Supporting Information

Electrochemical Acceptorless Dehydrogenation of N-Heterocycles Utilizing TEMPO as Organo-Electrocatalyst

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Content

1. General considerations

All glassware was oven dried at 110 ^{o}C for hours and cooled down under vacuum. Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All reactions were performed in resealable screw-capped Schlenk tube (approx. 20 mL volume) in the presence of Teflon-coated magnetic stirrer bar (4 mm × 10 mm). Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (bp. 60-90 ^{o}C). Gas chromatographic analyses were performed on SHIMADZU GC-2014 gas chromatography instrument with a FID detector and biphenyl was added as internal standard. GC-MS spectra were recorded on Varian GC MS 3900-2100T or SHIMADZU GC MS-2010. ^{1}H NMR spectra were recorded with ADVANCE III (400 MHz). Spectra were referenced internally to the residual proton resonance in $CDCl_3$ (δ 7.26 ppm), or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ^{13}C NMR spectra were referenced to $CDCl_3$ (δ 77.0 ppm, the middle peak). Coupling constants (*J*) were reported in Hertz (Hz).

2. Experimental details

2.1 General procedures for ECAD of N-heterocycles

In an oven-dried undivided three-necked bottle (25 mL) equipped with a stir bar, saturated N-heterocycles **1a**-**1n**, **1q**-**1r**, **3a**-**3g** (0.25 mmol), or **2o**-**2p**, **5a**-**5k** (0.5 mmol), Tempo (0.025 mmol), nBu_4NBF_4 (32.9 mg, 0.1 mmol), and CH_3CN/H_2O (6.0 mL /0.1 mL) were combined and added. The bottle was equipped with carbon cloth (15 mm × 20 mm) as the anode and platinum plate (15 mm × 15 mm) as the cathode and then charged with nitrogen. The reaction mixture was stirred and electrolyzed at a constant current of 7 mA (j ≈ 3.1 mA/cm^2) under room temperature for 4 h. When the reaction finished, the reaction mixture was washed with water and extracted with EA (10 mL × 3). The organic layers were combined, dried over Na_2SO_4, and concentrated. The pure product was obtained by column chromatography on silica gel.

2.2 Procedure for gram scale synthesis

In an oven-dried undivided three-necked bottle (250 mL) equipped with a stir bar, **1a**, **5a**, **1p** and **5h** (10 mmol), Tempo (1 mmol for **1a** or 0.5 mmol for **5a**, **1p** and **5h**), nBu_4NBF_4 (1.32 g, 4 mmol for **1a** or 0.66 g, 20 mmol for **5a**, **1p** and **5h**), and CH_3CN/H_2O (120 mL/5 mL for **1a** or 60 mL/2 mL for **5a**, **1p** and **5h**) were combined and added. The bottle was equipped with carbon cloth (20 mm × 30 mm) as the anode and platinum plate (15 mm × 15 mm) as the cathode and then charged with nitrogen. The reaction mixture was stirred and electrolyzed at a constant current of 100 mA for **1a** under room temperature for 13 h (or 75 mA for **6a**, **2q** and **6h** under room temperature for 8 h). When the reaction finished, the reaction mixture was washed with

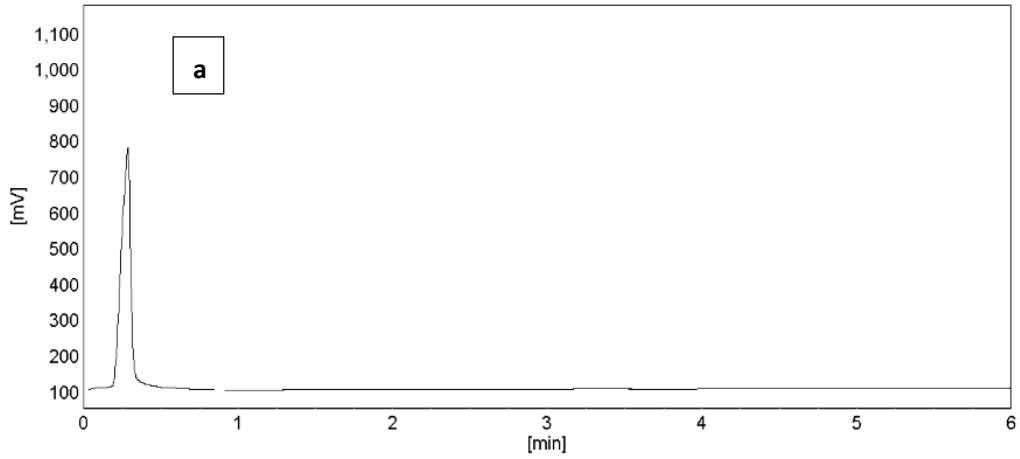
water and extracted with EA (50 mL × 3). The organic layers were combined, dried over Na_2SO_4, and concentrated. The pure product was obtained by column chromatography on silica gel.

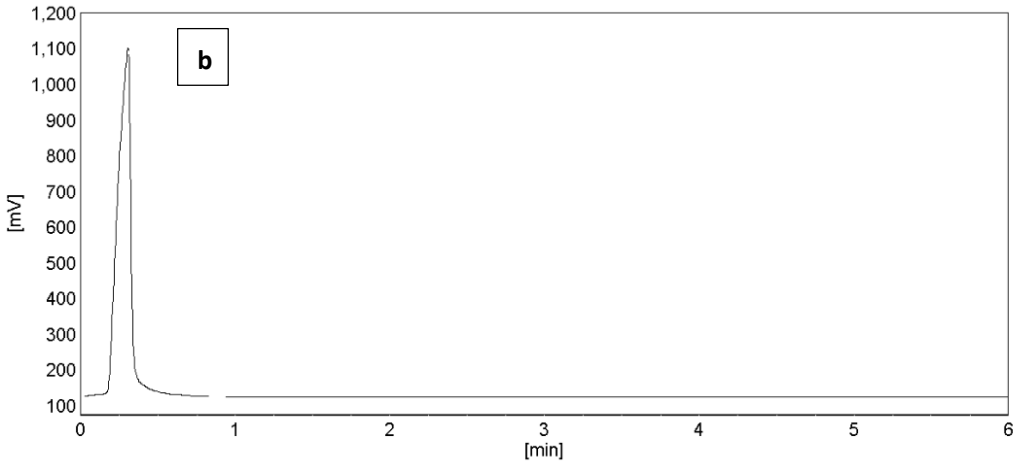
2.3 Procedure for the synthesis of 2-phenylquinazolin-4(3H)-one

A 20 mL oven-dried reaction Schlenk tube was charged with **4a** (20.6 mg, 0.1 mmol), H_2O_2 (6.8 mg, 0.2 mmol). The reaction tube was purged three times with O_2 balloon, and HOAc (0.5 mL) was added to the sealed reaction vessel by syringe. The resulting solution was stirred at 55 ℃ for 24 h. After cooling to room temperature, the volatiles were removed under vacuum and the residue was purified by column chromatography to give the product as pale yellow solid; yield: 21.0 mg (95%).

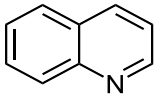
2.4 Procedure for the detection of H_2

After completion of the standard reaction, H_2 was analyzed by gas chromatography (9790, Fuli, China, oven temp. 90 ℃, TCD temp. 100 ℃, injection temp. 100 ℃,) Under this condition, the gas extracted from the sealed standard reaction was shown a sharp peak at 0.28 min (figure a) while the standard H_2 was shown as an obvious peak at 0.30 min (figure b).

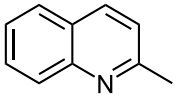




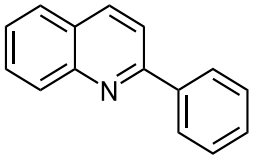
3. Detail descriptions for products



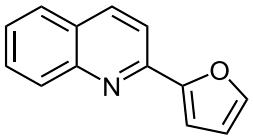
Quinoline (**2a**)[1]: colorless oil was obtained in 82% isolated yield. 1H NMR (400 MHz, $CDCl_3$) δ 8.91 (dd, J = 4.5, 1.9 Hz, 1H), 8.17 – 8.06 (m, 2H), 7.78 (td, J = 7.1, 6.4, 3.5 Hz, 1H), 7.71 (td, J = 6.8, 2.2 Hz, 1H), 7.53 (t, J = 7.4 Hz, 1H), 7.36 (dd, J = 8.1, 4.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.3, 148.1, 136.0, 129.4, 129.3, 128.1, 127.7, 126.4, 121.0.



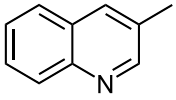
2-Methylquinoline (**2b**) [1]: colorless oil was obtained in 75% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 8.02 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.97 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.65 (ddt, *J* = 8.3, 6.8, 1.2 Hz, 1H), 7.44 (dd, *J* = 8.1, 6.9 Hz, 1H), 7.22 (dd, *J* = 8.3, 1.3 Hz, 1H), 2.72 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 147.6, 135.9, 129.2, 128.4, 127.3, 126.2, 125.4, 121.8, 25.2.



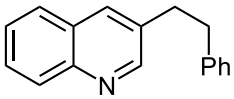
2-Phenylquinoline (**2c**) [1]: white solid was obtained in 70% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 8.20 – 8.09 (m, 4H), 7.79 (d, *J* = 8.6 Hz, 1H), 7.75 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.69 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.52 – 7.40 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 148.2, 139.6, 136.8, 129.7, 129.6, 129.3, 128.8, 127.5, 127.4, 127.1, 126.3, 119.0.



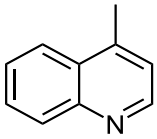
2-(Furan-2-yl)quinolone (**2d**) [1]: white solid was obtained in 74% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 8.10 (dd, *J* = 19.2, 8.7 Hz, 2H), 7.79 – 7.64 (m, 3H), 7.63 – 7.58 (m, 1H), 7.48 – 7.41 (m, 1H), 7.19 (dd, *J* = 3.5, 0.8 Hz, 1H), 6.55 (dd, *J* = 3.4, 1.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 148.8, 147.9, 143.9, 136.5, 129.7, 129.1, 127.4, 126.9, 126.0, 117.3, 112.0, 110.0.



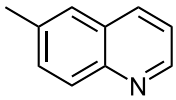
3-Methylquinoline (**2e**) [1]: colorless oil was obtained in 81% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 2.2 Hz, 1H), 8.07 (dd, *J* = 8.4, 1.1 Hz, 1H), 7.85 (dt, *J* = 2.3, 1.2 Hz, 1H), 7.70 (d, *J* = 8.2 Hz, 1H), 7.62 (ddd, *J* = 8.3, 6.7, 1.4 Hz, 1H), 7.53 – 7.43 (m, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 146.4, 134.5, 130.3, 129.0, 128.3, 128.0, 127.0, 126.4, 18.6.



