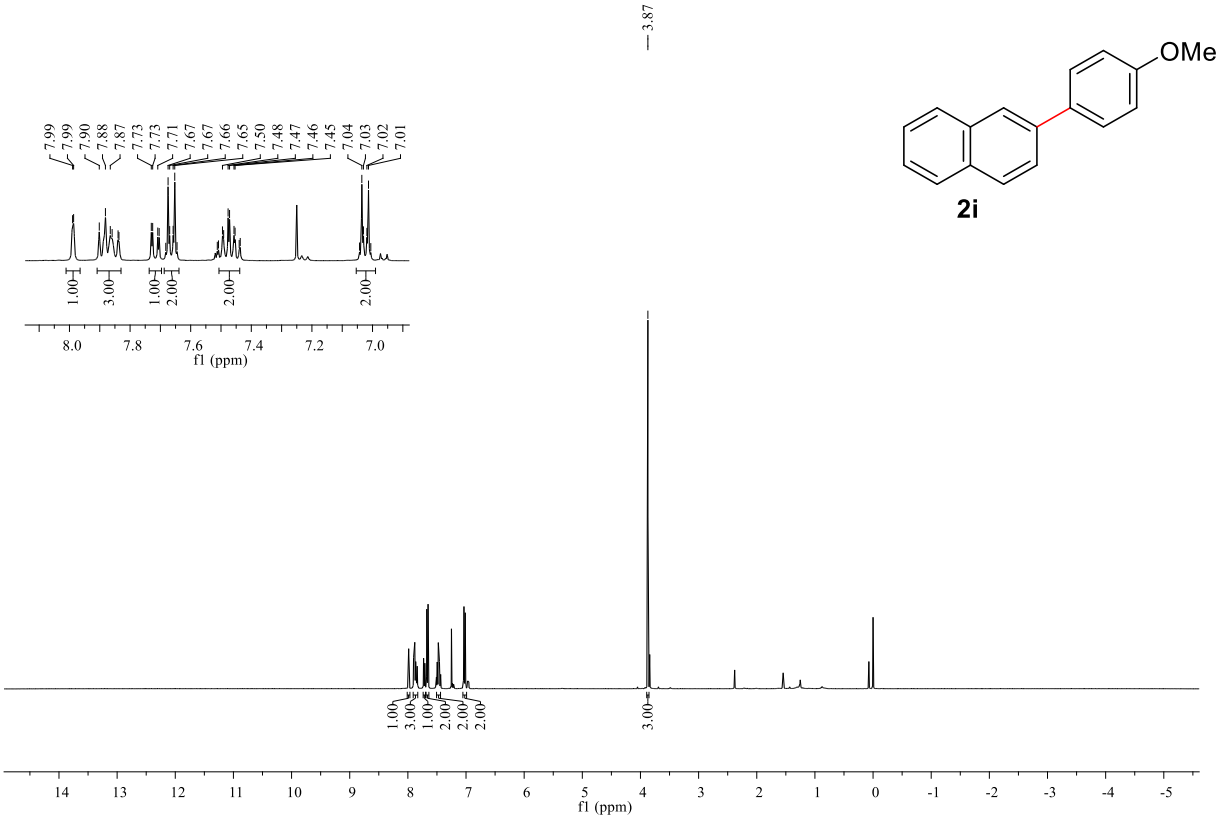

2-Np
2f
7.96
7.94
7.92
7.92
7.91
7.90
7.88
7.65
7.64
7.62
7.56
7.54
7.54
7.53
7.53
7.52
7.52
7.51
7.50
7.50
7.42
7.00
1.00
5.00
1.00
f1 (ppm)


140.32
138.48
133.98
133.57
132.73
131.91
128.91
128.66
128.50
128.25
127.93
127.83
127.42
126.48
126.29
126.26
126.22
126.00
125.60
f1 (ppm)


p-Tolyl
2g
2.42
8.02
7.91
7.89
7.88
7.87
7.85
7.84
7.75
7.75
7.73
7.73
7.64
7.62
7.51
7.50
7.50
7.48
7.47
7.46
7.31
7.29
1.00
3.00
1.00
2.00
2.00
2.00
f1 (ppm)
3.00


138.64
138.38
137.35
133.87
132.65
129.77
128.52
128.31
127.80
127.43
126.41
125.95
125.73
125.60
21.33
f1 (ppm)


Ph
2h
8.04
7.92
7.90
7.88
7.76
7.75
7.74
7.73
7.73
7.72
7.71
7.71
7.51
7.50
7.49
7.49
7.48
7.47
7.47
7.46
7.38
1.00
3.00
3.00
4.00
1.00
f1 (ppm)
141.29
138.72
133.83
132.77
129.04
128.59
128.37
127.82
127.61
127.53
126.46
126.11
125.98
125.77
f1 (ppm)


3.87
OMe
2i
7.99
7.99
7.90
7.88
7.87
7.73
7.73
7.71
7.67
7.67
7.66
7.65
7.50
7.48
7.47
7.46
7.45
7.04
7.03
7.02
7.01
1.00
3.00
1.00
2.00
2.00
2.00
8.0
7.8
7.6
7.4
7.2
7.0
f1 (ppm)
1.00
3.00
1.00
2.00
2.00
2.00
3.00
14
13
12
11
10
9
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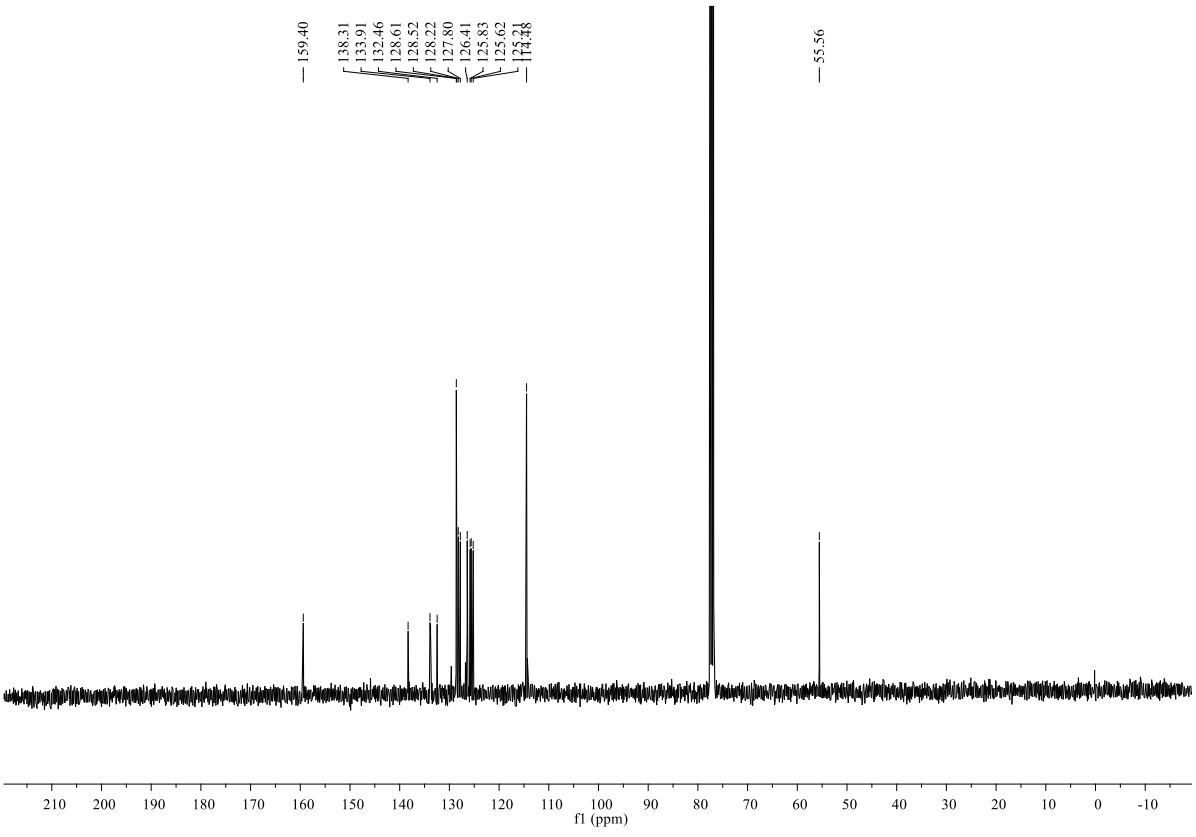
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)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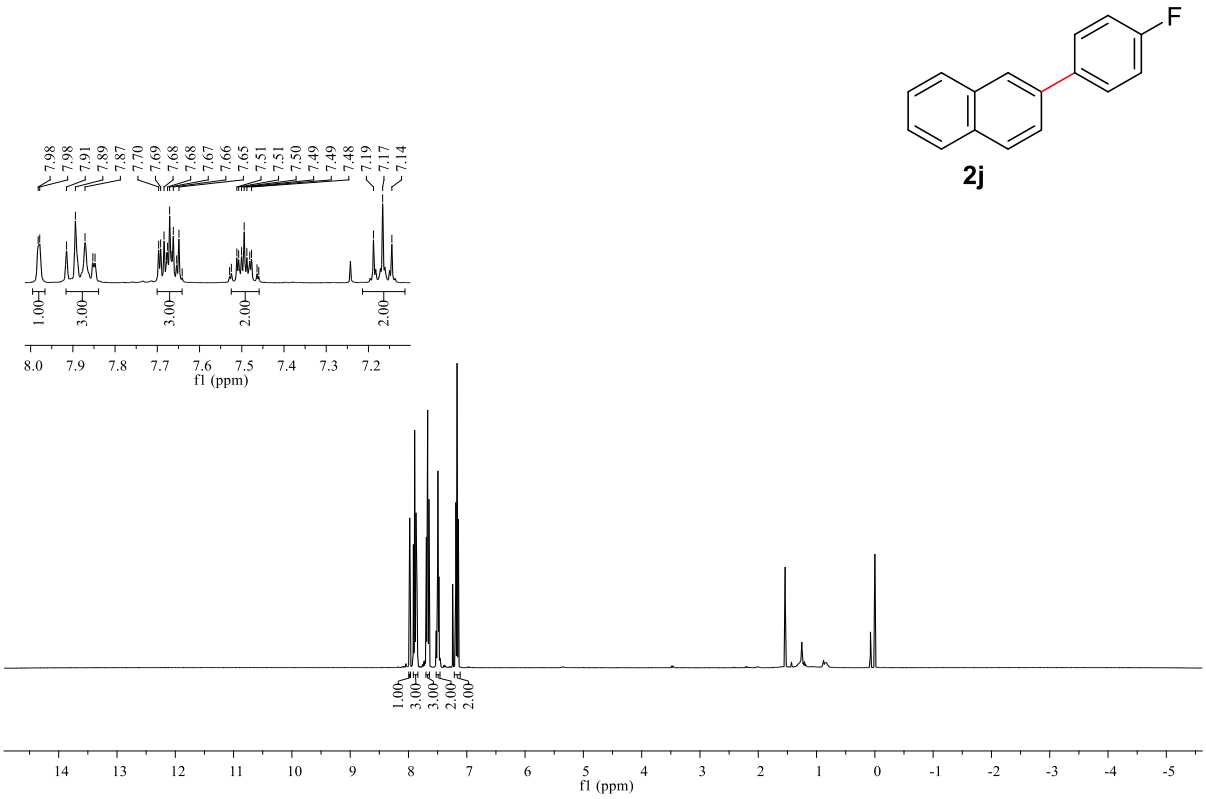
138.31
133.91
132.46
128.61
128.52
128.22
127.80
126.41
125.83
125.62
55.56
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