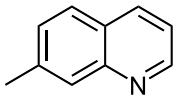
3-Phenethylquinoline (**2f**)[2]: colorless oil was obtained in 75% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 2.3 Hz, 1H), 8.08 (dd, *J* = 8.6, 1.1 Hz, 1H), 7.85 (d, *J* = 2.1 Hz, 1H), 7.73 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.65 (m, 1H), 7.51 (m, 1H), 7.32 – 7.15 (m, 5H), 3.14 – 3.07 (m, 2H), 3.05 – 2.98 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 146.6, 140.6, 134.3, 134.0, 128.9, 128.5, 128.3, 127.9, 127.2, 126.4, 126.0, 37.2, 34.9.



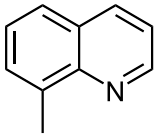
4-Methylquinoline (**2g**) [1]: colorless oil was obtained in 72% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (dt, *J* = 3.9, 1.6 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 8.01 – 7.92 (m, 1H), 7.69 (dd, *J* = 2.6, 1.5 Hz, 1H), 7.54 (d, *J* = 1.8 Hz, 1H), 7.25 – 7.14 (m, 1H), 2.66 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.8, 147.6, 143.9, 129.6, 128.7, 127.9, 125.9, 123.5, 121.5, 18.3.



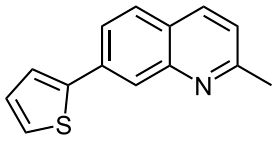
6-Methylquinoline (**2h**) [1]: colorless oil was obtained in 75% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (dd, *J* = 4.3, 1.6 Hz, 1H), 8.04 – 7.97 (m, 2H), 7.51 (d, *J* = 7.5 Hz, 2H), 7.31 (ddd, *J* = 8.3, 4.2, 1.5 Hz, 1H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.4, 146.7, 136.2, 135.2, 131.6, 128.9, 128.2, 126.4, 120.9, 21.4.



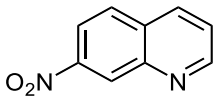
7-Methylquinoline (**2i**) [1]: colorless oil was obtained in 78% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (d, *J* = 2.4 Hz, 1H), 8.08 (m, 1H), 7.88 (s, 1H), 7.68 (m, 1H), 7.48 – 7.18 (m, 2H), 2.56 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.2, 148.3, 139.6, 135.6, 128.7, 128.2, 127.3, 126.2, 120.1, 21.8.



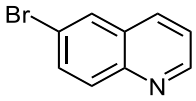
8-Methylquinoline (**2j**) [1]: colorless oil was obtained in 77% isolated yield.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (dd, *J* = 4.4, 2.4 Hz, 1H), 8.02 – 7.95 (m, 1H), 7.55 (t, *J* = 2.6 Hz, 1H), 7.47 (d, *J* = 4.0 Hz, 1H), 7.35 (d, *J* = 2.0 Hz, 1H), 7.30 – 7.21 (m, 1H), 2.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 147.0, 136.7, 135.9, 129.3, 127.9, 126.0, 125.6, 120.5, 17.9.



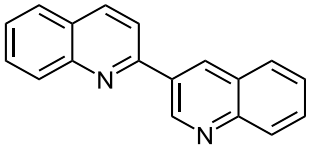
2-methyl-7-(thiophen-2-yl)quinolone (**2k**)[3]: light yellow oil was obtained in 61% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 1.2 Hz, 1H), 7.95 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.72 (d, *J* = 1.6 Hz, 2H), 7.48 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.33 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.20 (d, *J* = 8.3 Hz, 1H), 7.11 (dd, *J* = 5.1, 3.6 Hz, 1H), 2.72 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 148.0, 143.7, 135.7, 135.1, 128.2, 127.9, 125.7, 125.6, 124.4, 124.0, 123.9, 121.7, 25.3.



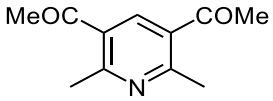
7-Nitroquinoline (**2l**) [2]: orange solid was obtained in 27% isolated yield. ^{1}H NMR (400 MHz, DMSO-*d*^{6}) δ 9.09 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.75 (d, *J* = 2.3 Hz, 1H), 8.54 (ddd, *J* = 8.4, 1.6, 0.8 Hz, 1H), 8.30 (dd, *J* = 9.0, 2.3 Hz, 1H), 8.23 (d, *J* = 9.0 Hz, 1H), 7.74 (dd, *J* = 8.4, 4.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-*d*^{6}) δ 154.2, 148.6, 147.2, 137.3, 132.3, 131.4, 125.6, 125.5, 120.8.



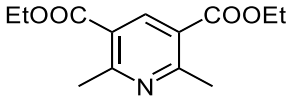
6-Bromoquinoline (**2m**) [1]: colorless oil was obtained in 65% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 – 8.85 (m, 1H), 8.10 – 8.02 (m, 1H), 8.00 – 7.91 (m, 2H), 7.82 – 7.72 (m, 1H), 7.41 (ddd, *J* = 8.3, 4.2, 1.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 146.7, 135.0, 132.9, 131.1, 129.7, 129.3, 121.8, 120.4.



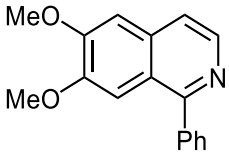
2,3'-Biquinoline (**2n**) [1]: white solid was obtained in 63% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (d, *J* = 8.6 Hz, 2H), 8.32 (dd, *J* = 8.6, 0.9 Hz, 2H), 8.23 (dt, *J* = 8.5, 1.0 Hz, 2H), 7.87 (dd, *J* = 8.1, 1.5 Hz, 2H), 7.75 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 2H), 7.57 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.2, 147.9, 136.7, 129.9, 129.5, 128.4, 127.6, 126.9, 119.4.



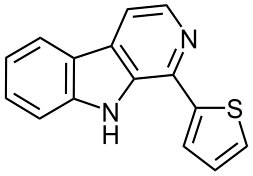
1,1'-(2,6-Dimethylpyridine-3,5-diyl)bis(ethan-1-one) (**2o**) [4]: white solid was obtained in 82% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 1H), 2.78 (t, *J* = 2.3 Hz, 6H), 2.65 (t, *J* = 1.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.1, 160.1, 137.7, 130.0, 29.3, 24.9.



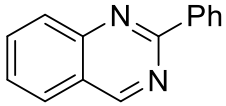
Diethyl 2,6-dimethylpyridine-3,5-dicarboxylate (**2p**) [5]: white solid was obtained in 90% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (s, 1H), 4.33 (q, *J* = 7.1 Hz, 4H), 2.77 (s, 6H), 1.35 (t, *J* = 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 162.0, 140.7, 122.8, 61.2, 24.8, 14.1.



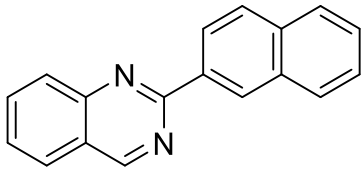
6,7-Dimethoxy-1-phenylisoquinoline (**2q**)[6]: white solid was obtained in 82% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 5.6 Hz, 1H), 7.75 – 7.67 (m, 2H), 7.57 – 7.44 (m, 4H), 7.37 (s, 1H), 7.11 (s, 1H), 4.03 (s, 3H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 152.4, 149.8, 141.2, 139.9, 133.6, 129.4, 128.3, 122.3, 118.6, 105.3, 104.8, 55.9, 55.7.



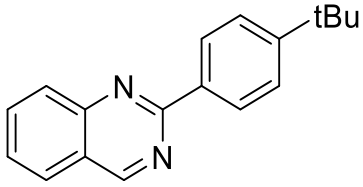
1-(Thiophen-2-yl)-9H-pyrido[3,4-b]indole (**2r**)[7]: white solid was obtained in 59% isolated yield.^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 (s, 1H), 8.40 (d, *J* = 5.2 Hz, 1H), 8.03 (d, *J* = 7.9 Hz, 1H), 7.78 (d, *J* = 5.2 Hz, 1H), 7.70 (d, *J* = 3.6 Hz, 1H), 7.50 – 7.37 (m, 2H), 7.32 (d, *J* = 5.1 Hz, 1H), 7.23 (t, *J* = 7.0 Hz, 1H), 7.00 (dd, *J* = 5.1, 3.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 140.5, 139.0, 137.0, 132.1, 130.3, 128.5, 127.9, 127.1, 125.1, 121.64, 121.58, 120.4, 113.7, 111.7.



2-Phenylquinazoline (**4a**) [8]: white solid was obtained in 70% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.62 (dd, *J* = 6.7, 1.6 Hz, 2H), 8.10 – 8.01 (m, 1H), 7.91 – 7.81 (m, 2H), 7.61 – 7.45 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 160.4, 150.6, 137.9, 134.0, 130.5, 128.6, 128.56, 128.51, 127.2, 127.0, 123.5.

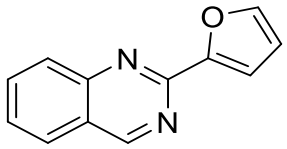


2-(Naphthalen-2-yl)quinazoline (**4b**) [8]: white solid was obtained in 71% isolated yield. ^{1}H NMR (400 MHz, DMSO-d^6) δ 9.76 (s, 1H), 9.19 (d, *J* = 1.7 Hz, 1H), 8.70 (dd, *J* = 8.6, 1.7 Hz, 1H), 8.23 – 7.99 (m, 6H), 7.77 (t, *J* = 7.4 Hz, 1H), 7.62 (td, *J* = 7.4, 6.7, 3.7 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d^6) δ 162.4, 160.7, 150.9, 135.9, 135.9, 135.2, 133.9, 130.1, 129.4, 129.3, 128.9, 128.9, 128.8, 128.7, 128.5, 127.6, 126.0, 124.4.

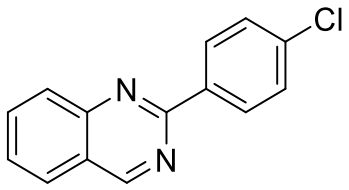


2-(4-(Tert-butyl)phenyl)quinazoline (**4c**): white solid was obtained in 76% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.44 (s, 1H), 8.59 – 8.50 (m, 2H), 8.07 (dd, *J* =

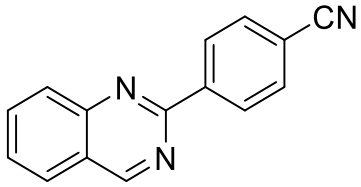
8.3, 1.0 Hz, 1H), 7.97 – 7.82 (m, 2H), 7.56 (d, *J* = 8.6 Hz, 3H), 1.39 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1, 160.4, 153.9, 150.7, 135.2, 134.0, 128.5, 128.3, 127.1, 127.0, 125.6, 123.4, 34.8, 31.2.



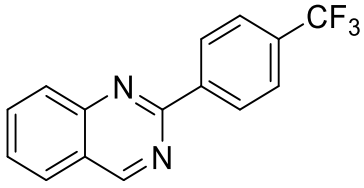
2-(Furan-2-yl)quinazoline (**4d**) [8]: white solid was obtained in 68% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.36 (s, 1H), 8.08 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.95 – 7.82 (m, 2H), 7.78 – 7.67 (m, 1H), 7.57 (ddd, *J* = 8.0, 6.9, 1.1 Hz, 1H), 7.46 (dd, *J* = 3.4, 0.9 Hz, 1H), 6.62 (dd, *J* = 3.4, 1.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 153.9, 152.3, 150.2, 145.2, 134.4, 128.2, 127.1, 123.2, 114.0, 112.2.



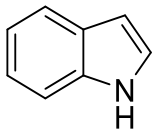
2-(4-Chlorophenyl)quinazoline (**4e**) [8]: white solid was obtained in 58% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.61 – 8.50 (m, 2H), 8.10 – 8.02 (m, 1H), 7.97 – 7.87 (m, 2H), 7.66 – 7.57 (m, 1H), 7.54 – 7.45 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 159.9, 150.6, 136.8, 136.4, 134.2, 129.8, 128.8, 128.5, 127.4, 127.1, 123.5.



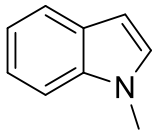
4-(Quinazolin-2-yl)benzonitrile (**4f**) [8]: white solid was obtained in 53% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.49 (s, 1H), 8.80 – 8.70 (m, 2H), 8.11 (dt, *J* = 8.2, 1.1 Hz, 1H), 8.02 – 7.92 (m, 2H), 7.86 – 7.78 (m, 2H), 7.73 – 7.65 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 159.0, 150.5, 142.1, 134.5, 132.3, 128.9, 128.7, 128.1, 127.2, 123.8, 118.9, 113.7.



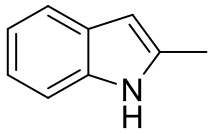
2-(4-(Trifluoromethyl)phenyl)quinazoline (**4g**) [8]: white solid was obtained in 54% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.46 (s, 1H), 8.72 (d, *J* = 8.1 Hz, 2H), 8.09 (d, *J* = 8.7 Hz, 1H), 7.97 – 7.87 (m, 2H), 7.77 (d, *J* = 8.2 Hz, 2H), 7.64 (t, *J* = 7.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.6, 159.5, 150.6, 141.2, 134.3, 132.0 (q, *J* = 32 Hz), 128.8, 128.7, 127.8, 127.1, 125.5 (q, *J* = 3.9 Hz), 124.2 (q, *J* = 271.7 Hz) 123.8. ^{19}F NMR (377 MHz, $CDCl_3$) δ -62.6.



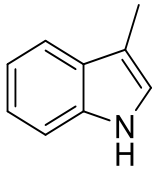
1H-indole (**6a**) [1]: colorless oil was obtained in 85% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.64 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.27 (dq, *J* = 8.1, 1.0 Hz, 1H), 7.18 (ddd, *J* = 8.2, 6.9, 1.3 Hz, 1H), 7.11 (ddd, *J* = 8.1, 6.3, 1.2 Hz, 1H), 7.04 (t, *J* = 2.8 Hz, 1H), 6.52 (ddd, *J* = 3.1, 2.0, 1.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.6, 127.7, 124.2, 121.8, 120.6, 119.7, 111.0, 102.3.



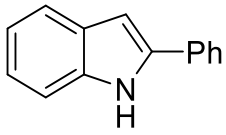
1-Methyl-1H-indole (**6b**) [1]: colorless oil was obtained in 65% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.77 (m, 1H), 7.60 – 7.44 (m, 2H), 7.43 – 7.33 (m, 1H), 7.20 (td, *J* = 3.4, 1.3 Hz, 1H), 6.83 – 6.66 (m, 1H), 3.88 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.5, 128.7, 128.3, 121.3, 120.7, 119.1, 109.1, 100.7, 32.5.



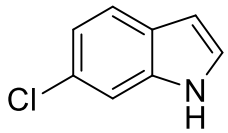
2-Methyl-1H-indole (**6c**) [1]: colorless oil was obtained in 86% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (t, *J* = 5.7 Hz, 1H), 7.41 (s, 1H), 7.14 – 7.03 (m, 3H), 6.21 – 6.13 (m, 1H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.9, 135.1, 128.8, 120.7, 119.5, 110.3, 100.1, 13.4.



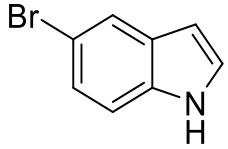
3-Methyl-1H-indole (**6d**) [1]: colorless oil was obtained in 76% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.24 – 7.16 (m, 1H), 7.15 – 7.08 (m, 1H), 6.93 (d, *J* = 1.1 Hz, 1H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.2, 128.2, 121.8, 121.5, 119.0, 118.8, 111.6, 110.9, 9.6.



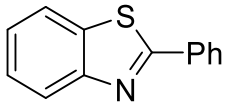
2-Phenyl-1H-indole (**6e**) [1]: white solid was obtained in 79% isolated yield.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.63 (d, *J* = 7.5 Hz, 3H), 7.47 – 7.08 (m, 6H), 6.82 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.8, 136.7, 132.3, 129.2, 129.0, 127.7, 125.1, 122.3, 120.6, 120.2, 110.9, 99.9.



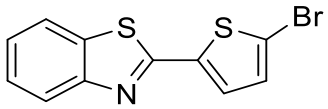
6-Chloro-1H-indole (**6f**) [8]: white solid was obtained in 82% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.35 (dd, *J* = 1.7, 0.9 Hz, 1H), 7.19 – 7.13 (m, 2H), 6.58 (td, *J* = 2.1, 1.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.0, 127.7, 126.3, 124.9, 121.5, 120.5, 110.9, 102.6.



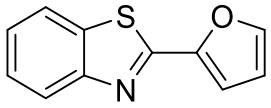
5-Bromo-1H-indole (**6g**) [1]: white solid was obtained in 73% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.76 (d, *J* = 1.9 Hz, 1H), 7.27 – 7.12 (m, 3H), 6.47 (d, *J* = 2.1 Hz, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ 134.3, 129.5, 125.4, 124.7, 123.1, 112.9, 112.4, 102.2.



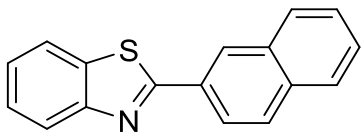
2-Phenylbenzo[d]thiazole (**6h**) [1]: light yellow solid was obtained in 81% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 – 8.03 (m, 3H), 7.87 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.50 – 7.44 (m, 4H), 7.40 – 7.33 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 154.0, 134.9, 133.4, 130.8, 128.9, 127.4, 126.2, 125.1, 123.1, 121.5.



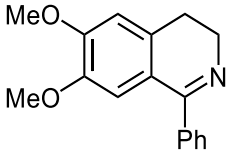
2-(5-Bromothiophen-2-yl)benzo[d]thiazole (**6i**) [10]: light yellow solid was obtained in 67% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (ddd, *J* = 8.2, 1.2, 0.7 Hz, 1H), 7.82 (ddd, *J* = 8.0, 1.3, 0.7 Hz, 1H), 7.50 – 7.43 (m, 1H), 7.39 – 7.32 (m, 2H), 7.07 (d, *J* = 4.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 153.4, 138.6, 134.4, 130.9, 128.4, 126.5, 125.4, 123.0, 121.4, 117.1.



2-(Furan-2-yl)benzo[d]thiazole (**6j**) [11]: light yellow solid was obtained in 82% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.01 (m, 1H), 7.89 – 7.81 (m, 1H), 7.60 – 7.55 (m, 1H), 7.47 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 7.35 (ddd, *J* = 8.2, 7.2, 1.2 Hz, 1H), 7.17 (dd, *J* = 3.5, 0.7 Hz, 1H), 6.56 (dd, *J* = 3.5, 1.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 153.6, 148.6, 144.6, 134.1, 126.4, 125.1, 123.0, 121.5, 112.4, 111.3.



2-(Naphthalen-2-yl)benzo[d]thiazole (**6k**) [1]: light yellow solid was obtained in 84% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.18 – 8.05 (m, 2H), 7.92 – 7.77 (m, 4H), 7.52 – 7.42 (m, 3H), 7.33 (td, *J* = 7.6, 7.2, 1.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.0, 154.1, 135.0, 134.5, 133.0, 130.8, 128.71, 128.70, 127.8, 127.5, 127.3, 126.8, 126.3, 125.1, 124.3, 123.1, 121.5.



6,7-Dimethoxy-1-phenyl-3,4-dihydroisoquinoline (**7**) [9]: light yellow oil was obtained with 37% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.54 (m, 2H), 7.44 (dd, *J* = 5.1, 1.9 Hz, 3H), 6.79 (d, *J* = 2.6 Hz, 2H), 3.95 (s, 3H), 3.85 – 3.77 (m, 2H), 3.73 (s, 3H), 2.77 – 2.70 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 150.8, 147.0, 139.0, 132.5, 129.2, 128.7, 128.1, 121.5, 111.4, 110.1, 56.1, 56.0, 47.6, 25.9.

References

[1] K. H. He, F. F. Tan, C. Z. Zhou, G. J. Zhou, X. L. Yang, Y. Li, *Angew. Chem. Int. Ed.* **2017**, *56*, 3080-3084.

[2] M. Planellas, W. Guo, F. Alonso, M. Yus, A. Shafir, R. Pleixats, T. Parella, *Adv. Synth. Catal.* **2014**, *356*, 179-188.

[3] S. S. Kulkarni, A. H. Newman, *Bioorg. Med. Chem. Lett.* **2007**, *17*, 2987-2991.

[4] A. F. Maier, S. Tussing, T. Schneider, U. Florke, Z. W. Qu, S. Grimme, J. Paradies, *Angew. Chem. Int. Ed.* **2016**, *55*, 12219-12223.

[5] M. Hayashi, N. Nakamichi, Y. Kawashita, *Synthesis* **2004**, *7*, 1015-1020.

[6] S. Hati, S. Sen, *Eur. J. Org. Chem.* **2017**, *2017*, 1277-1280.

[7] P. Rocca, F. Marsais, A. Godard, G. Queguiner, *Tetrahedron* **1993**, *49*, 3325-3342.

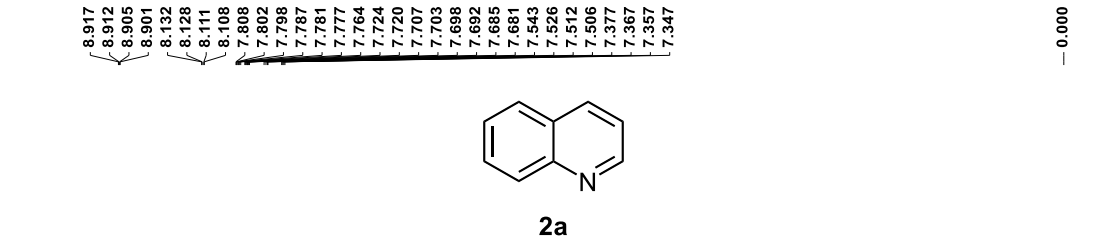
[8] J. Zhang, S. Chen, F. Chen, W. Xu, G.-J. Deng, H. Gong, *Adv. Synth. Catal.* **2017**, *359*, 2358-2363

[9] A. E. Wendlandt, S. S. Stahl, *J. Am. Chem. Soc.* **2014**, *136*, 506-512.