F
2j
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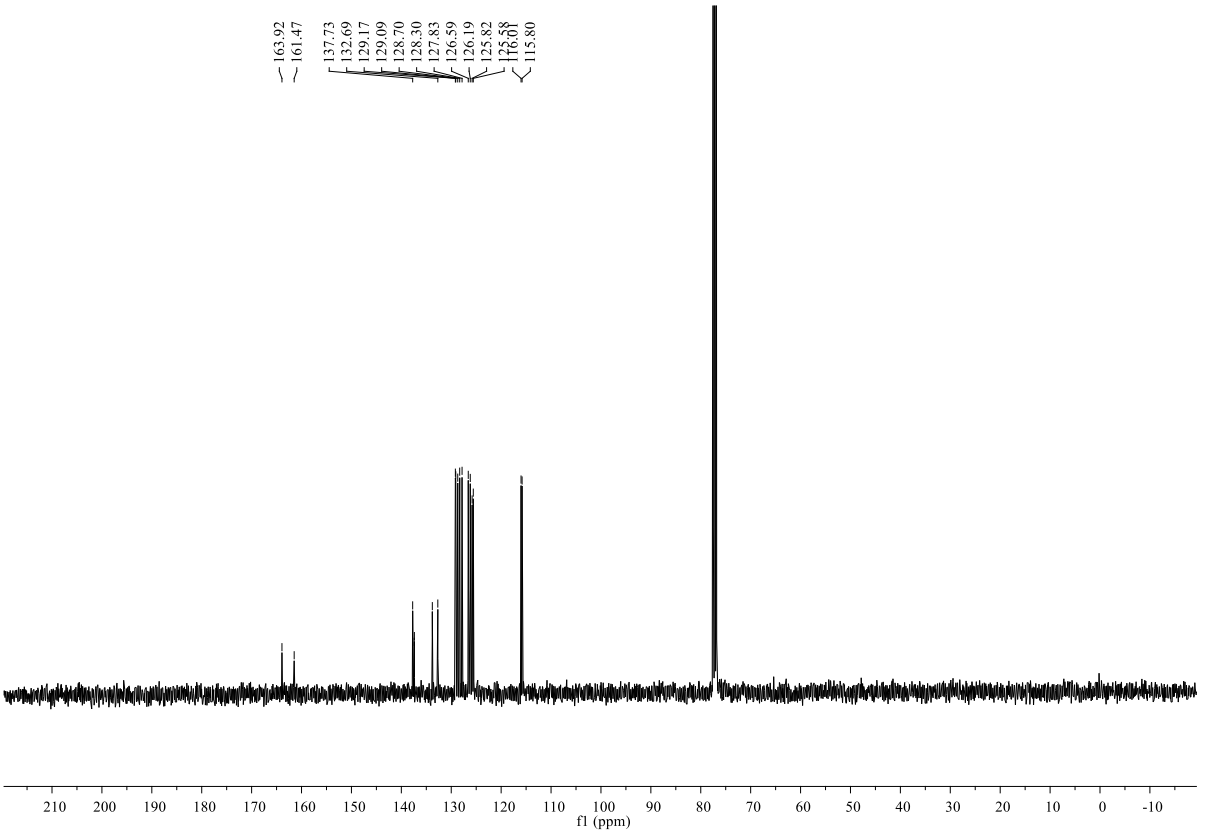
7.98
7.91
7.89
7.87
7.70
7.69
7.68
7.68
7.67
7.66
7.65
7.51
7.51
7.50
7.49
7.49
7.48
7.19
7.17
7.14
1.00
3.00
3.00
2.00
2.00
f1 (ppm)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132.69
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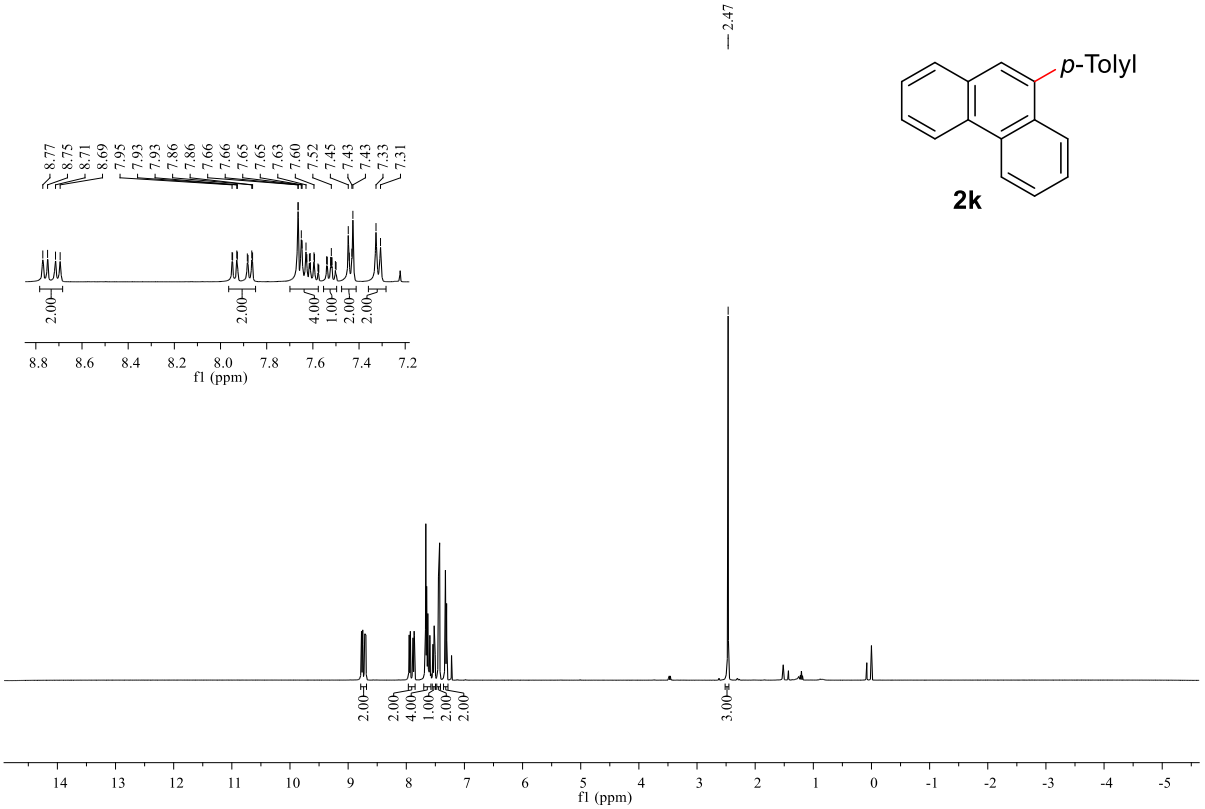
128.70
128.30
127.83
126.59
126.19
125.82
115.80
f1 (ppm)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p-Tolyl
2k
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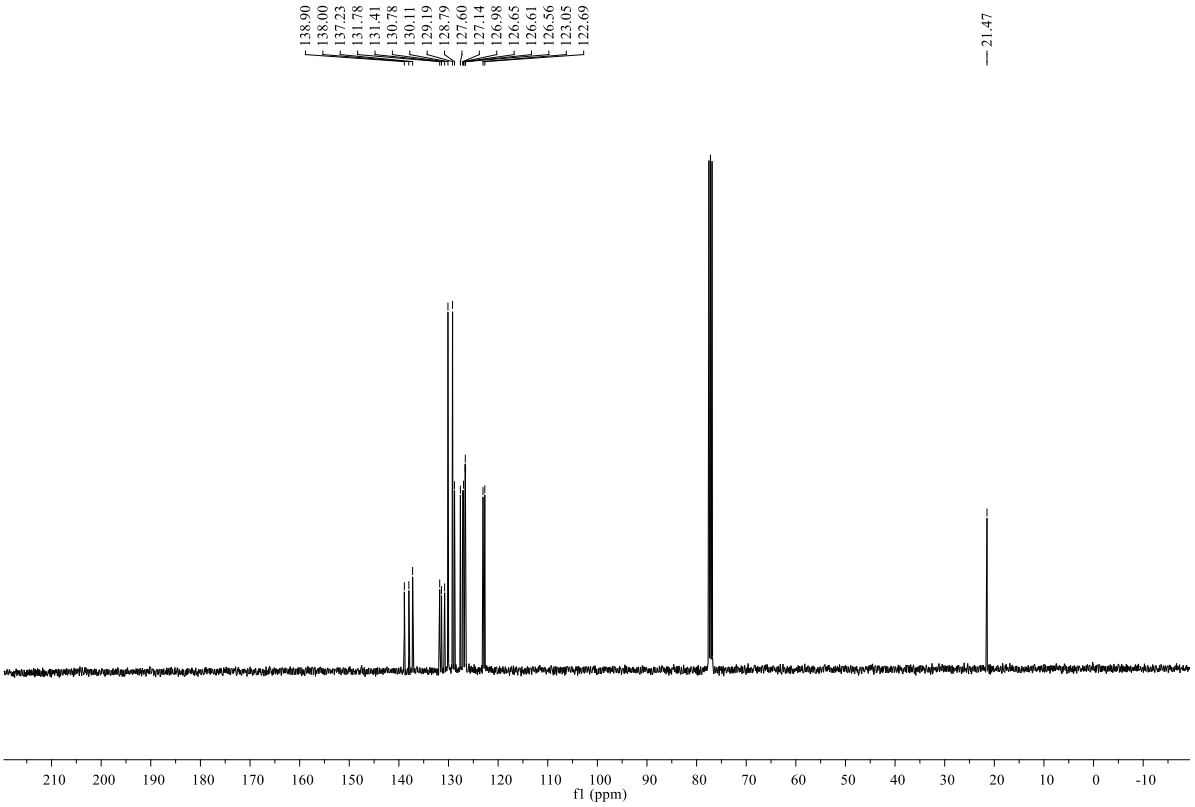
8.71
8.69
7.95
7.93
7.93
7.86
7.86
7.66
7.66
7.65
7.65
7.63
7.60
7.52
7.45
7.43
7.43
7.33
7.31
2.00
2.00
4.00
1.00
2.00
2.00
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
f1 (ppm)
2.00
2.00
4.00
1.00
2.00
2.00
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)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138.00
137.23
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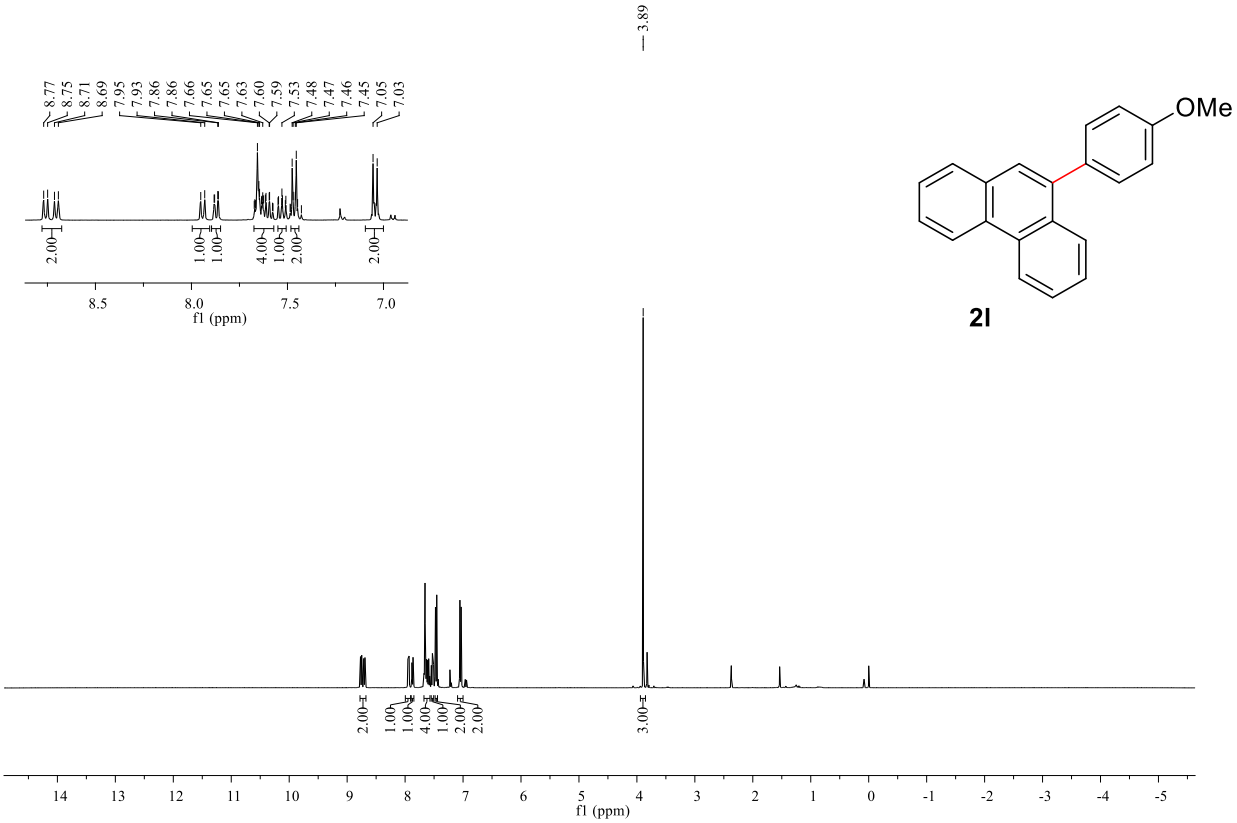
130.78
130.11
129.19
128.79
127.60
127.14
126.98
126.65
126.61
126.56
123.05
122.69
21.47
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


3.89
8.77
8.75
8.71
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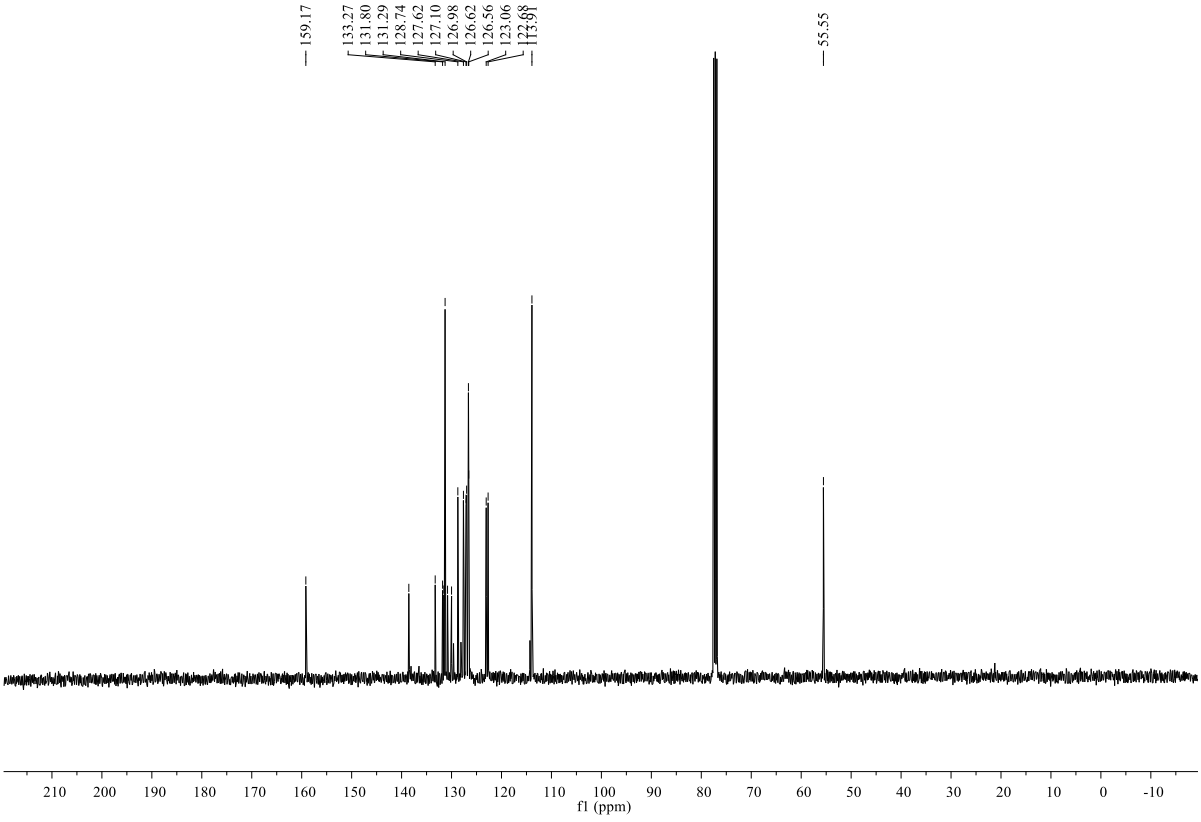
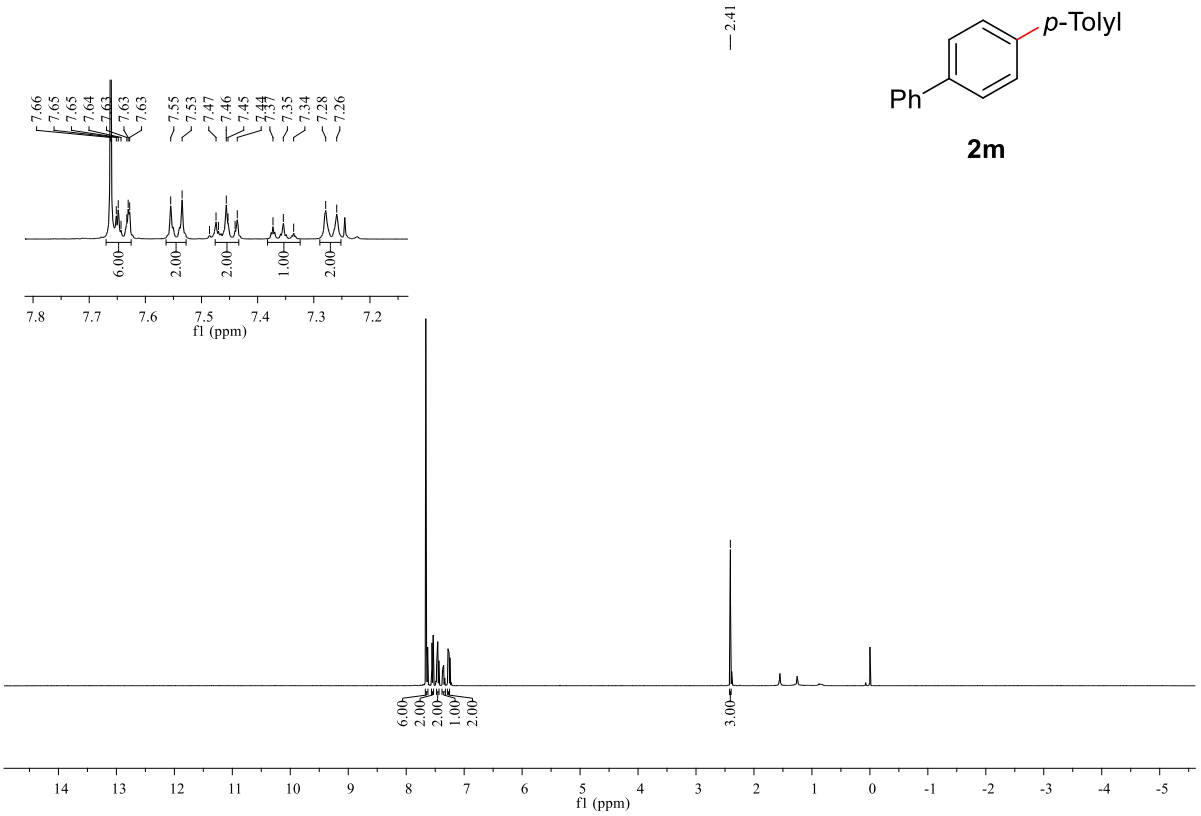
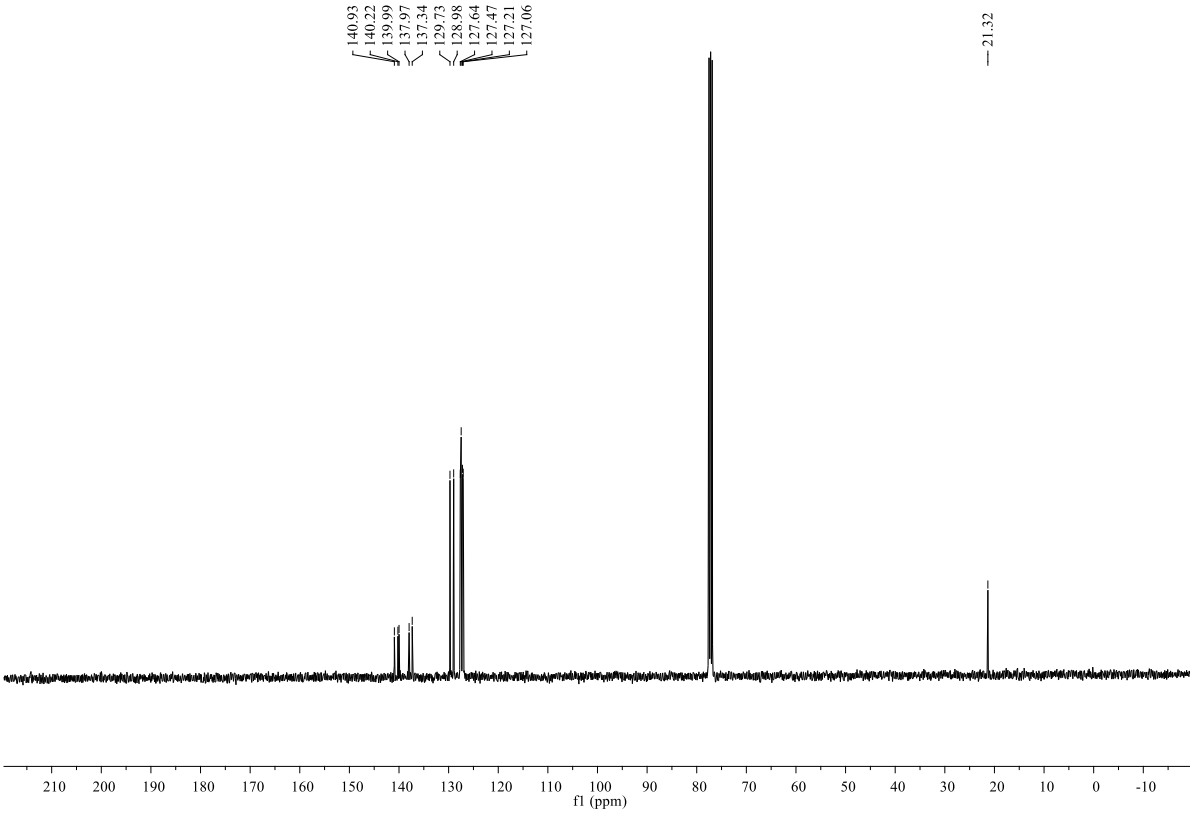
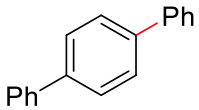
7.93
7.86
7.86
7.66
7.65
7.65
7.63
7.60
7.59
7.53
7.48
7.47
7.46
7.45
7.05
7.03
2.00
1.00
1.00
4.00
1.00
2.00
2.00
8.5
8.0
7.5
7.0
f1 (ppm)
OMe
2l
2.00
1.00
1.00
4.00
1.00
2.00
2.00
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)