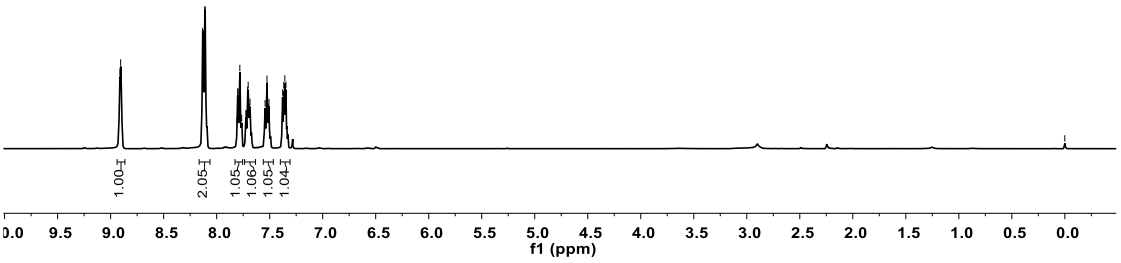
[10] X. Chen, X. Huang, Q. He, Y. Xie, C. Yang, *Chem. Commun.* **2014**, *50*, 3996-3999.

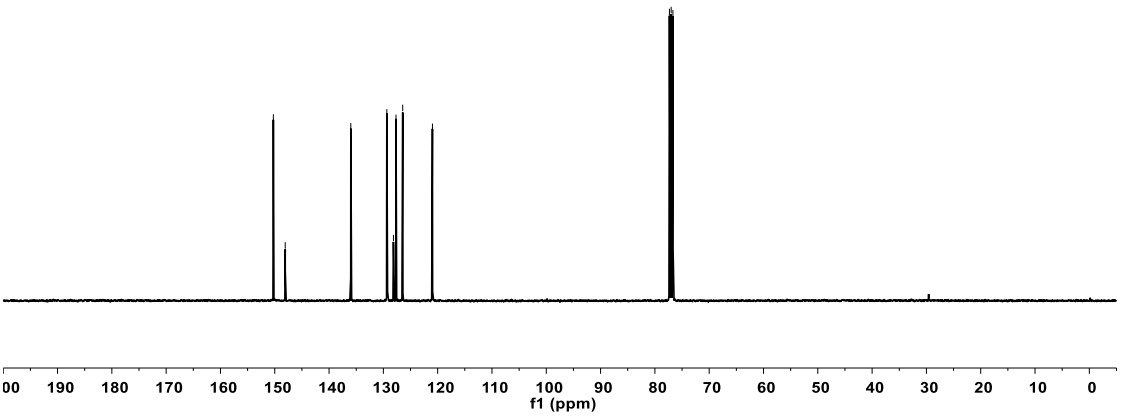
[11] X. Shi, J. Guo, J. Liu, M. Ye, Q. Xu, *Chem. Eur. J.* **2015**, *21*, 9988-9993.

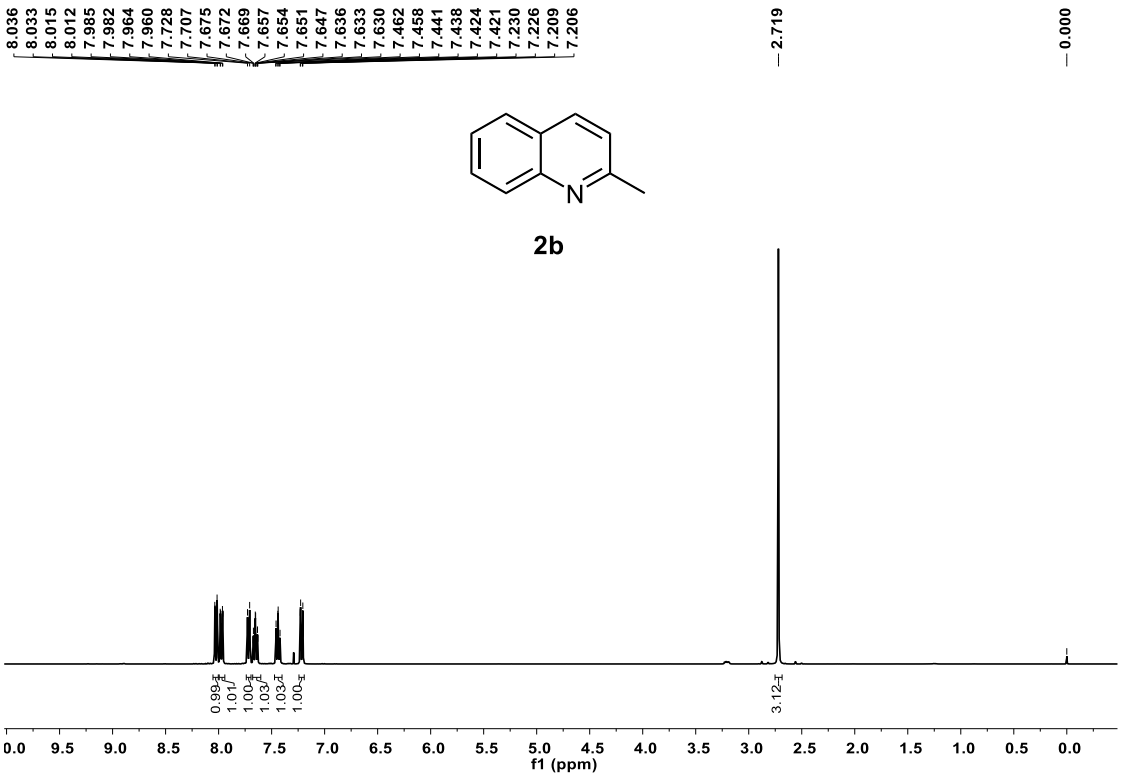
Copies of product NMR spectra



2a



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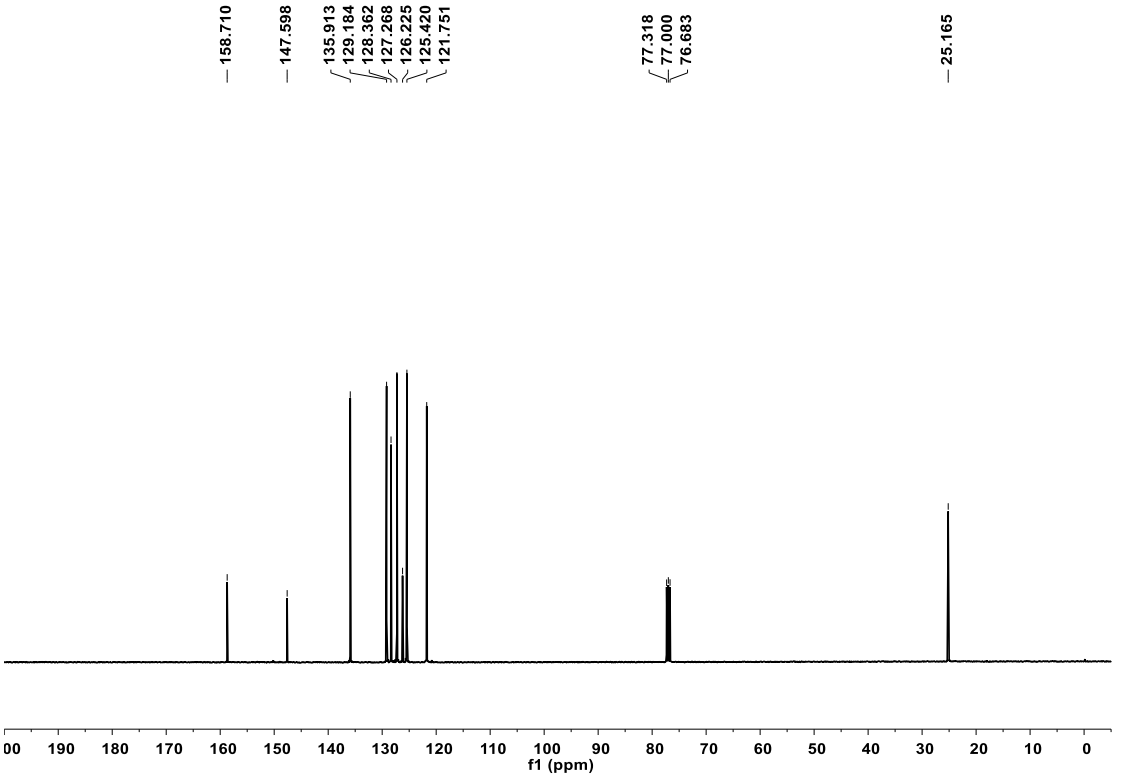
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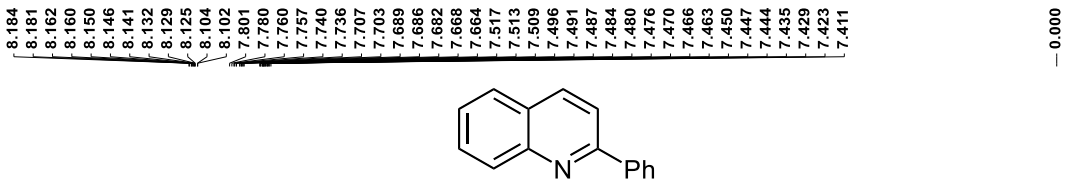
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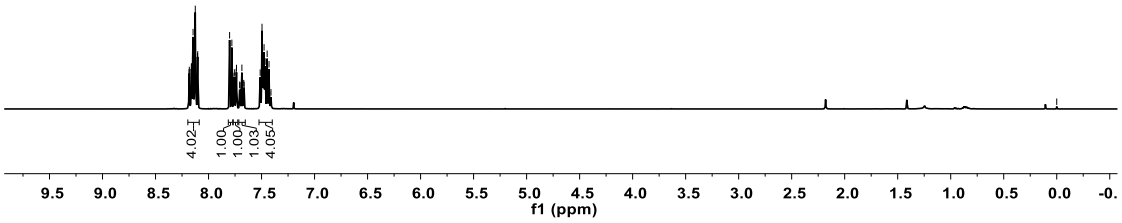
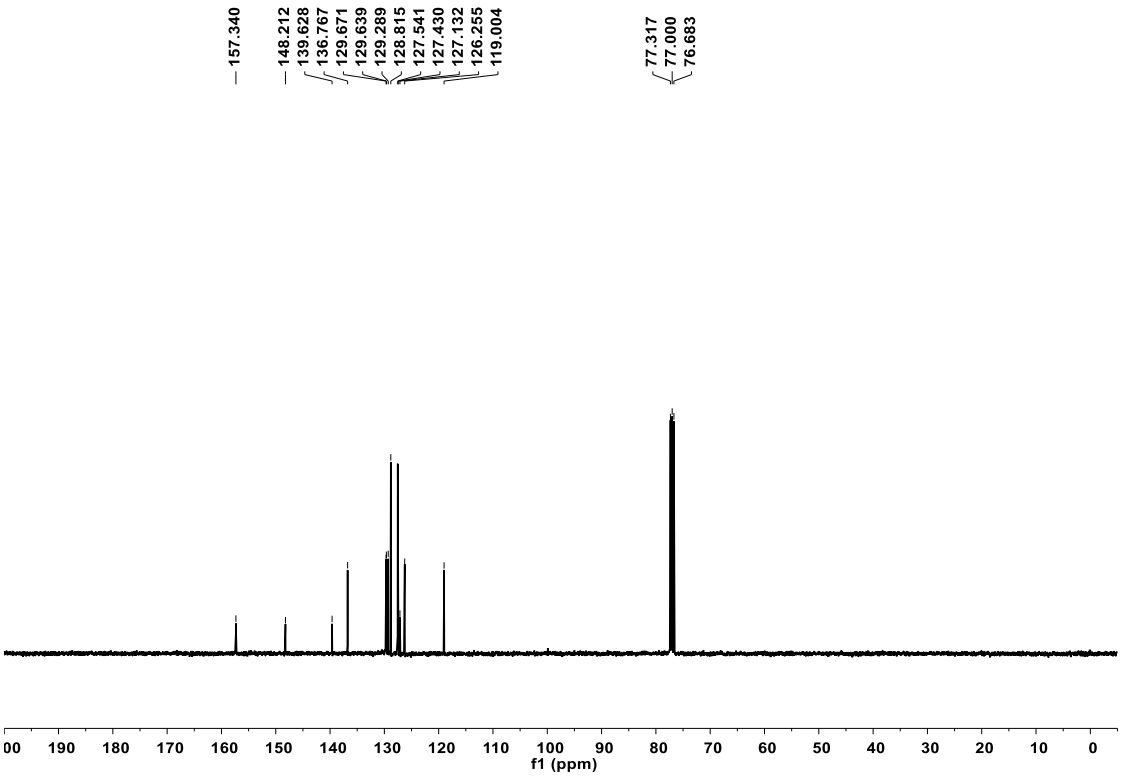
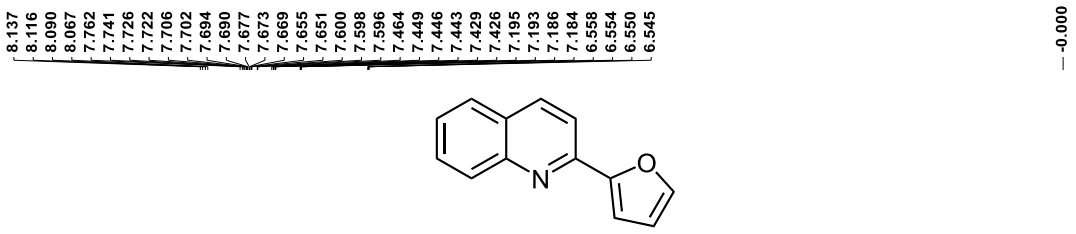
0.000
N
Ph