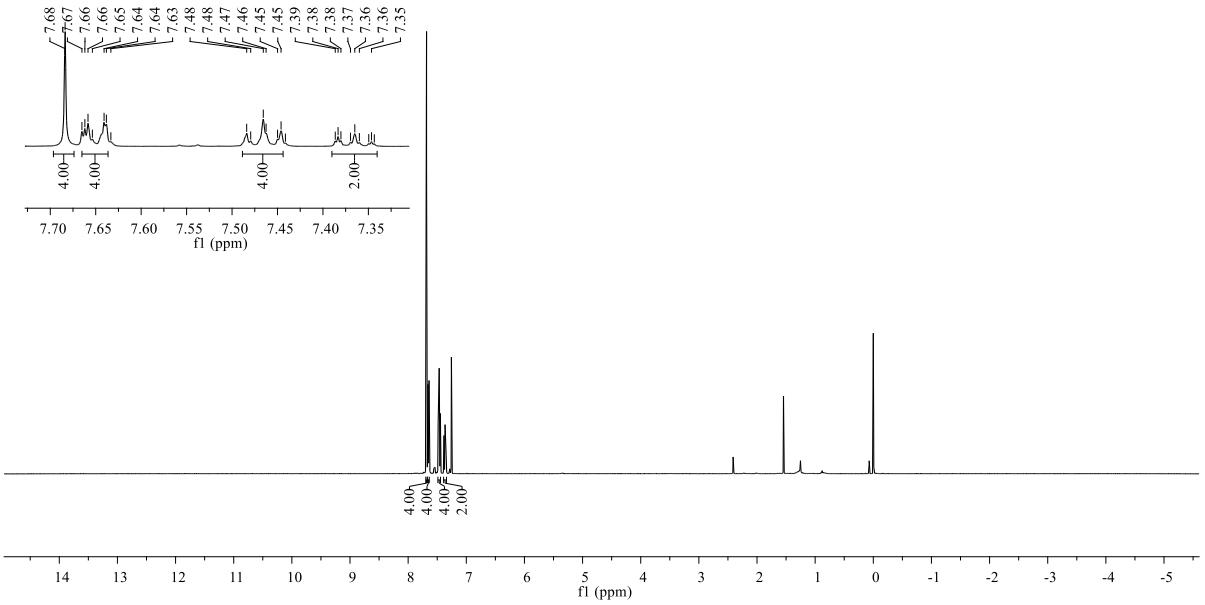

159.17
133.27
131.80
131.29
128.74
127.62
127.10
126.98
126.62
126.56
123.06
122.68
113.91
55.55
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

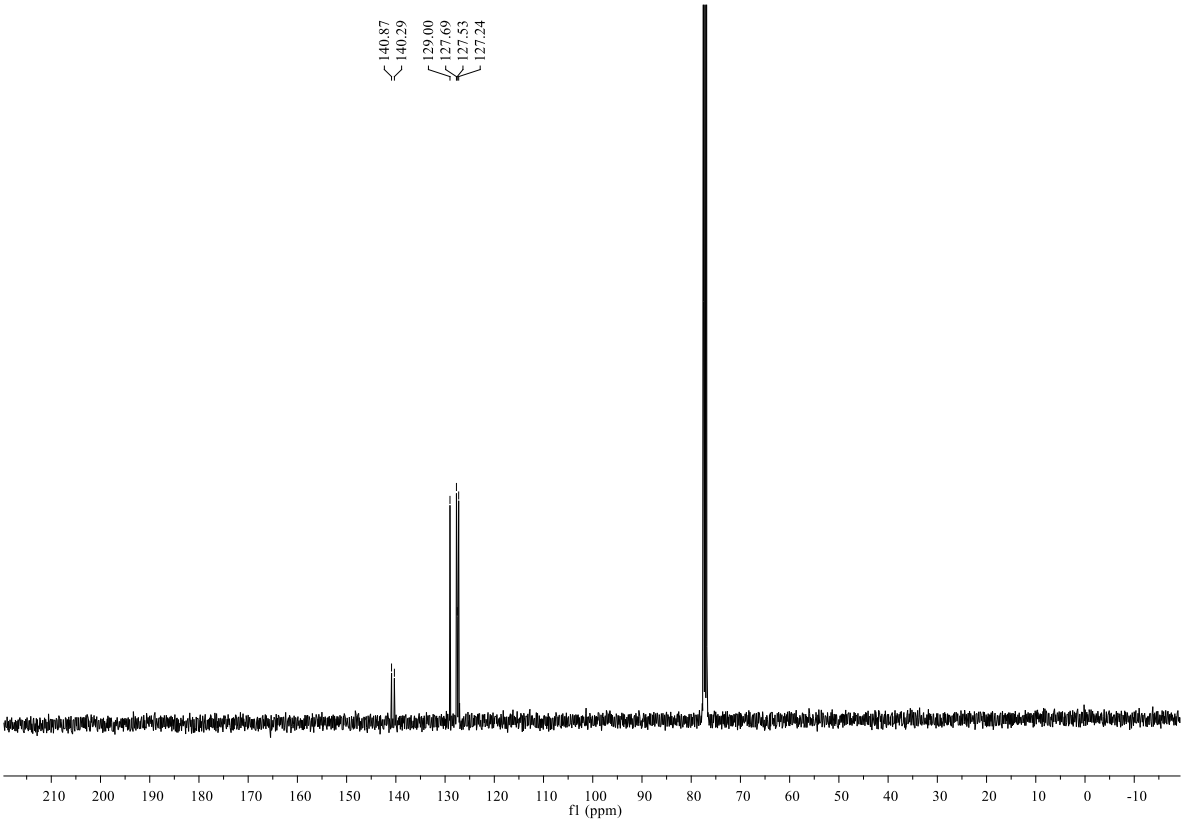

2.41
p-Tolyl
Ph
2m
7.66
7.65
7.65
7.64
7.63
7.63
7.63
7.55
7.53
7.47
7.46
7.45
7.44
7.37
7.35
7.34
7.28
7.26
6.00
2.00
2.00
1.00
2.00
7.8
7.7
7.6
7.5
7.4
7.3
7.2
f1 (ppm)
6.00
2.00
2.00
1.00
2.00
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)

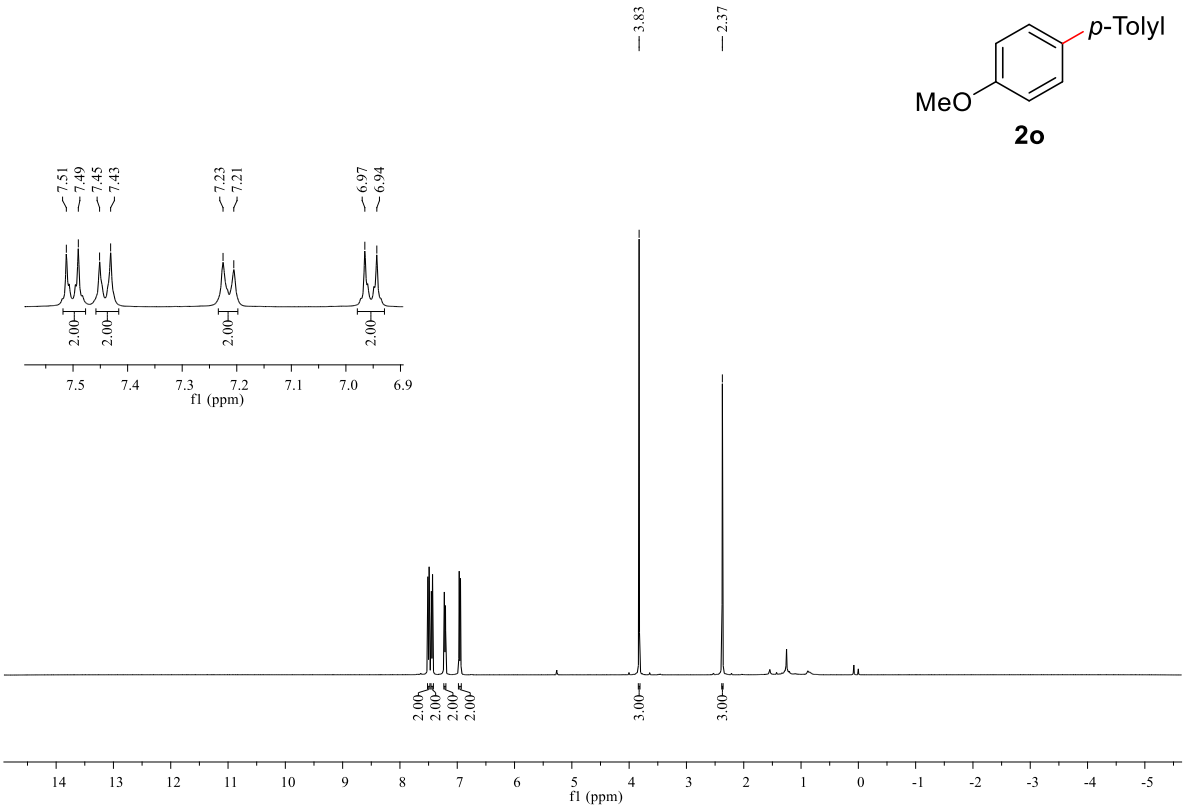

140.93
140.22
139.99
137.97
137.34
129.73
128.98
127.64
127.47
127.21
127.06
21.32
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

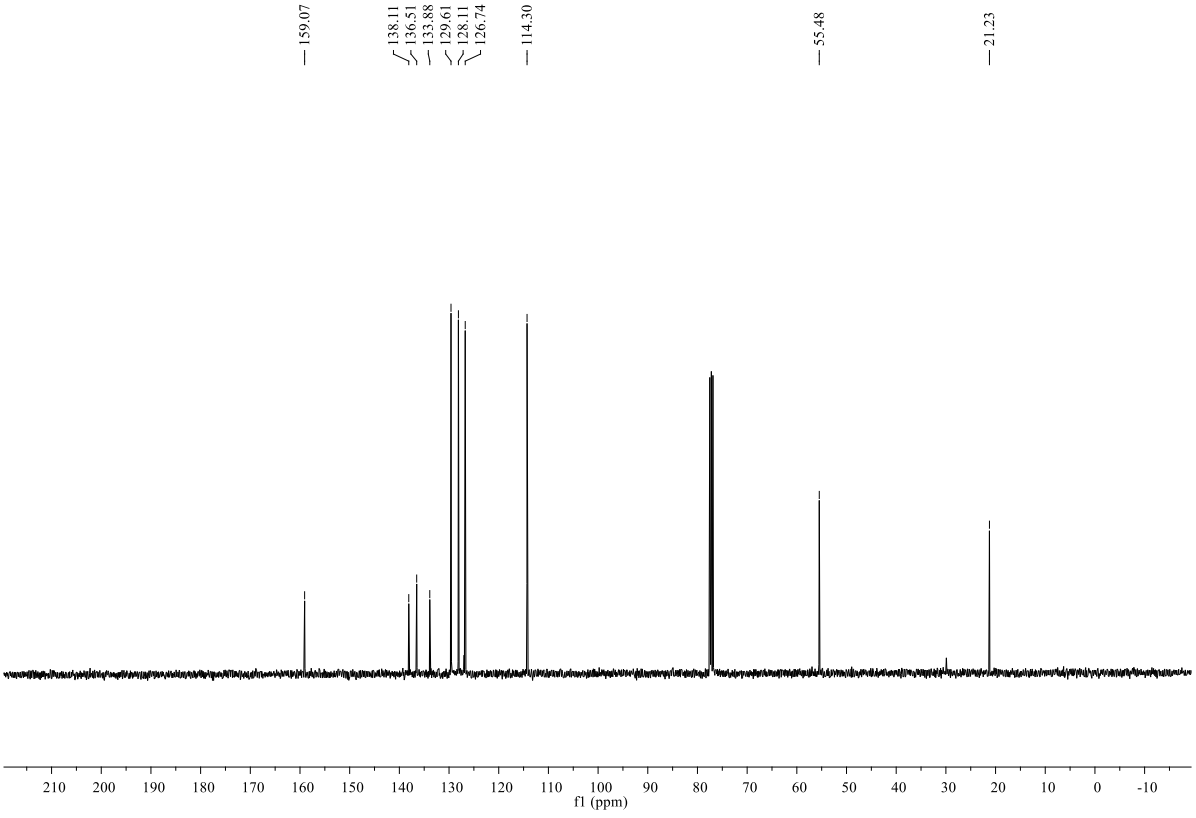

Ph
Ph

2n


7.68
7.67
7.66
7.66
7.65
7.64
7.64
7.63
7.48
7.48
7.47
7.46
7.45
7.45
7.39
7.38
7.38
7.37
7.36
7.36
7.35
4.00
4.00
4.00
2.00
7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35
f1 (ppm)
4.00
4.00
4.00
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5
f1 (ppm)


140.87
140.29
129.00
127.69
127.53
127.24
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)


3.83
2.37
p-Tolyl
MeO
2o
7.51
7.49
7.45
7.43
7.23
7.21
6.97
6.94
2.00
f1 (ppm)
3.00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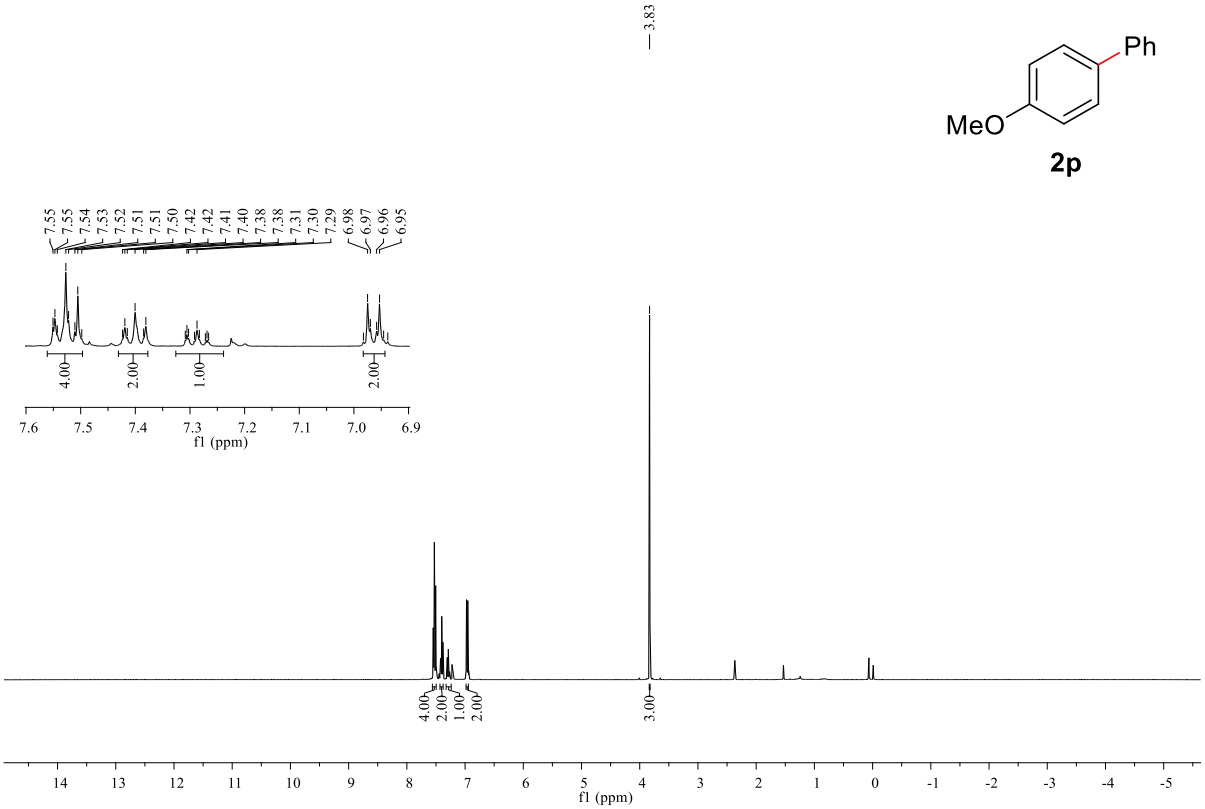
138.11
136.51
133.88
129.61
128.11
126.74
114.30
55.48
21.23
f1 (ppm)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Ph
MeO
2p
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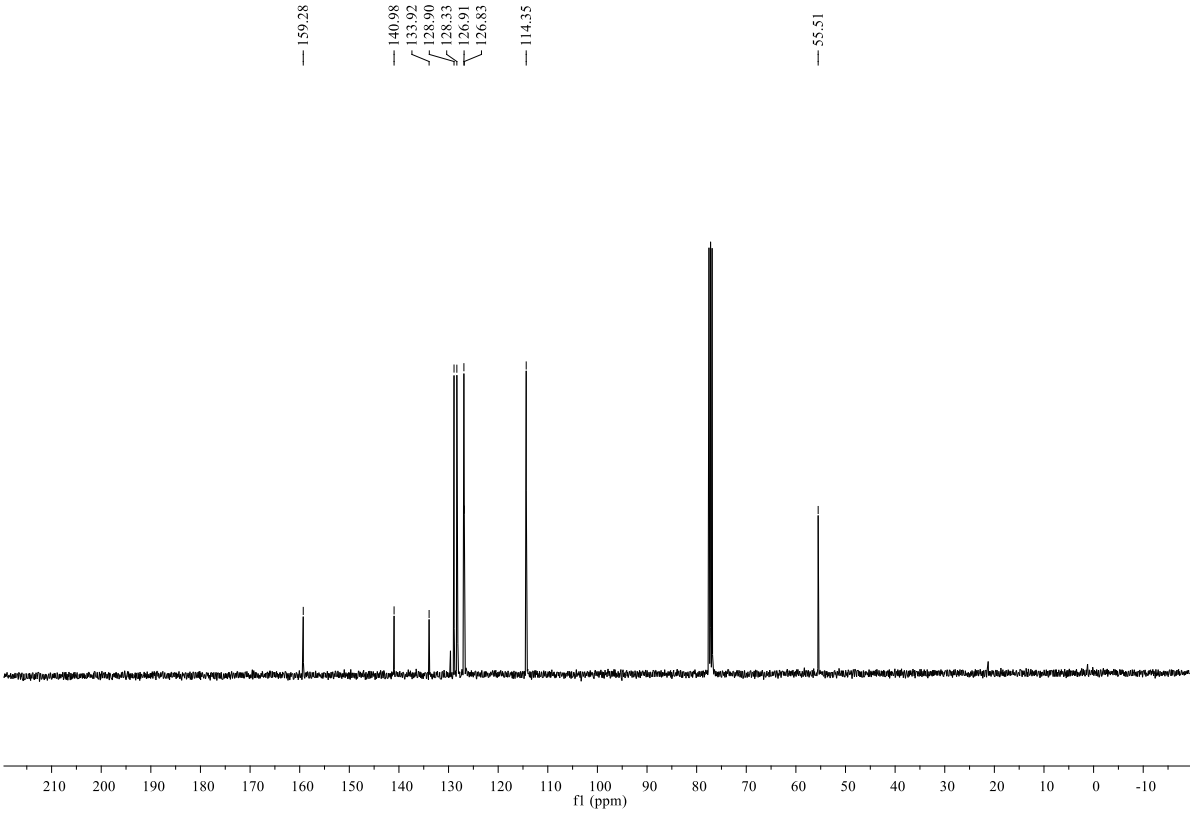
7.55
7.54
7.53
7.52
7.51
7.51
7.50
7.42
7.42
7.41
7.40
7.38
7.38
7.31
7.30
7.29
6.98
6.97
6.96
6.95
4.00
2.00
1.00
2.00
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
4.00
2.00
1.00
2.00
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)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140.98
133.92
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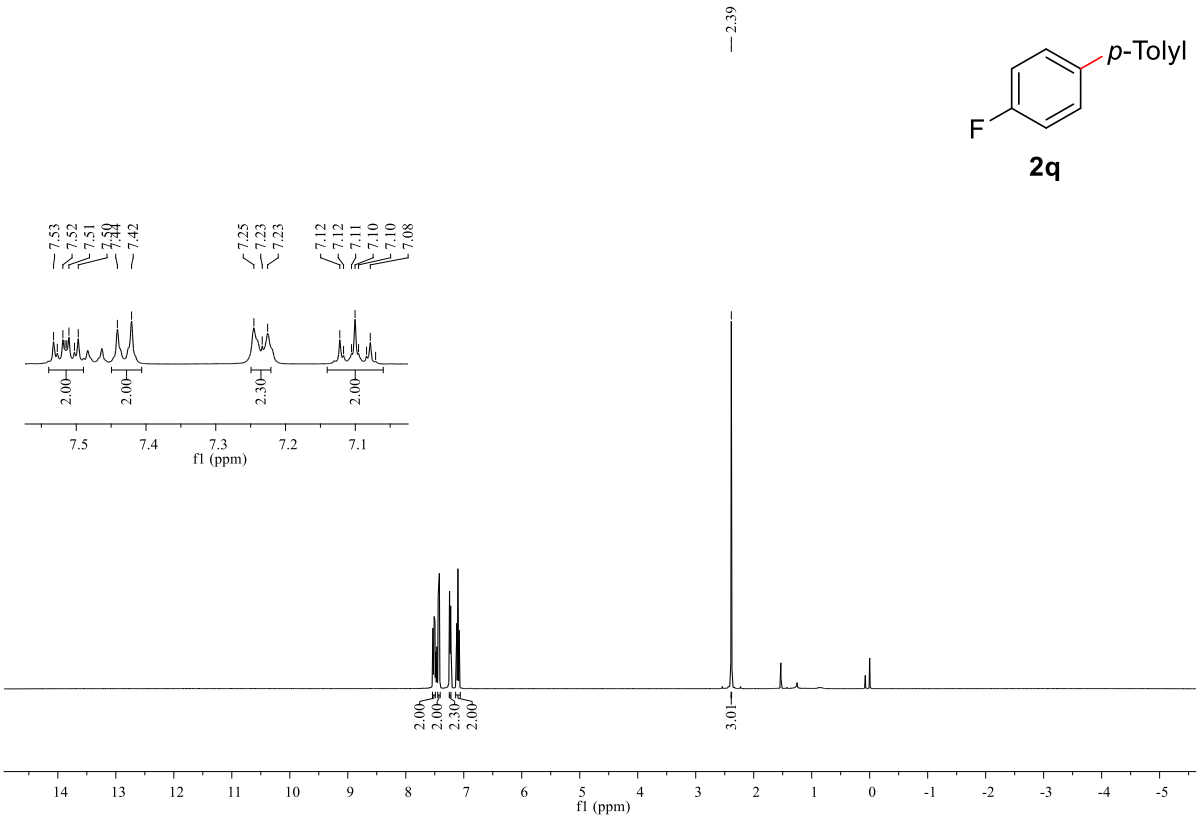
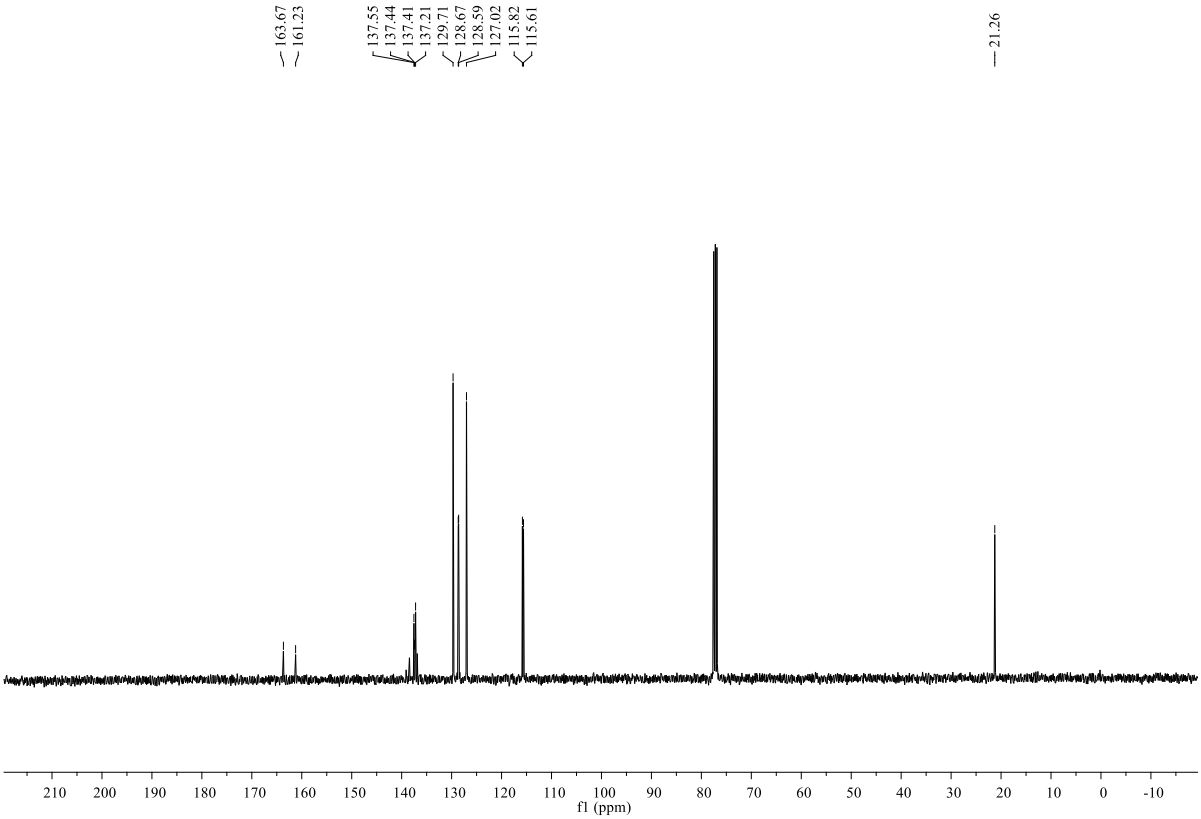
128.33
126.91
126.83
114.35
55.51
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