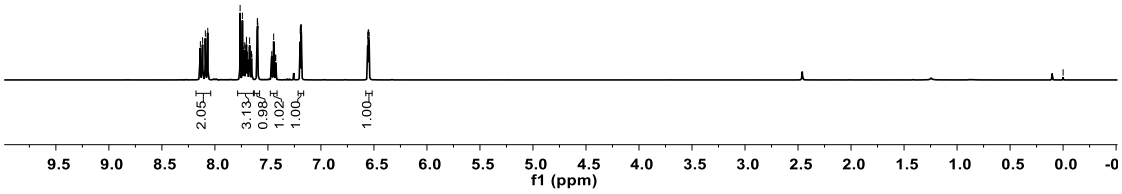
2c

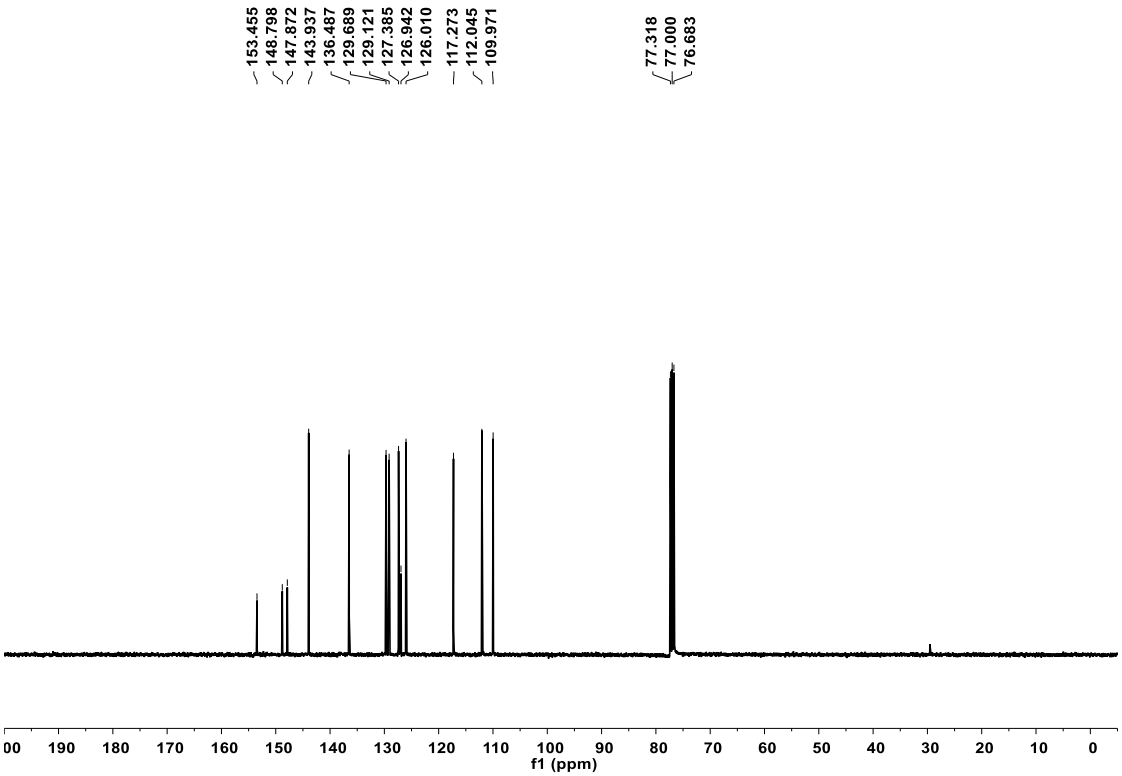

4.02
1.00
1.00
1.03
4.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

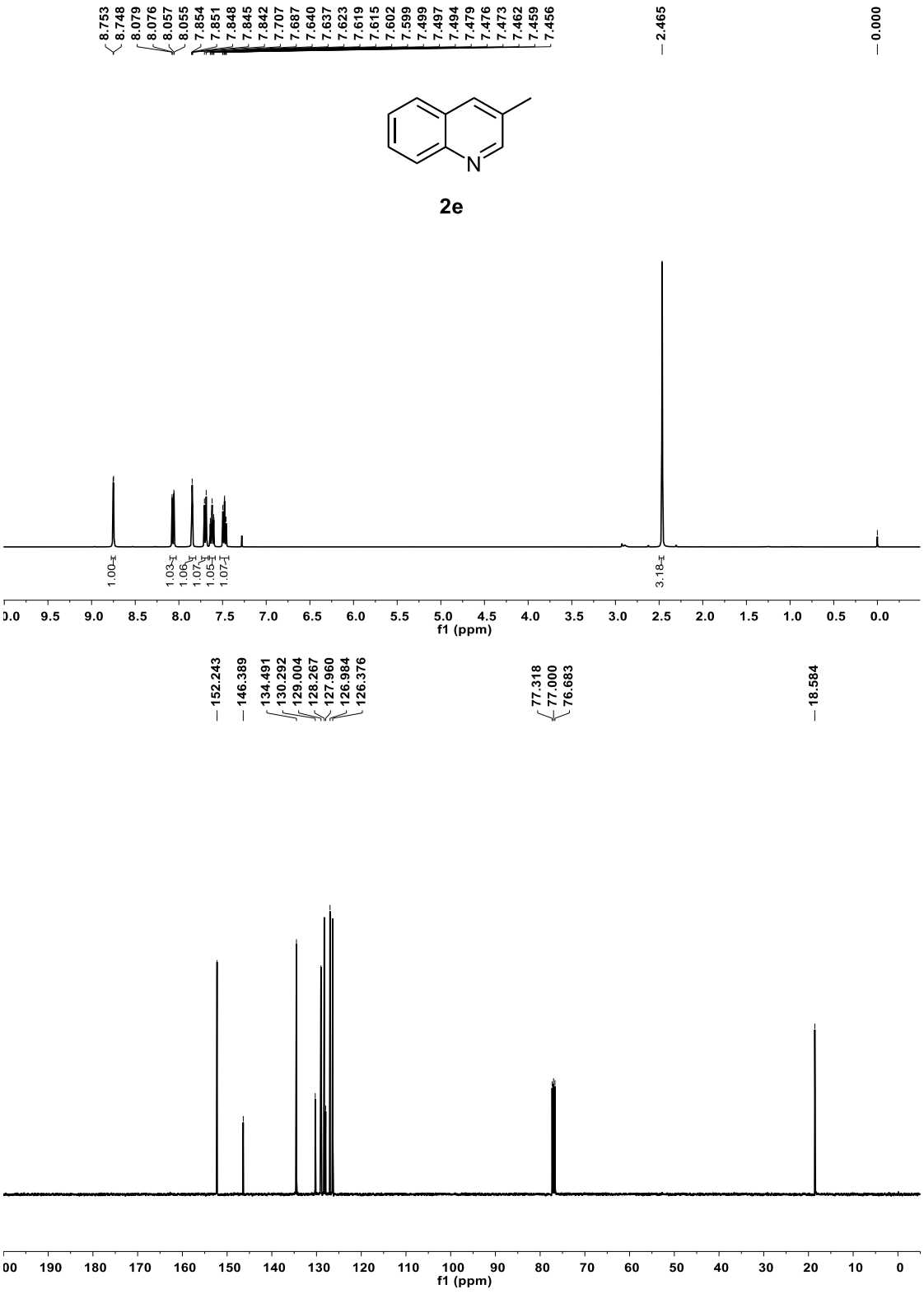

157.340
148.212
139.628
136.767
129.671
129.639
129.289
128.815
127.541
127.430
127.132
126.255
119.004
77.317
77.000
76.683
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

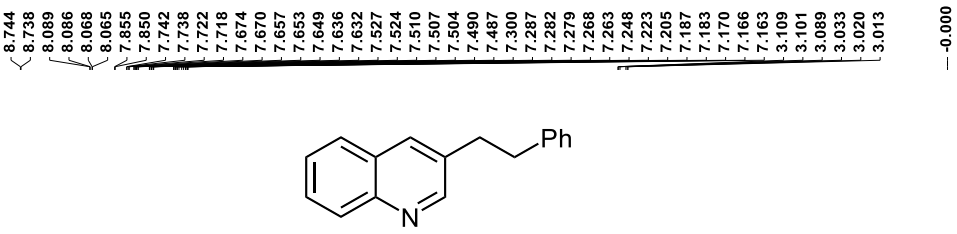

8.137
8.116
8.090
8.067
7.762
7.741
7.726
7.722
7.706
7.702
7.694
7.690
7.677
7.673
7.669
7.655
7.651
7.600
7.598
7.596
7.464
7.449
7.446
7.443
7.429
7.426
7.195
7.193
7.186
7.184
6.558
6.554
6.550
6.545
-0.000
N
O

2d

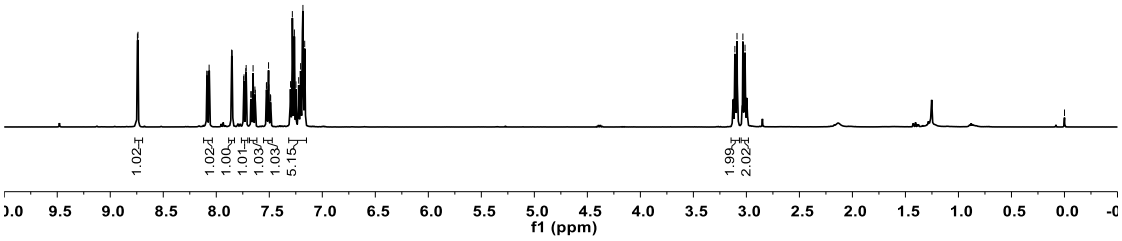

2.05
3.13
0.98
1.02
1.00
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

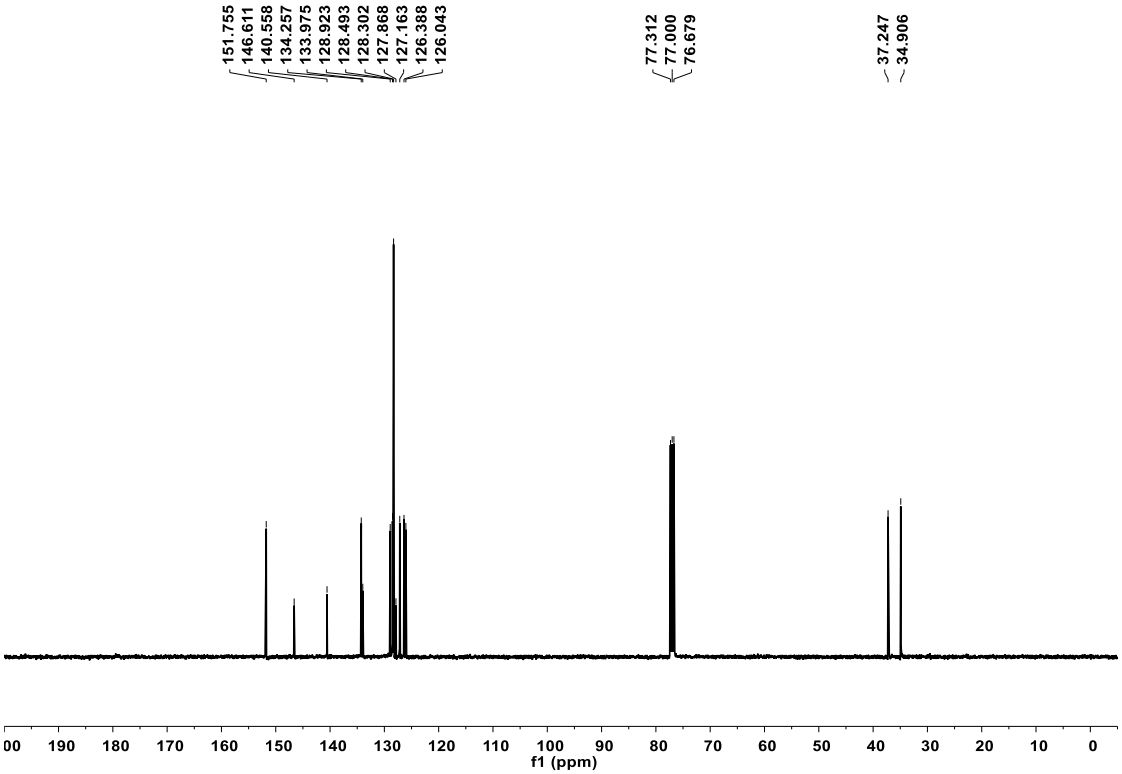

153.455
148.798
147.872
143.937
136.487
129.689
129.121
127.385
126.942
126.010
117.273
112.045
109.971
77.318
77.000
76.683
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

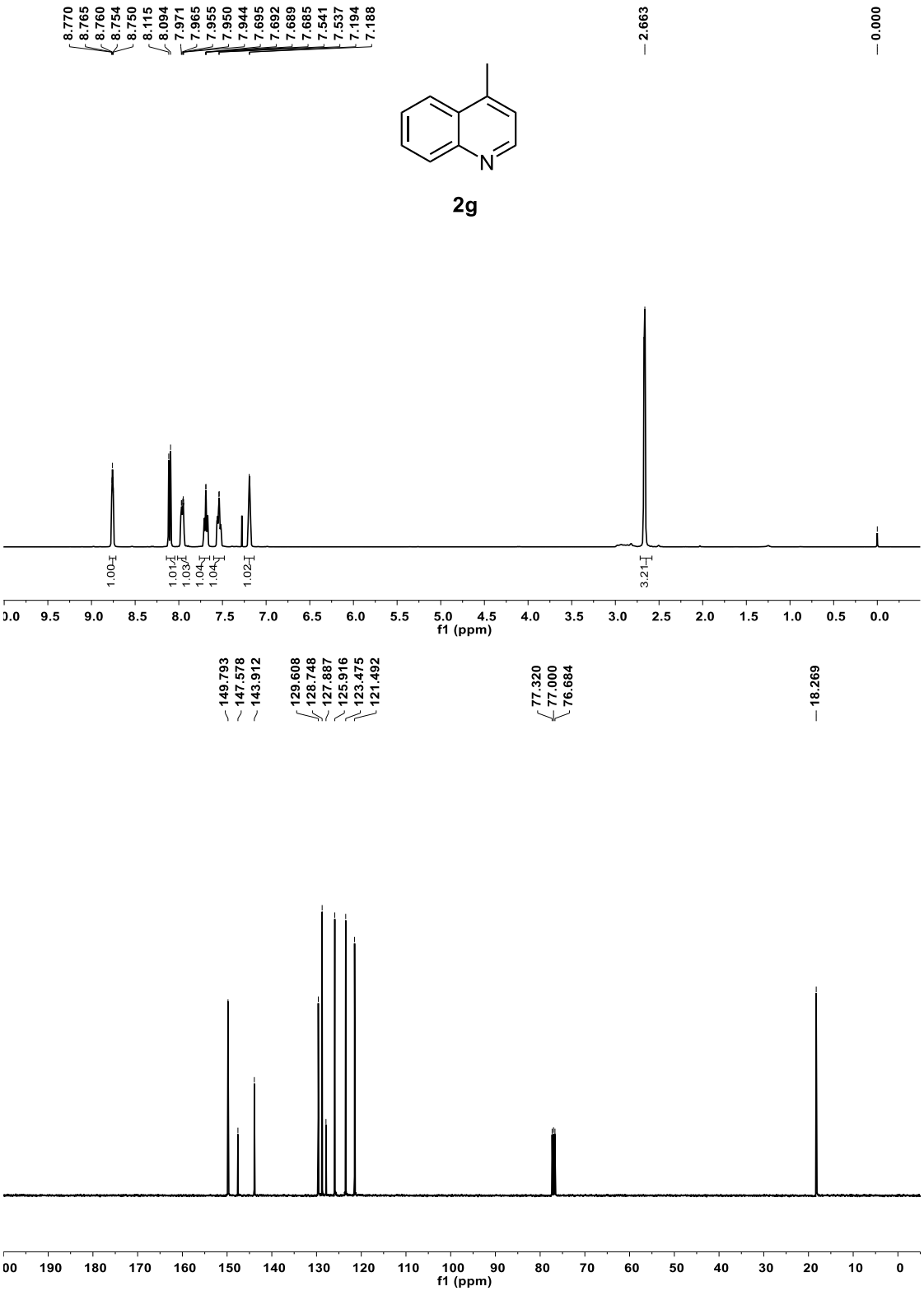

8.753
8.748
8.079
8.076
8.057
8.055
7.854
7.851
7.848
7.845
7.842
7.707
7.687
7.640
7.637
7.623
7.619
7.615
7.602
7.599
7.499
7.497
7.494
7.479
7.476
7.473
7.462
7.459
7.456
2.465
0.000
N
2e
1.00
1.03
1.06
1.07
1.05
1.07
3.18
f1 (ppm)
152.243
146.389
134.491
130.292
129.004
128.267
127.960
126.984
126.376
77.318
77.000
76.683
18.584
f1 (ppm)


8.744
8.738
8.089
8.086
8.068
8.065
7.855
7.850
7.742
7.738
7.722
7.718
7.674
7.670
7.657
7.653
7.649
7.636
7.632
7.527
7.524
7.510
7.507
7.504
7.490
7.487
7.300
7.287
7.282
7.279
7.268
7.263
7.248
7.223
7.205
7.187
7.183
7.170
7.166
7.163
3.109
3.101
3.089
3.033
3.020
3.013
-0.000
Ph
N

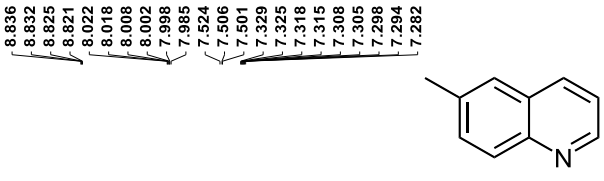
2f


1.02
1.02
1.00
1.01
1.03
5.15
1.99
2.02
f1 (ppm)