2.39
p-Tolyl
F
2q
7.53
7.52
7.51
7.50
7.44
7.42
7.25
7.23
7.23
7.12
7.12
7.11
7.10
7.10
7.08
2.00
2.00
2.30
2.00
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
2.00
2.00
2.30
2.00
3.01
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)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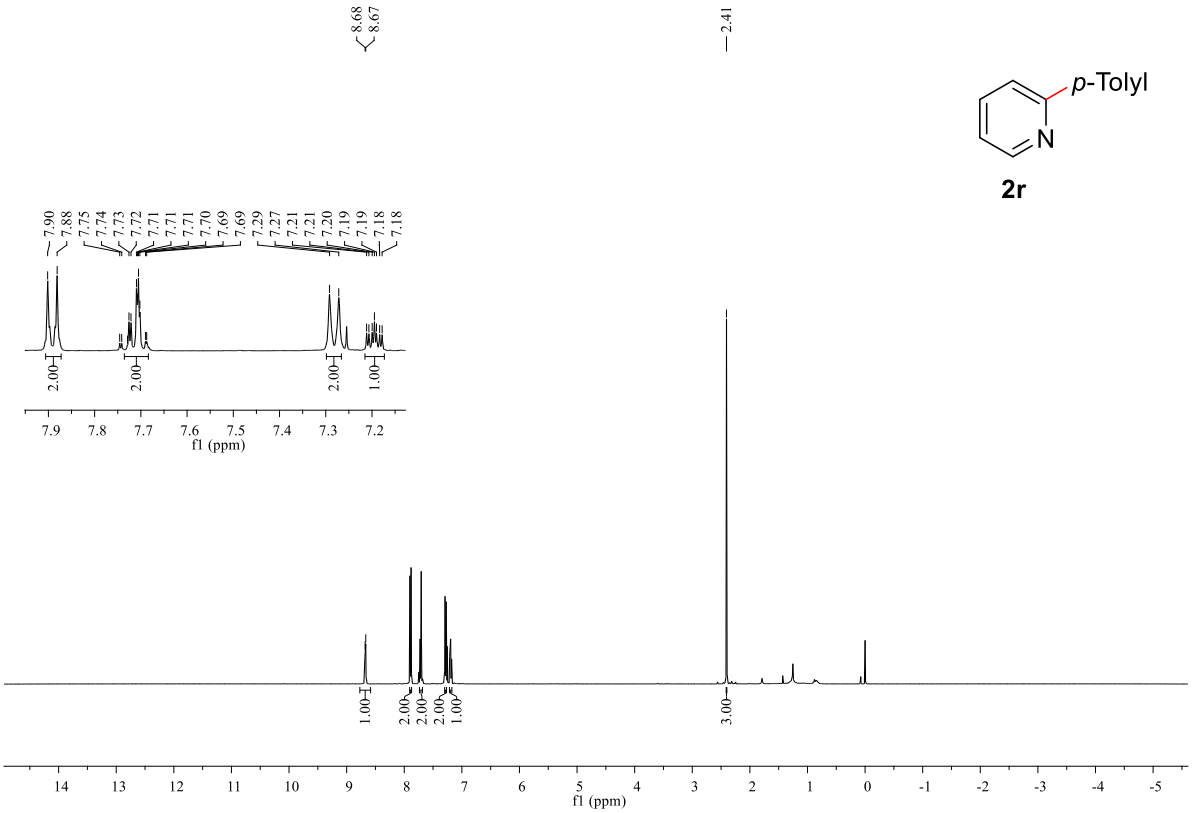
137.55
137.44
137.41
137.21
129.71
128.67
128.59
127.02
115.82
115.61
21.26
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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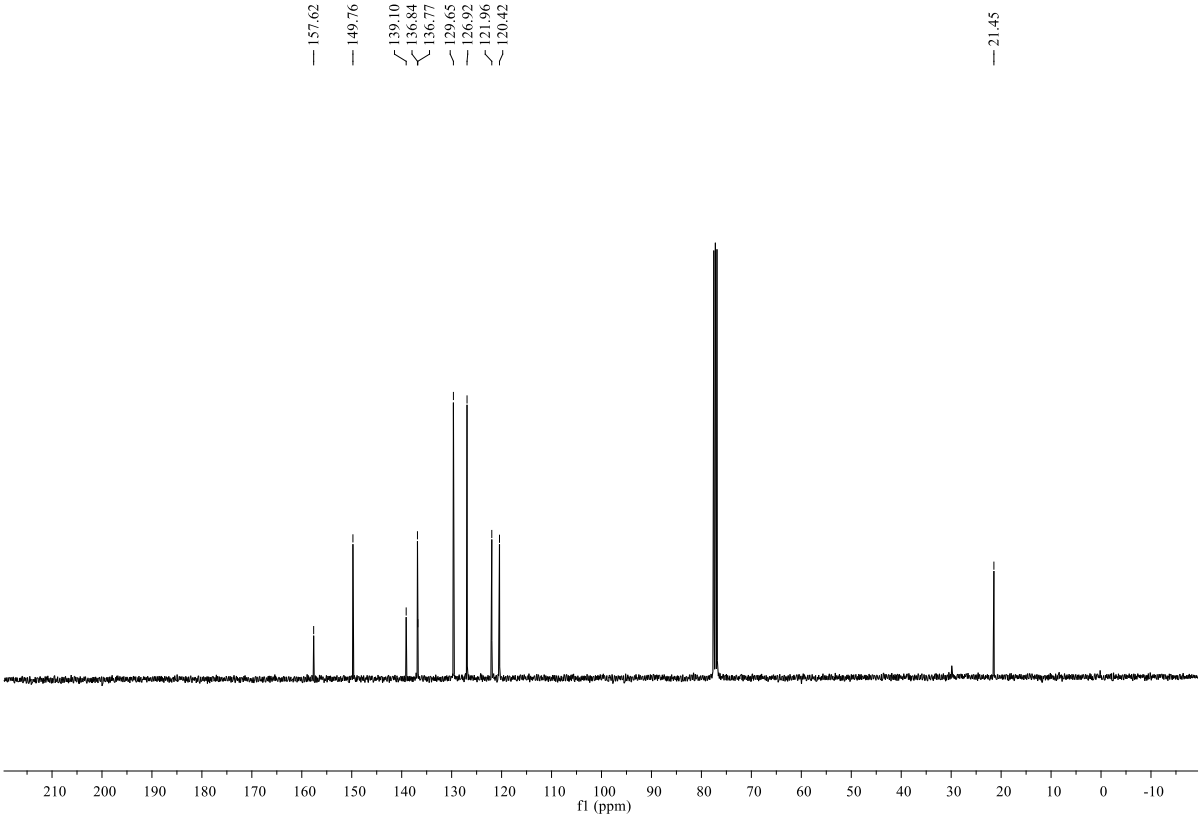
8.67
2.41
p-Tolyl
N
2r
7.90
7.88
7.75
7.74
7.73
7.72
7.71
7.71
7.71
7.71
7.70
7.69
7.69
7.29
7.27
7.21
7.21
7.20
7.19
7.19
7.18
7.18
2.00
2.00
2.00
1.00
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
f1 (ppm)
1.00
2.00
2.00
2.00
1.00
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)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139.10
136.84
136.77
129.65
126.92
121.96
120.42
21.45
210
200
190
180
170
160
150
140
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120
110
100
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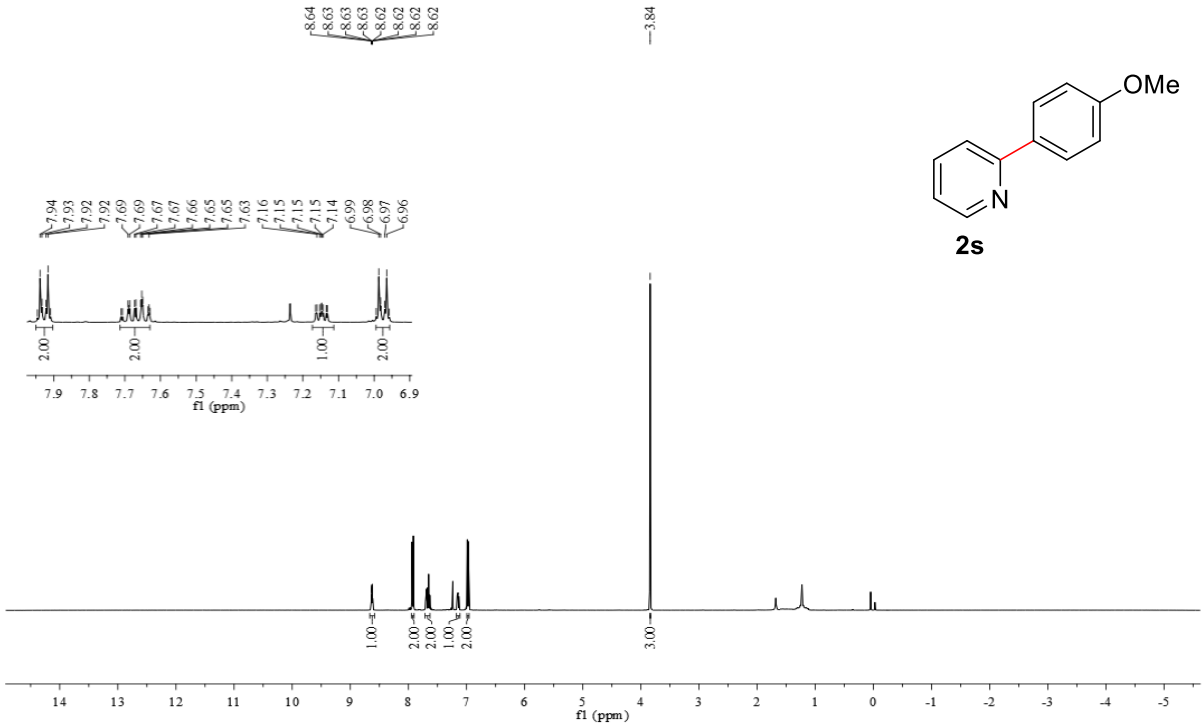
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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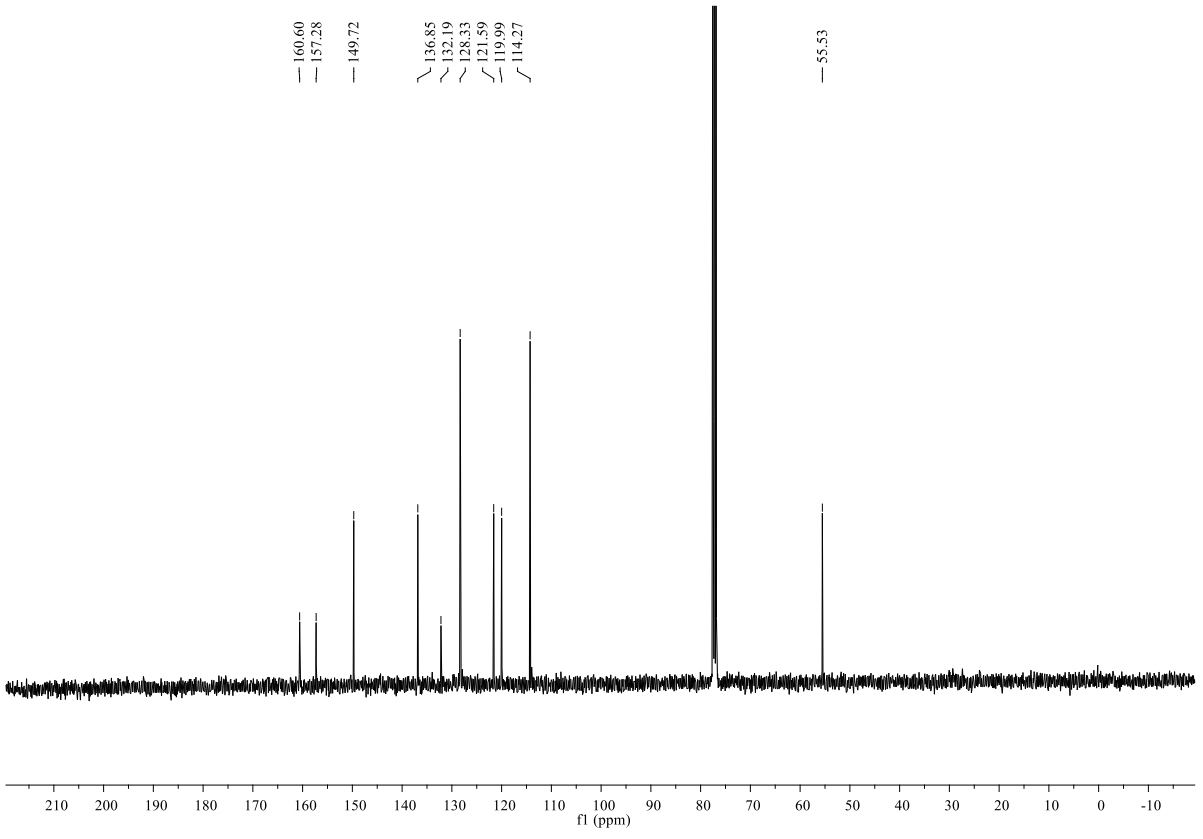
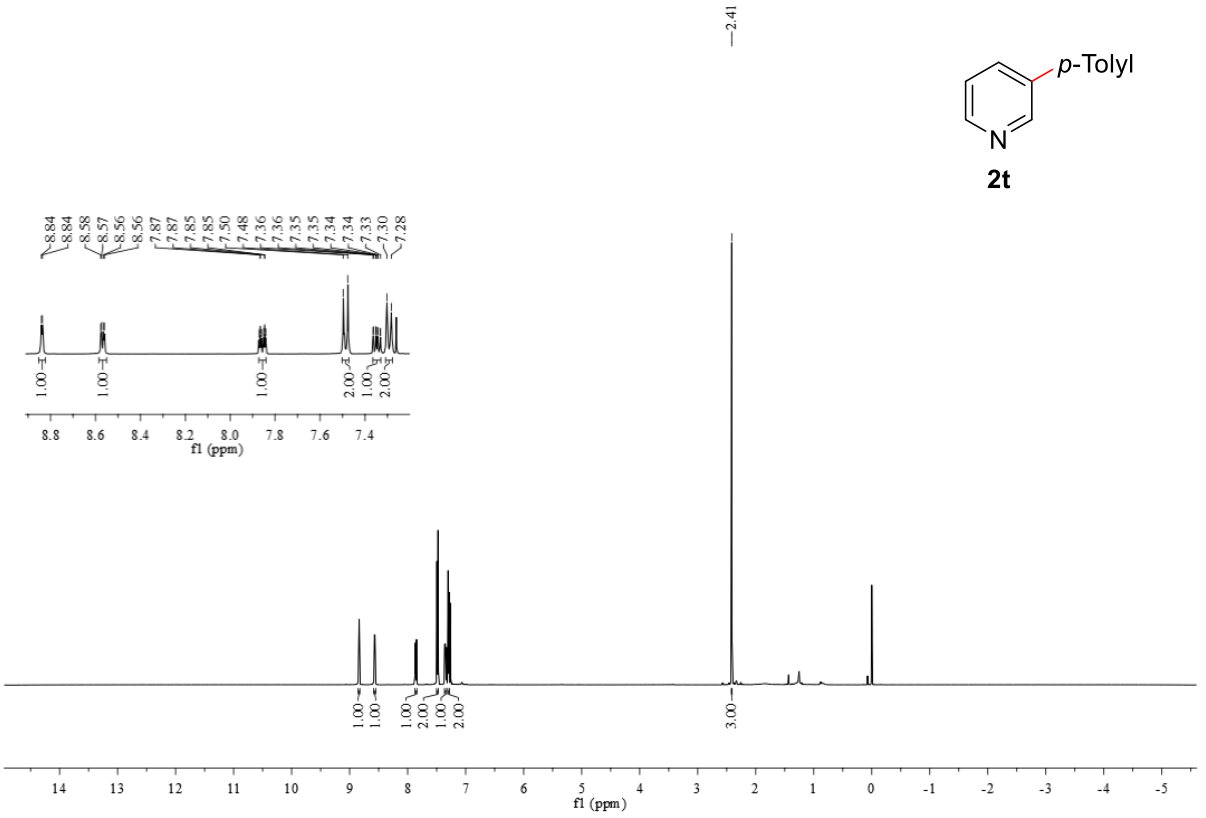
8.63
8.63
8.62
8.62
8.62
8.62
3.84
OMe
N
2s
7.94
7.93
7.92
7.92
7.69
7.69
7.67
7.67
7.66
7.65
7.65
7.63
7.16
7.15
7.15
7.15
7.14
6.99
6.98
6.97
6.96
2.00
2.00
1.00
2.00
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
1.00
2.00
2.00
1.00
2.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5
f1 (ppm)


160.60
157.28
149.72
136.85
132.19
128.33
121.59
119.99
114.27
55.53
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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p-Tolyl
N
2t
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8.84
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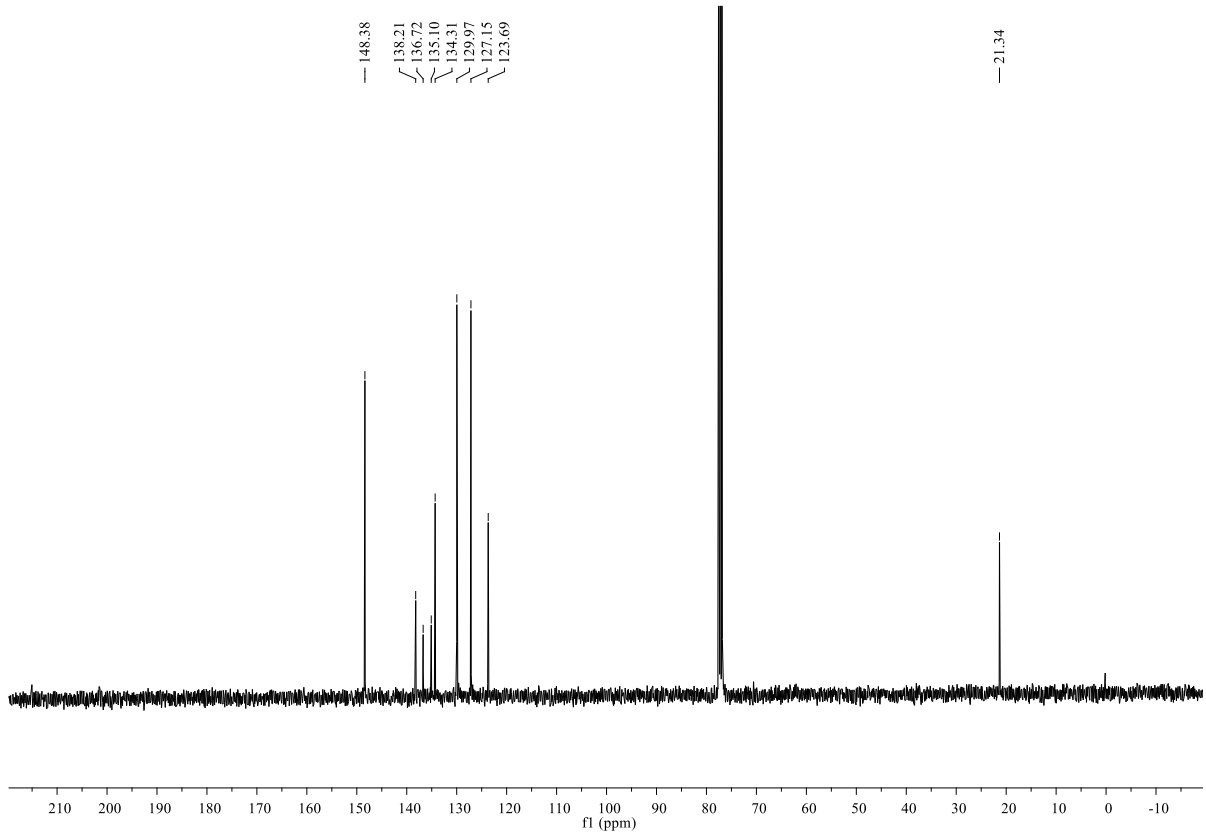
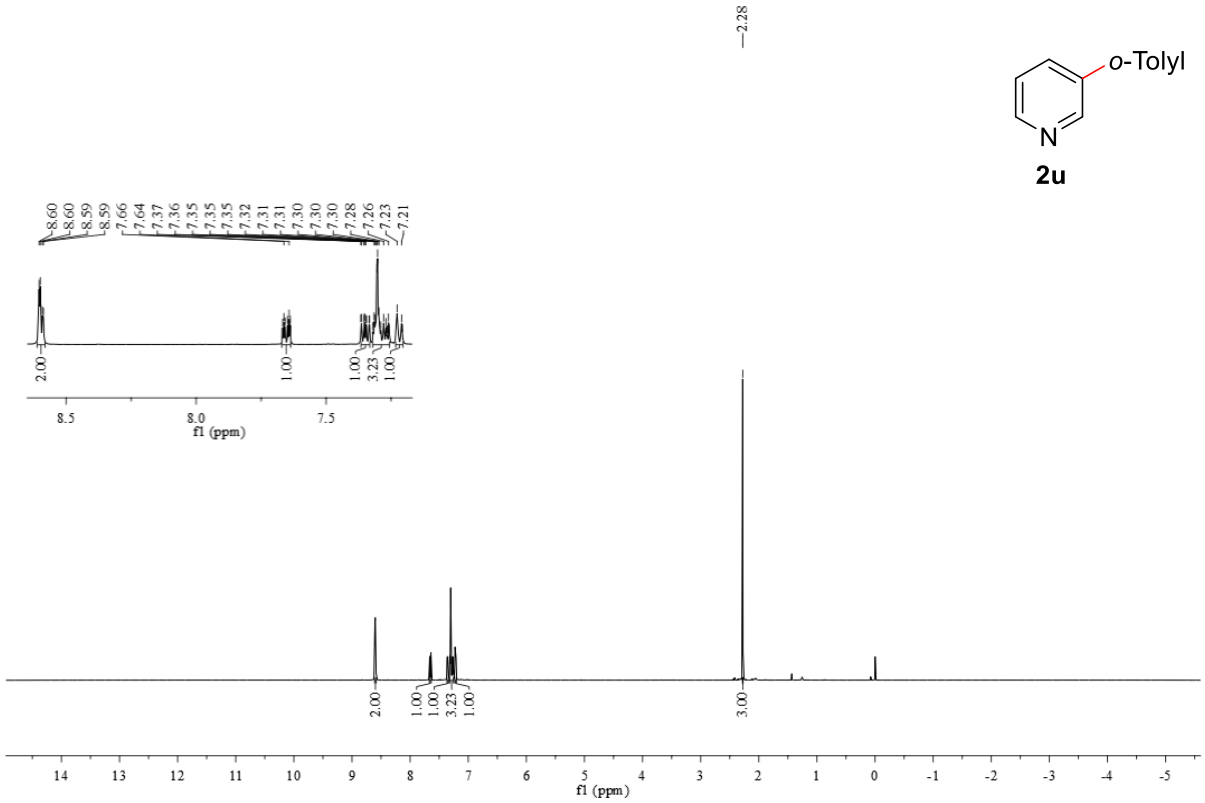
8.56
7.87
7.87
7.85
7.85
7.50
7.48
7.36
7.36
7.35
7.35
7.34
7.34
7.33
7.30
7.28
1.00
1.00
1.00
2.00
1.00
2.00
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
f1 (ppm)
1.00
1.00
1.00
2.00
1.00
2.00
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)


148.38
138.21
136.72
135.10
134.31
129.97
127.15
123.69
21.34
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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o-Tolyl
N
2u
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8.60
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8.59
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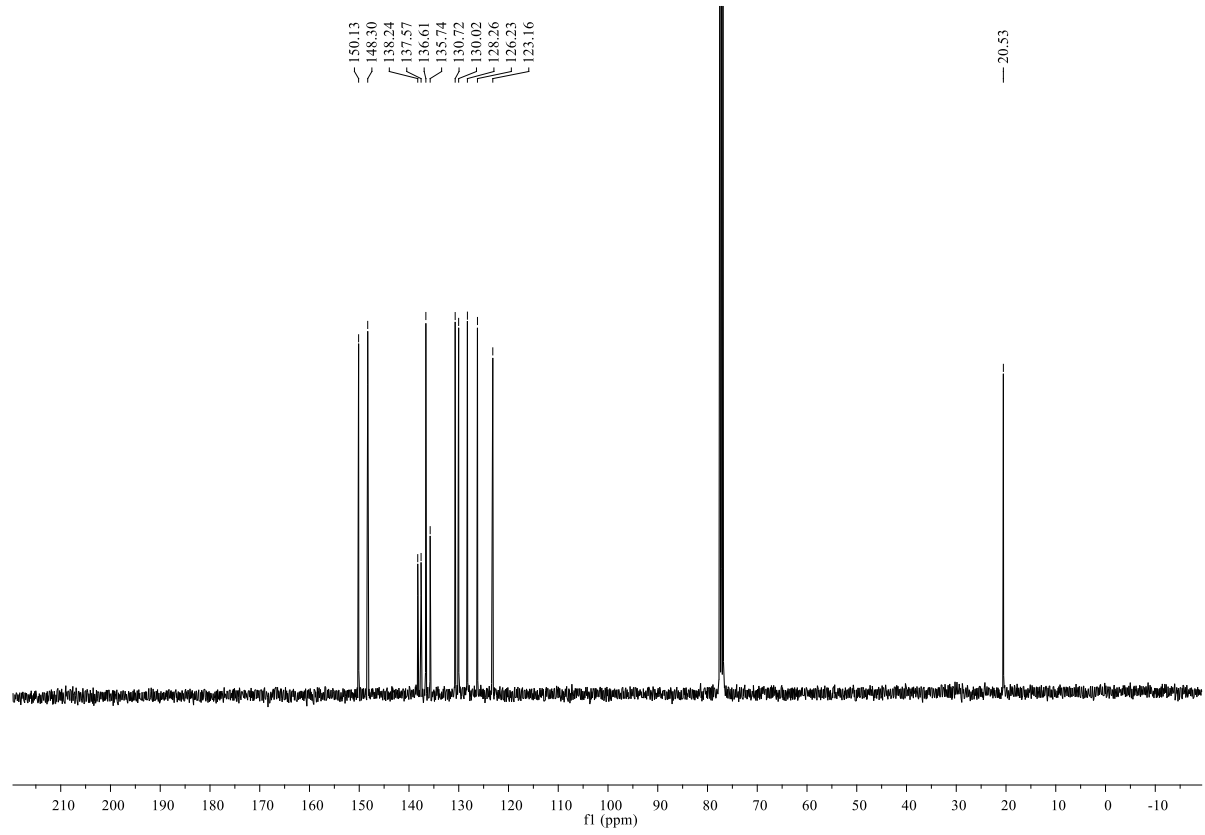
7.64
7.37
7.36
7.35
7.35
7.35
7.32
7.31
7.31
7.30
7.30
7.30
7.28
7.26
7.23
7.21
2.00
1.00
1.00
3.23
1.00
8.5
8.0
7.5
f1 (ppm)
2.00
1.00
1.00
3.23
1.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5
f1 (ppm)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135.74
130.72
130.02
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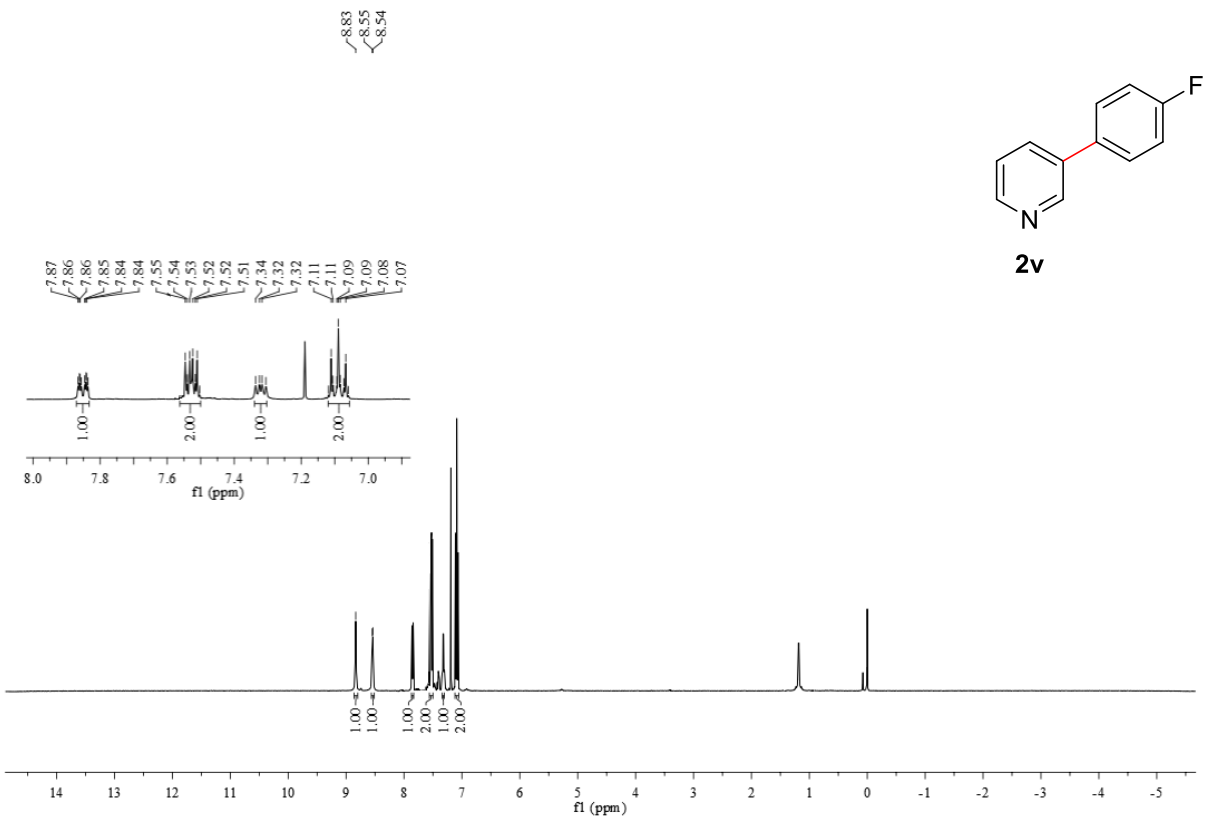
126.23
123.16
20.53
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.86
7.85
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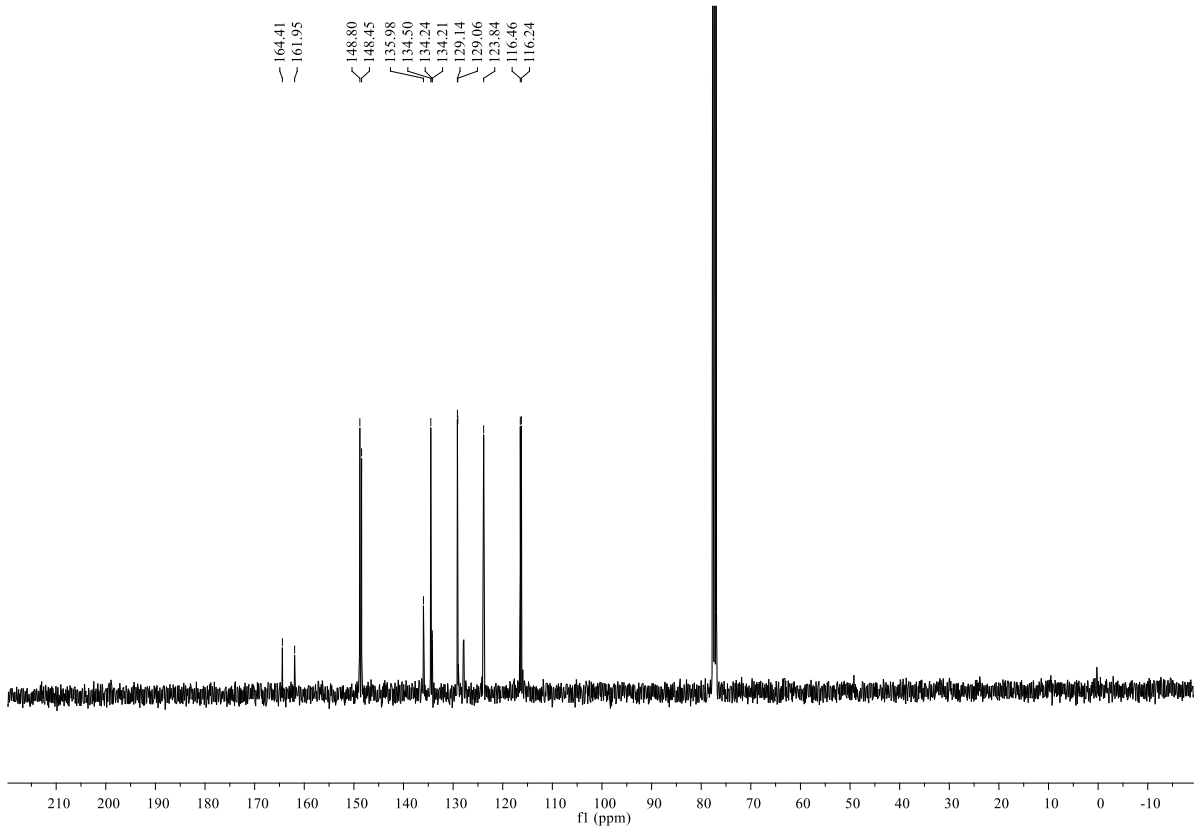
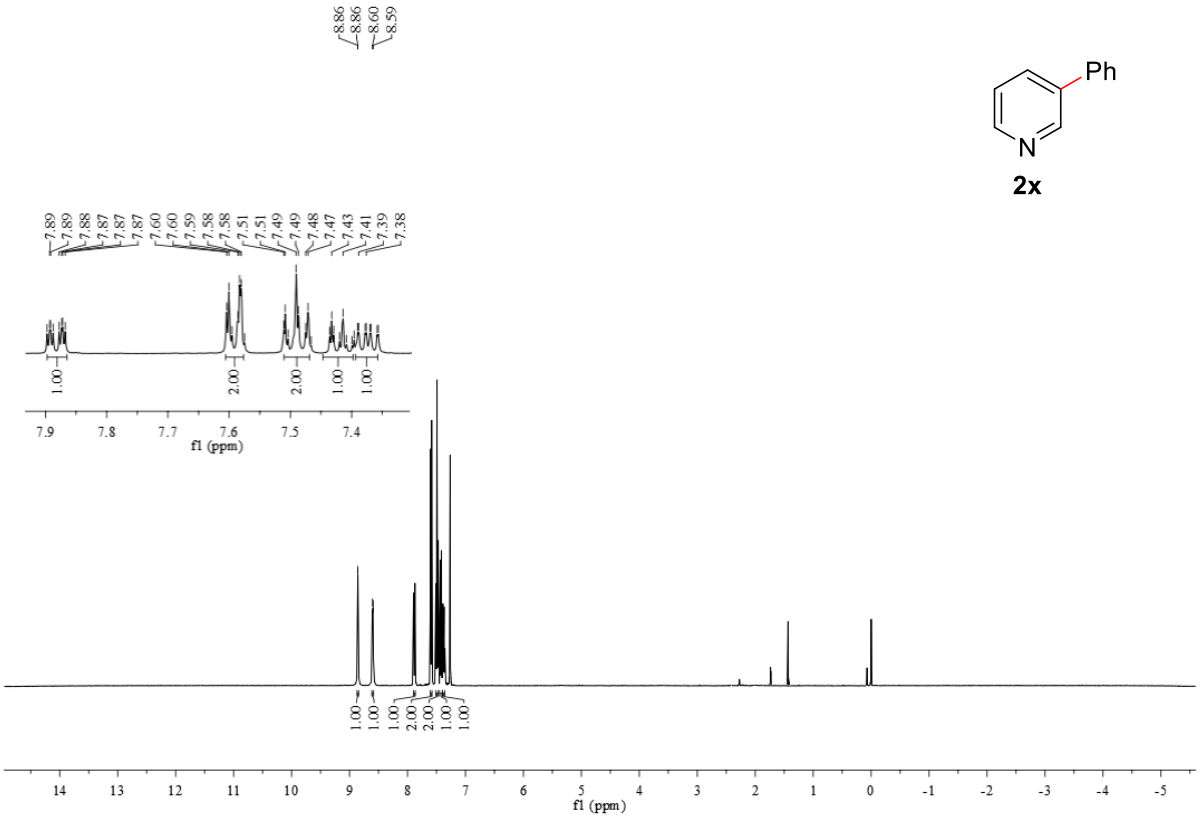
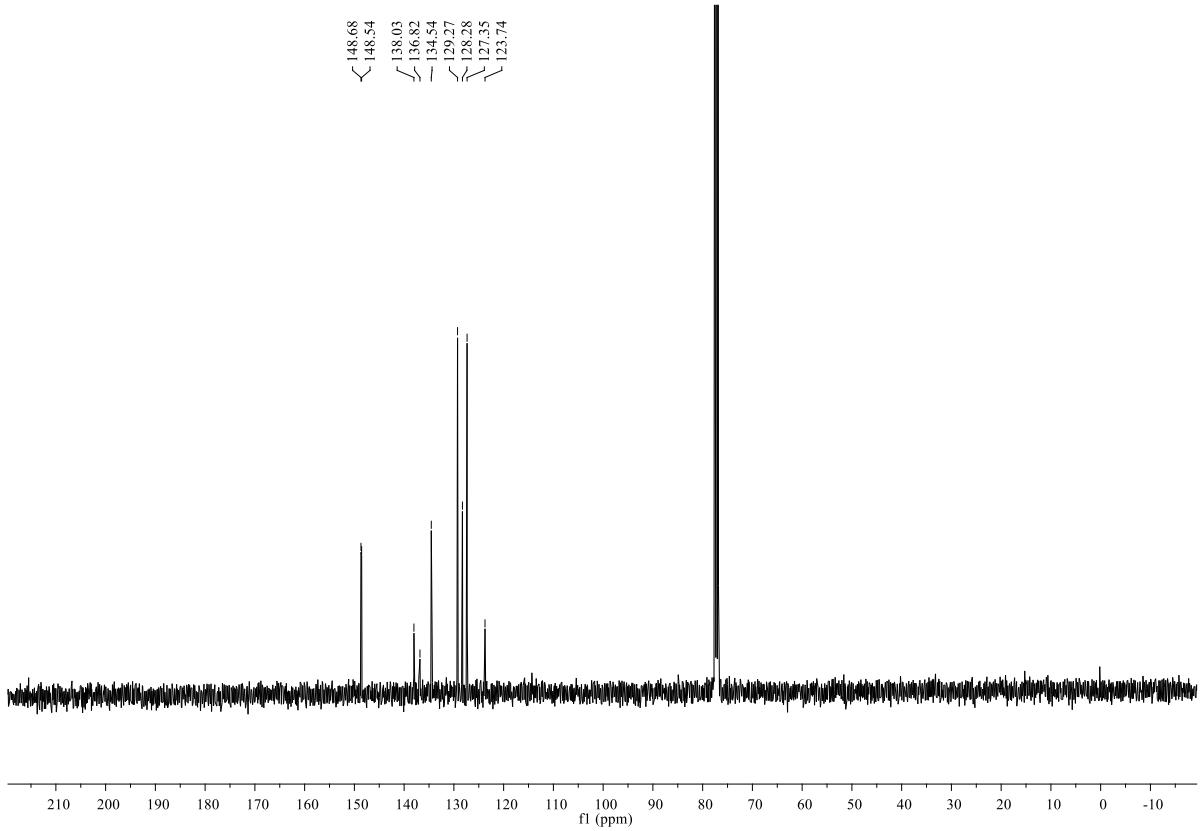
7.54
7.53
7.52
7.52
7.51
7.34
7.32
7.32
7.11
7.11
7.09
7.09
7.08
7.07
1.00
2.00
1.00
2.00
8.0
7.8
7.6
7.4
7.2
7.0
f1 (ppm)
1.00
1.00
1.00
2.00
1.00
2.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)