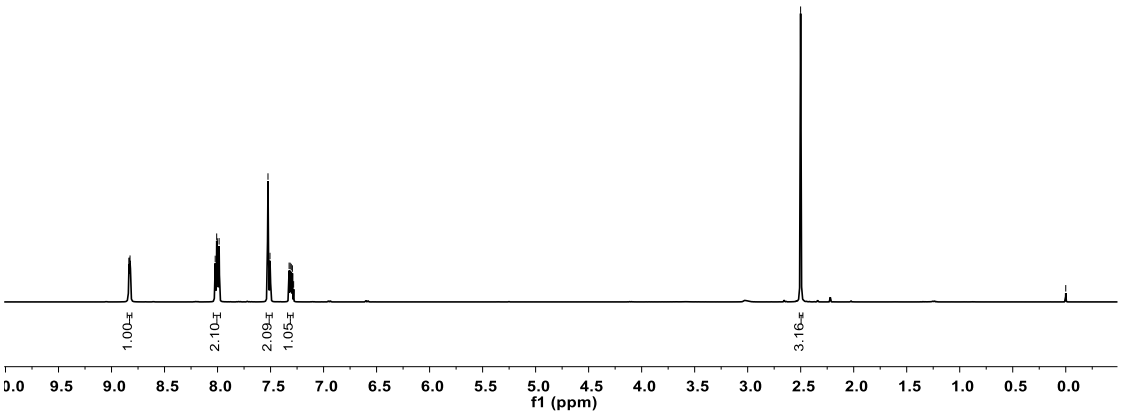

151.755
146.611
140.558
134.257
133.975
128.923
128.493
128.302
127.868
127.163
126.388
126.043
77.312
77.000
76.679
37.247
34.906
f1 (ppm)

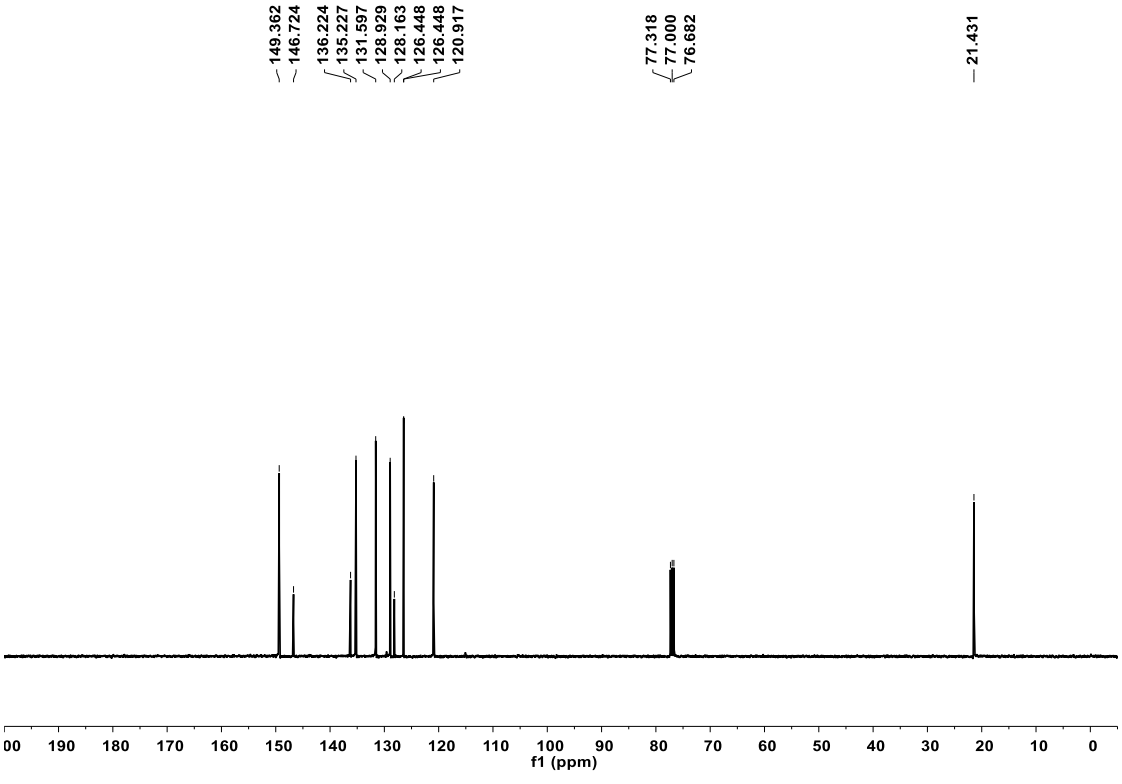

8.770
8.765
8.760
8.754
8.750
8.115
8.094
7.971
7.965
7.955
7.950
7.944
7.695
7.692
7.689
7.685
7.541
7.537
7.194
7.188
2.663
0.000
N
1.00
1.01
1.03
1.04
1.04
1.02
3.21
f1 (ppm)
149.793
147.578
143.912
129.608
128.748
127.887
125.916
123.475
121.492
77.320
77.000
76.684
18.269
f1 (ppm)

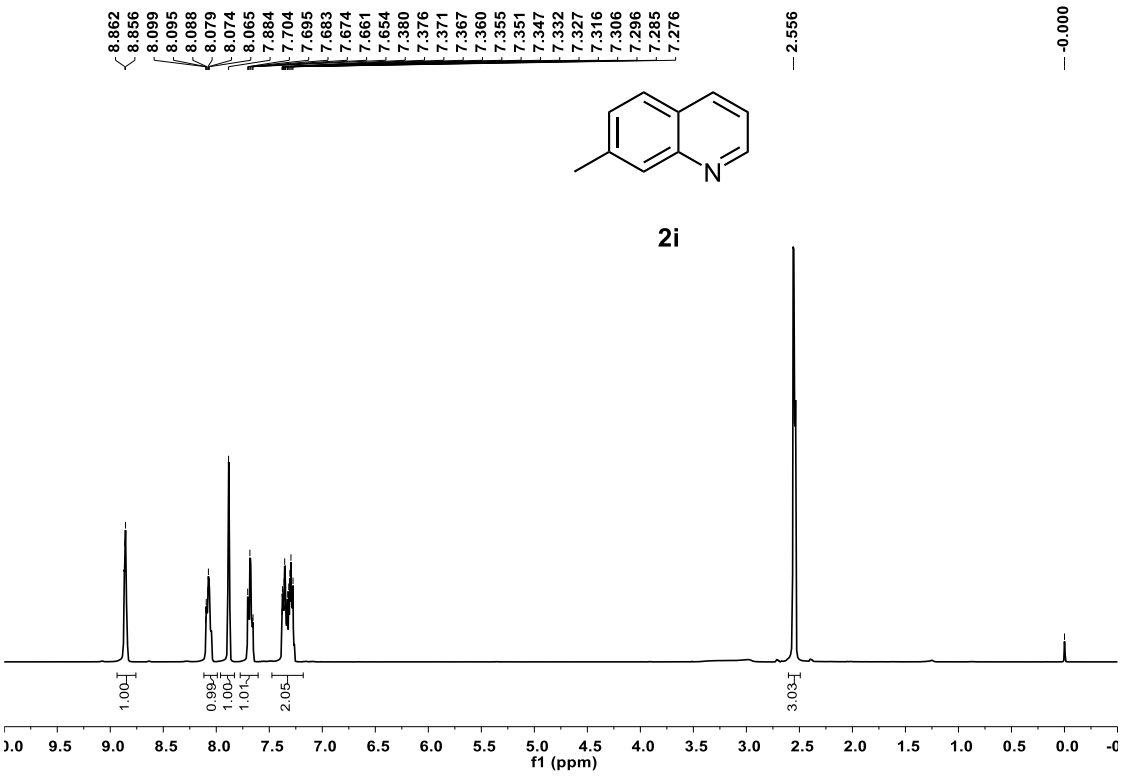
2g

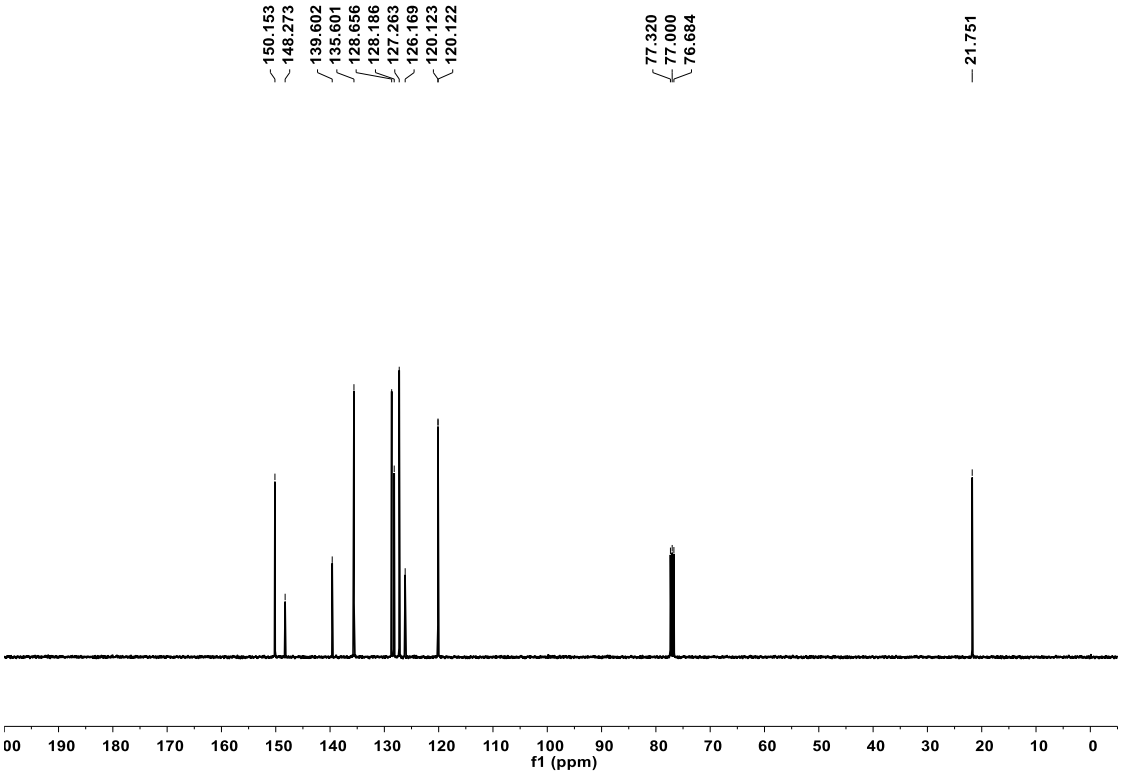

8.836
8.832
8.825
8.821
8.022
8.018
8.008
8.002
7.998
7.985
7.524
7.506
7.501
7.329
7.325
7.318
7.315
7.308
7.305
7.298
7.294
7.282
2.501
0.000
N