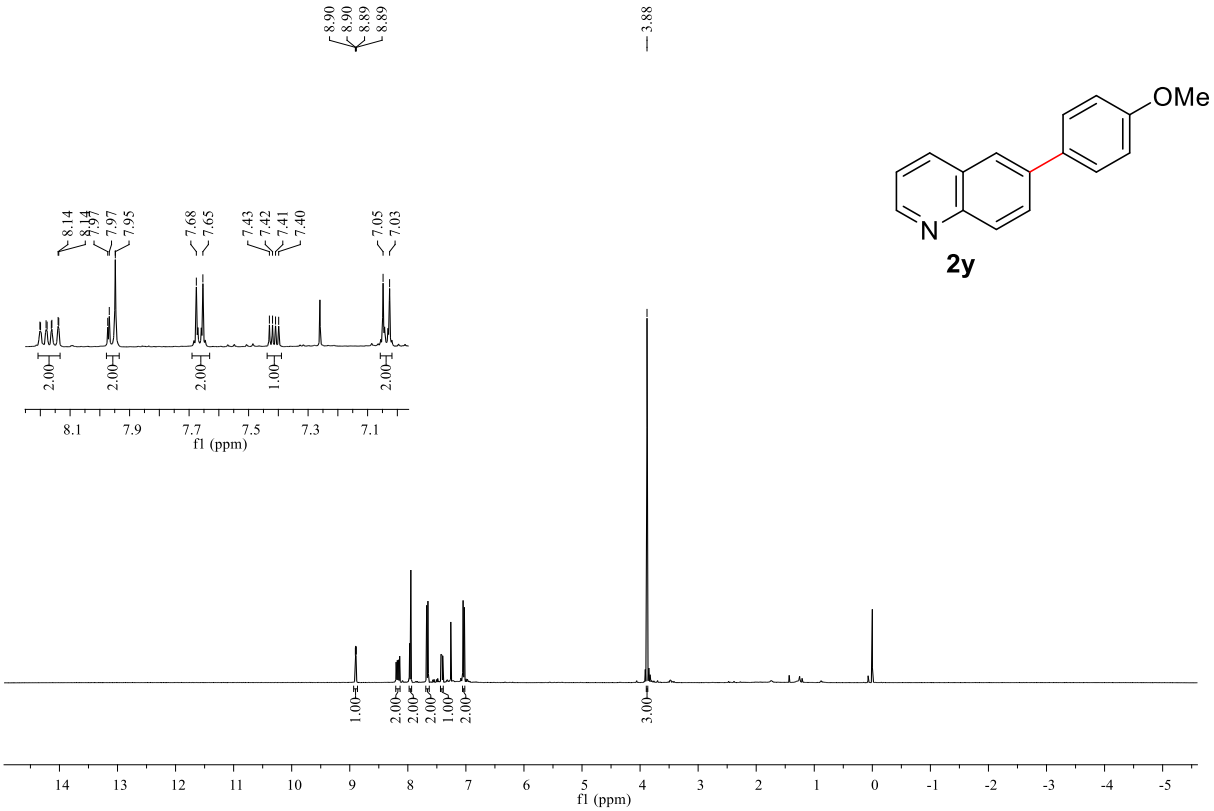
F
N

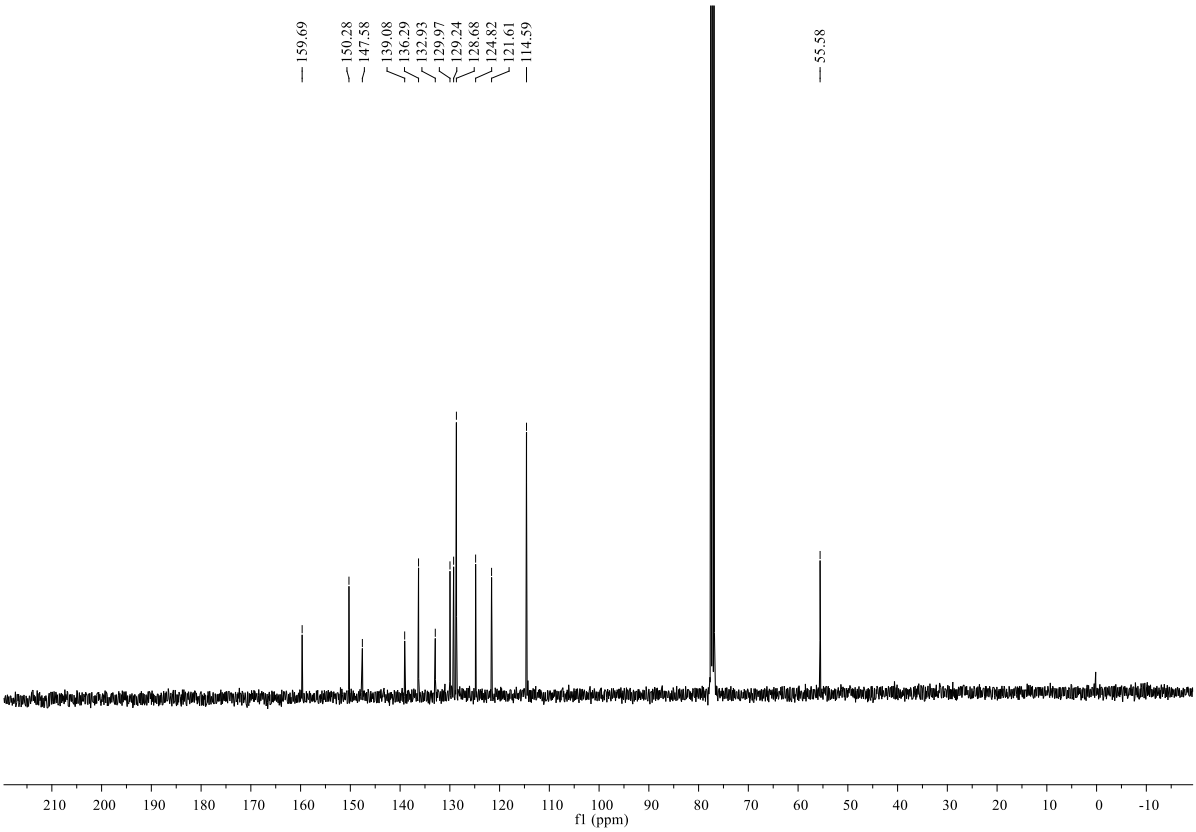
2v


164.41
161.95
148.80
148.45
135.98
134.50
134.24
134.21
129.14
129.06
123.84
116.46
116.24
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.86
8.86
8.60
8.59
Ph
N
2x
7.89
7.89
7.88
7.87
7.87
7.87
7.60
7.60
7.59
7.58
7.58
7.51
7.51
7.49
7.49
7.48
7.47
7.43
7.41
7.39
7.38
1.00
2.00
2.00
1.00
1.00
7.9
7.8
7.7
7.6
7.5
7.4
f1 (ppm)
1.00
1.00
1.00
2.00
2.00
1.00
1.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)


148.68
148.54
138.03
136.82
134.54
129.27
128.28
127.35
123.74
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.90
8.90
8.89
8.89
3.88
OMe
N
2y
8.14
8.14
7.97
7.97
7.95
7.68
7.65
7.43
7.42
7.41
7.40
7.05
7.03
2.00
2.00
2.00
1.00
2.00
8.1
7.9
7.7
7.5
7.3
7.1
f1 (ppm)
1.00
2.00
2.00
2.00
1.00
2.00
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
f1 (ppm)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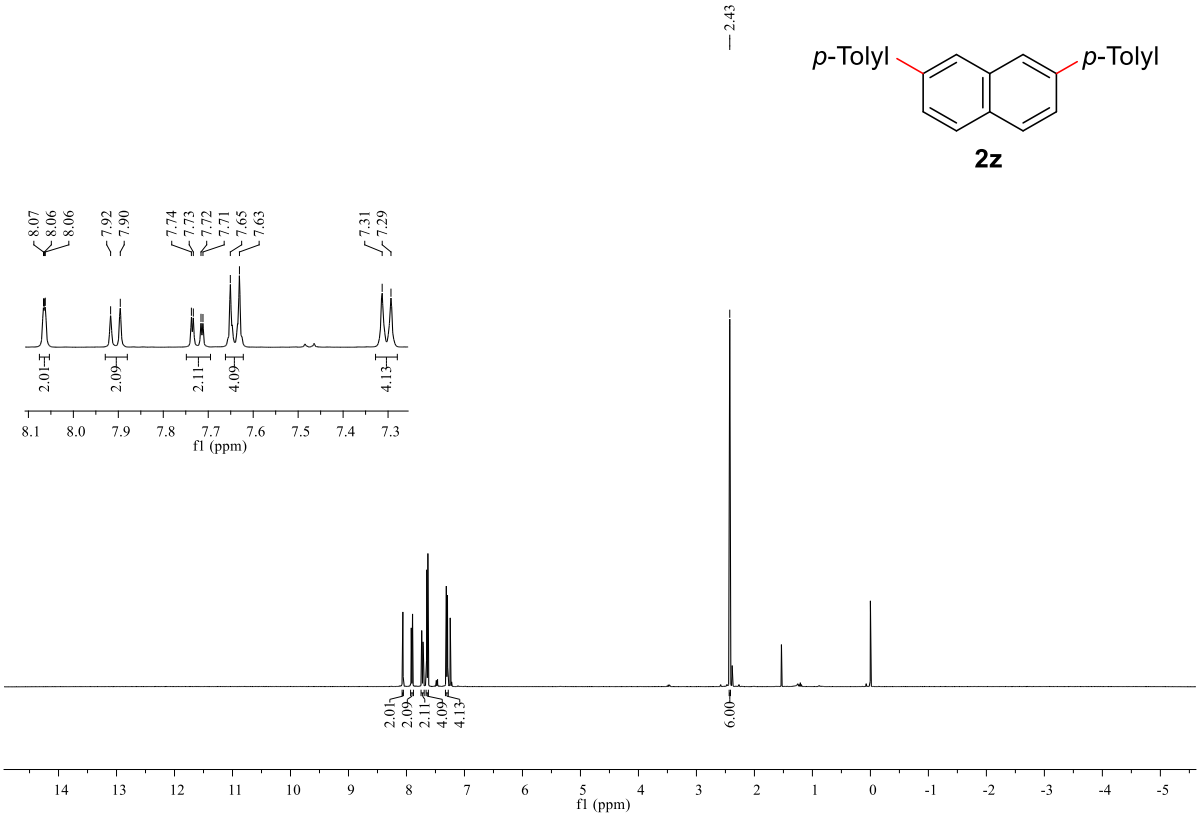
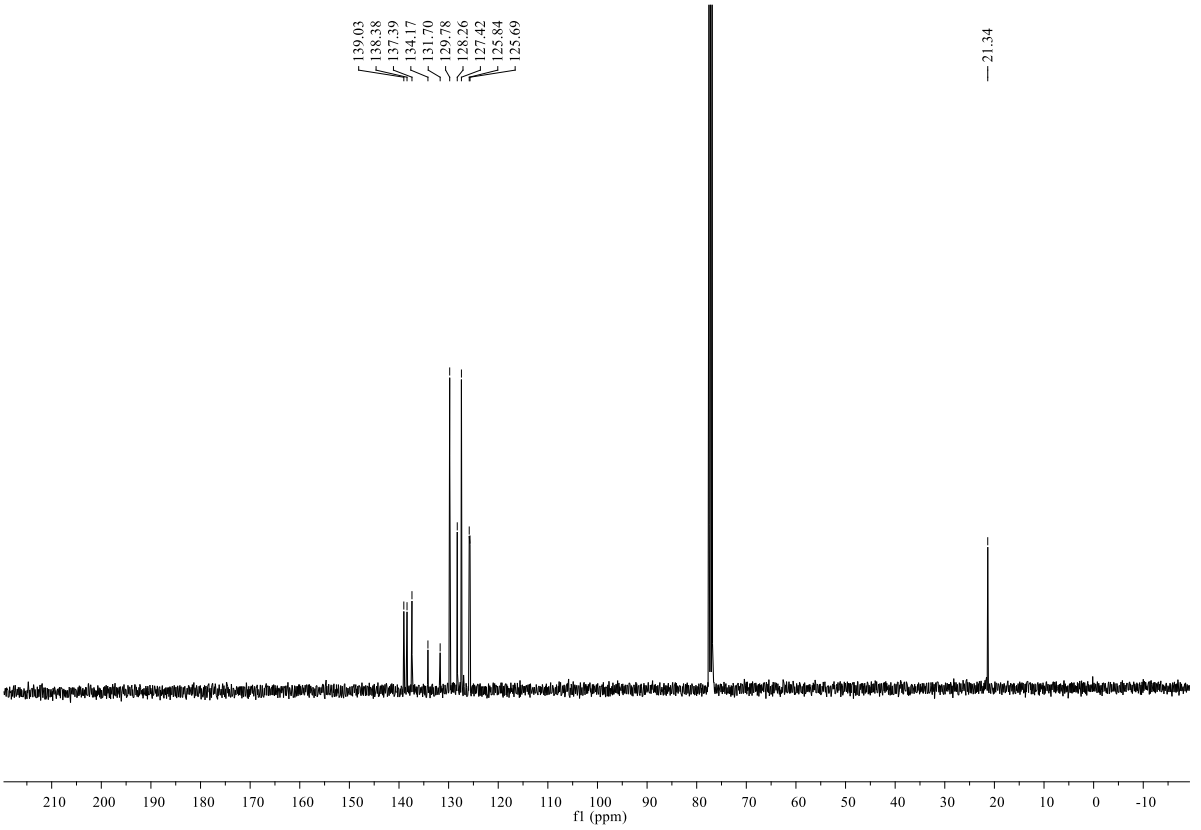
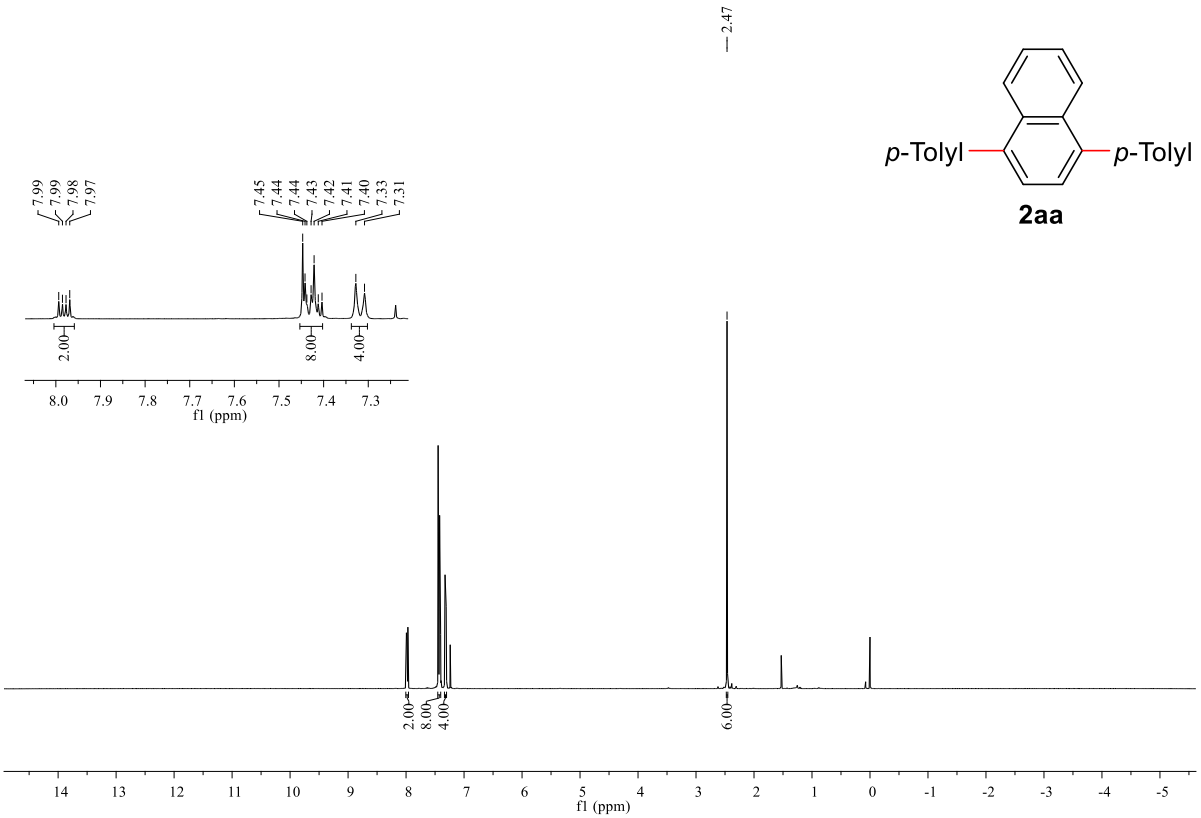
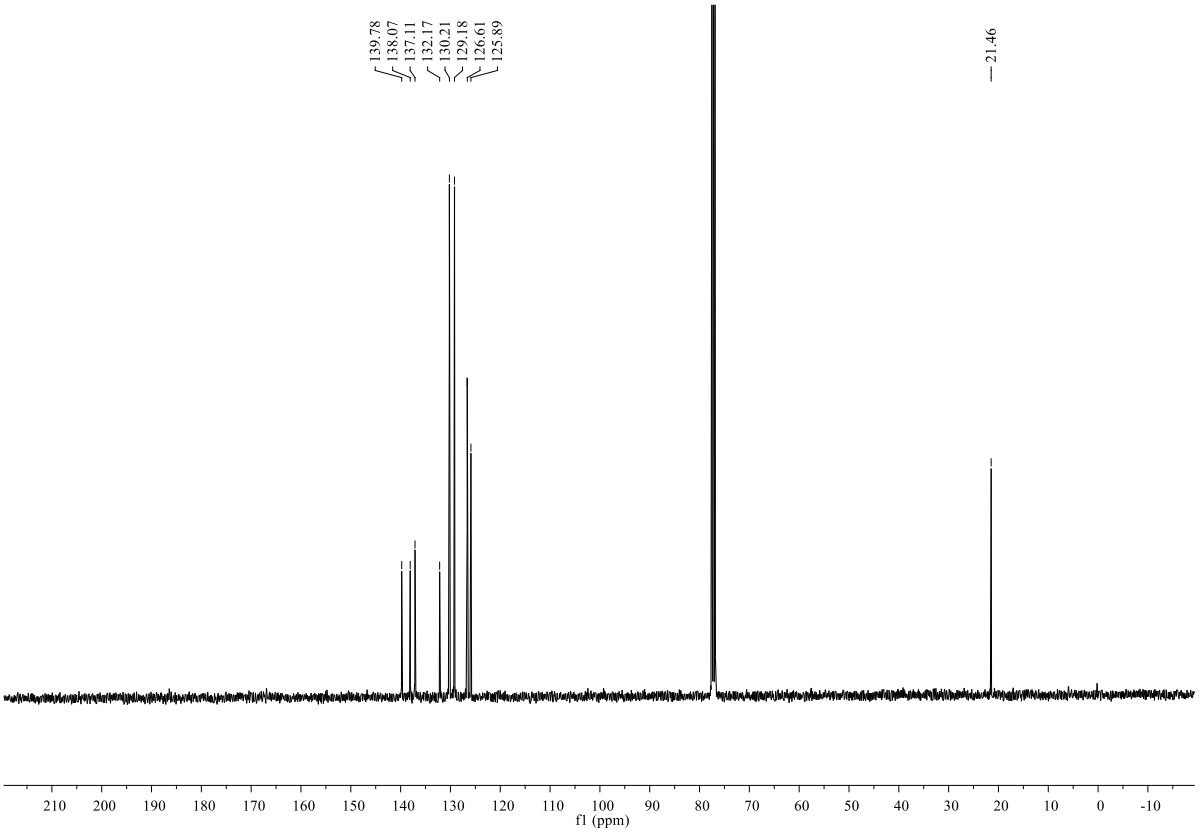
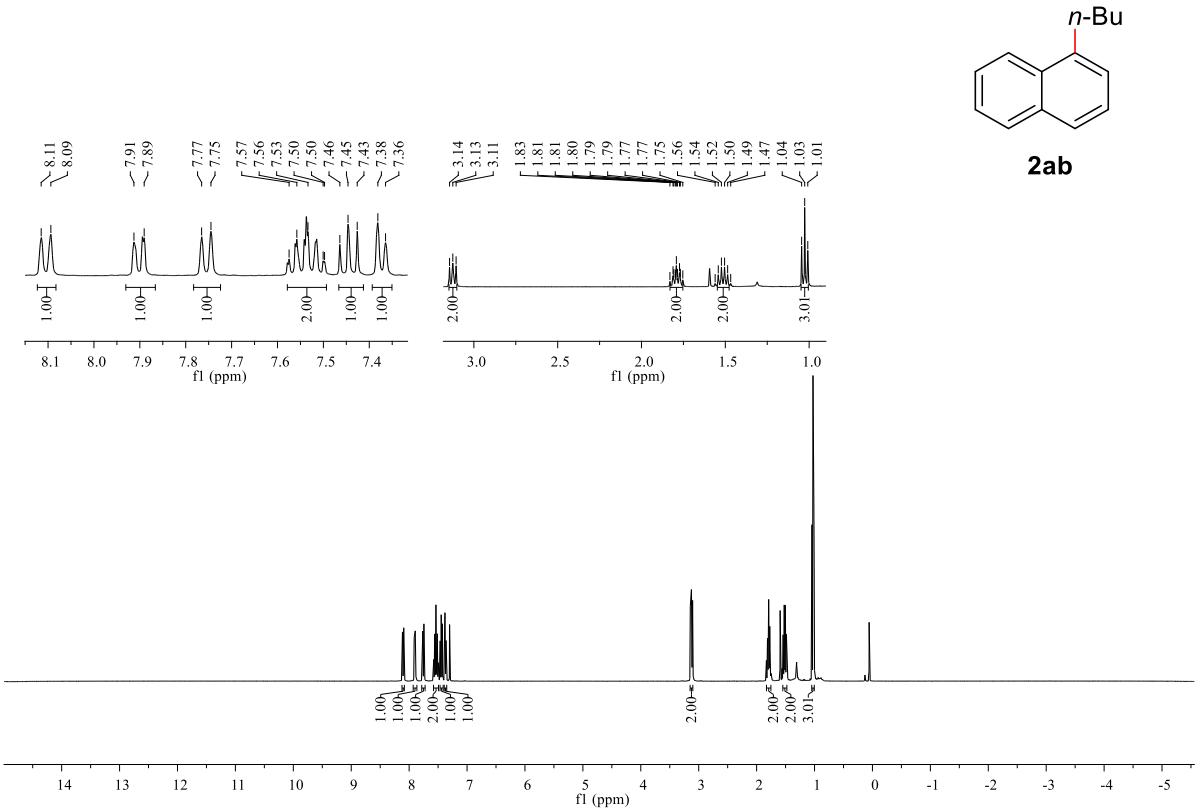
150.28
147.58
139.08
136.29
132.93
129.97
129.24
128.68
124.82
121.61
114.59
55.58
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

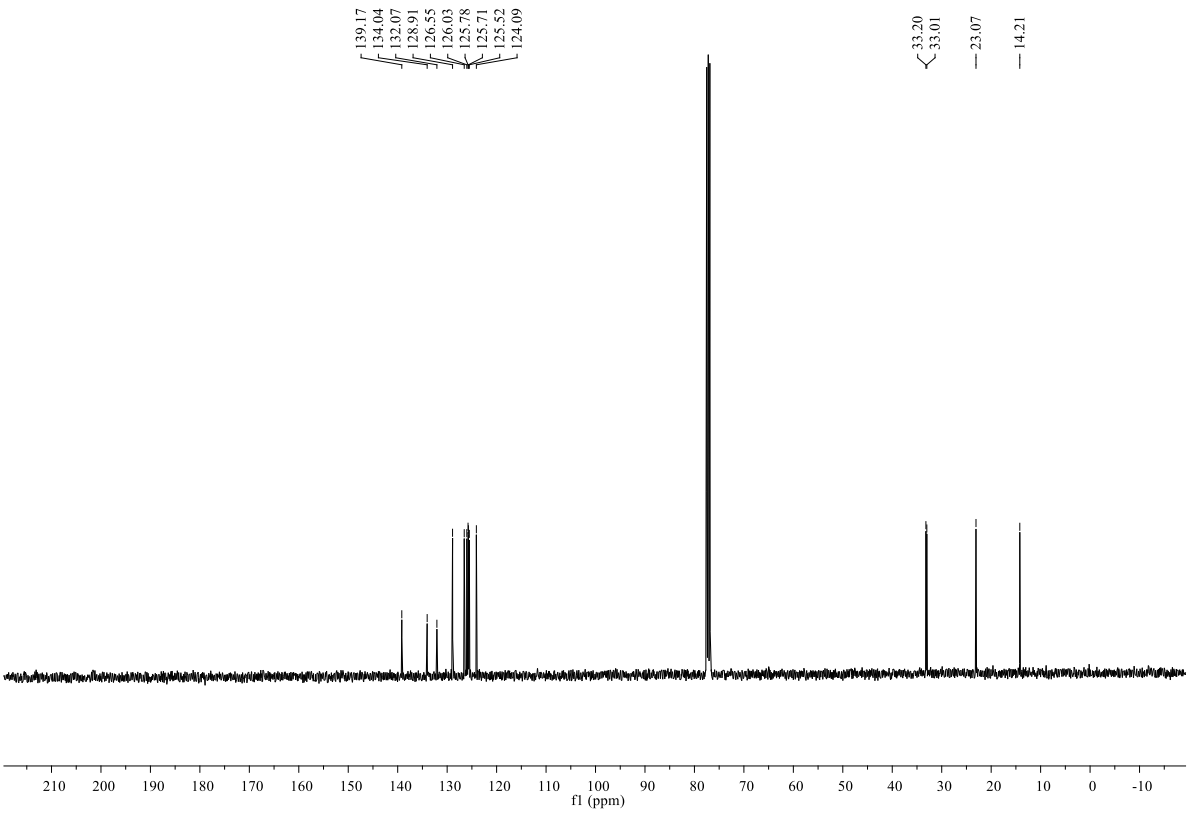

2.43
p-Tolyl
p-Tolyl
2z
8.07
8.06
8.06
7.92
7.90
7.74
7.73
7.72
7.71
7.65
7.63
7.31
7.29
2.01
2.09
2.11
4.09
4.13
6.00
f1 (ppm)


139.03
138.38
137.39
134.17
131.70
129.78
128.26
127.42
125.84
125.69
21.34
f1 (ppm)


2.47
p-Tolyl
p-Tolyl
2aa
7.99
7.99
7.98
7.97
7.45
7.44
7.44
7.43
7.42
7.41
7.40
7.33
7.31
2.00
8.00
4.00
6.00
f1 (ppm)


139.78
138.07
137.11
132.17
130.21
129.18
126.61
125.89
21.46
f1 (ppm)


n-Bu
2ab
8.11
8.09
7.91
7.89
7.77
7.75
7.57
7.56
7.53
7.50
7.50
7.46
7.45
7.43
7.38
7.36
3.14
3.13
3.11
1.83
1.81
1.81
1.80
1.79
1.79
1.77
1.77
1.75
1.56
1.54
1.52
1.50
1.49
1.47
1.04
1.03
1.01
f1 (ppm)
f1 (ppm)
f1 (ppm)


139.17
134.04
132.07
128.91
126.55
126.03
125.78
125.71
125.52
124.09
33.20
33.01
23.07
14.21
f1 (ppm)