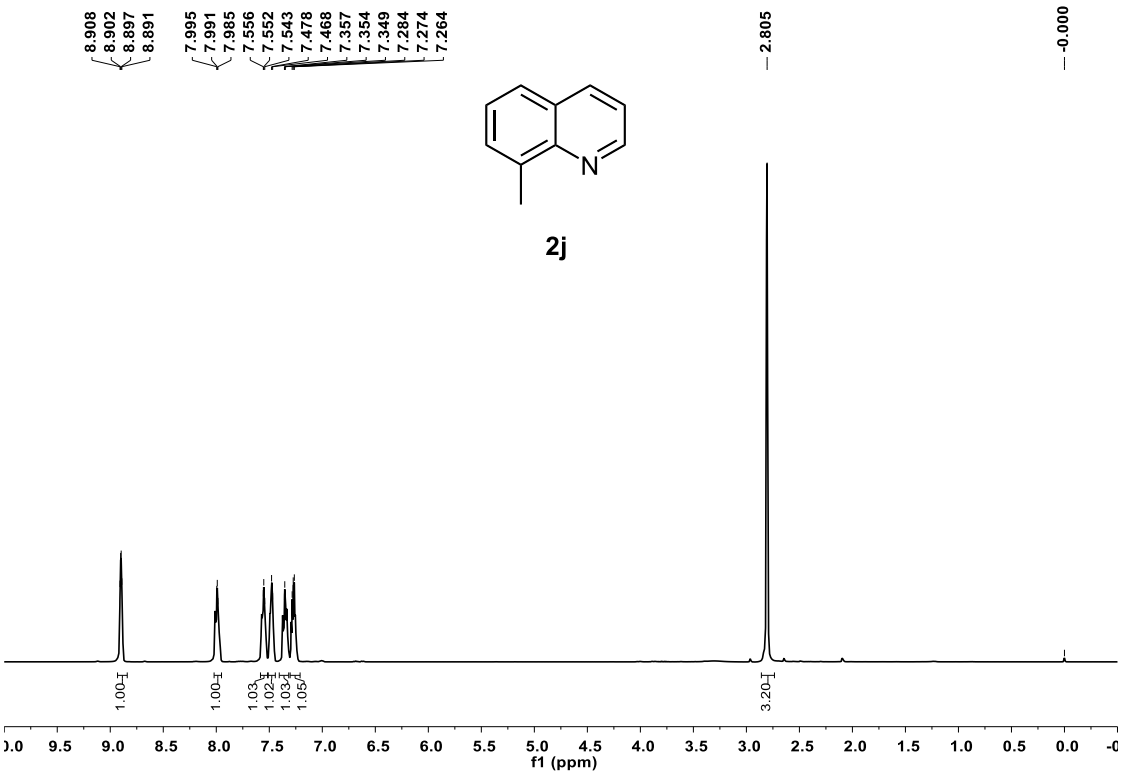
2h

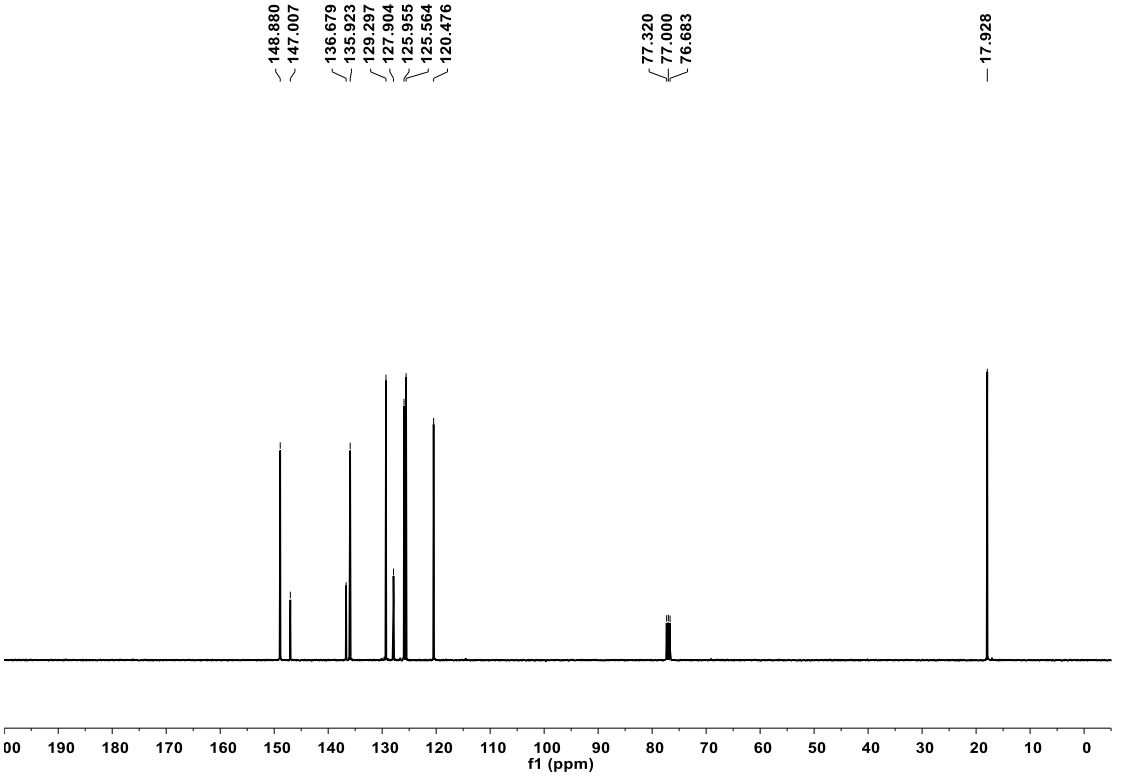

1.00
2.10
2.09
1.05
3.16
f1 (ppm)

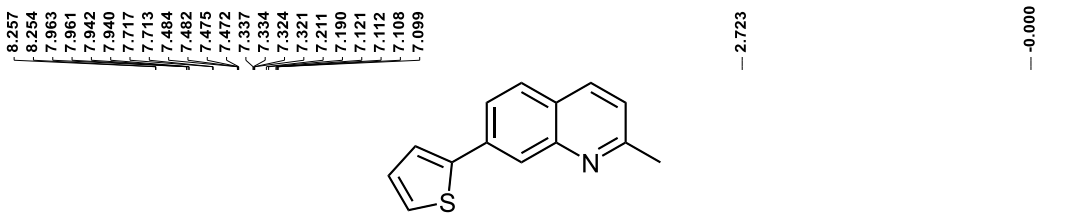

149.362
146.724
136.224
135.227
131.597
128.929
128.163
126.448
126.448
120.917
77.318
77.000
76.682
21.431
f1 (ppm)


8.862
8.856
8.099
8.095
8.088
8.079
8.074
8.065
7.884
7.704
7.695
7.683
7.674
7.661
7.654
7.380
7.376
7.371
7.367
7.360
7.355
7.351
7.347
7.332
7.327
7.316
7.306
7.296
7.285
7.276
2.556
-0.000
N
2i
1.00
0.99
1.00
1.01
2.05
3.03
f1 (ppm)

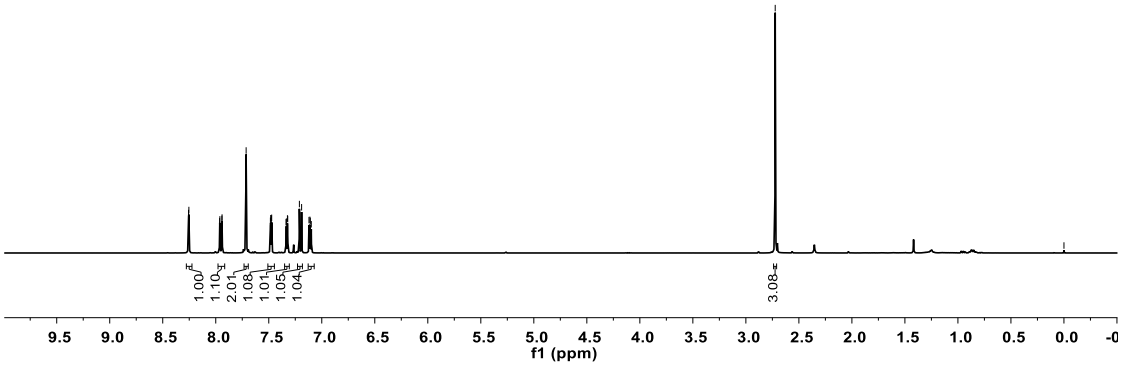

150.153
148.273
139.602
135.601
128.656
128.186
127.263
126.169
120.123
120.122
77.320
77.000
76.684
21.751
f1 (ppm)

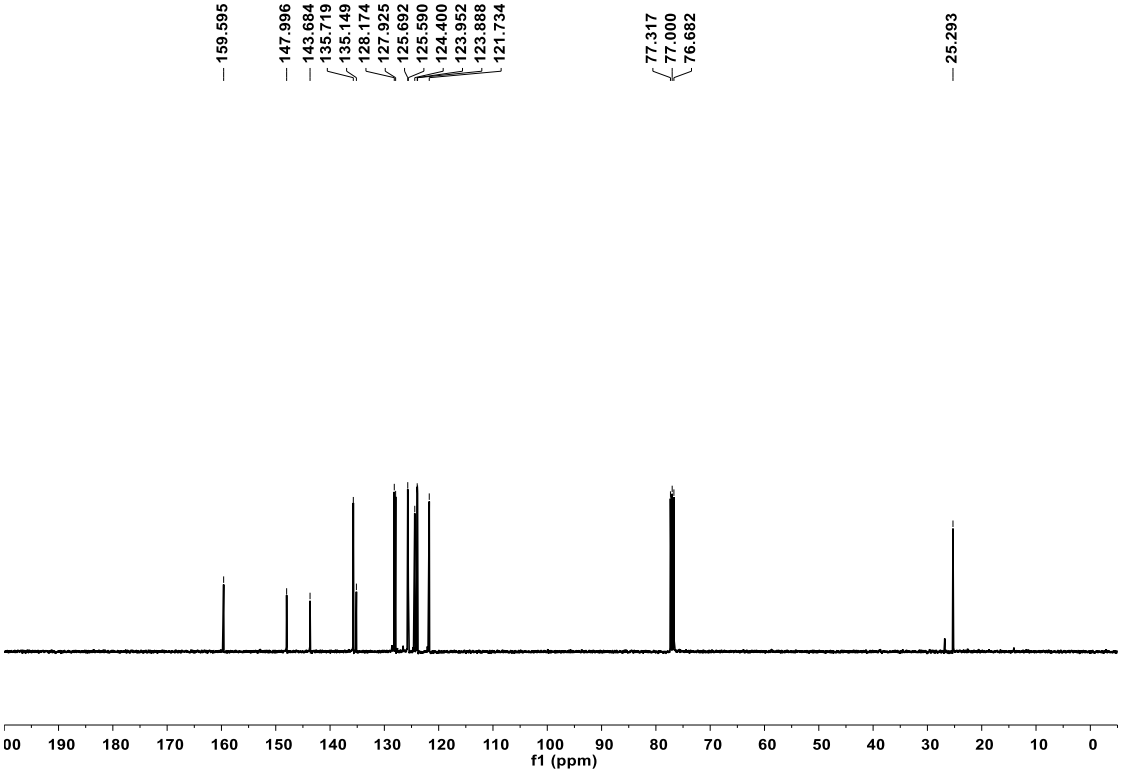

8.908
8.902
8.897
8.891
7.995
7.991
7.985
7.556
7.552
7.543
7.478
7.468
7.357
7.354
7.349
7.284
7.274
7.264
2.805
-0.000
N
2j
1.00
1.00
1.03
1.02
1.03
1.05
3.20
f1 (ppm)

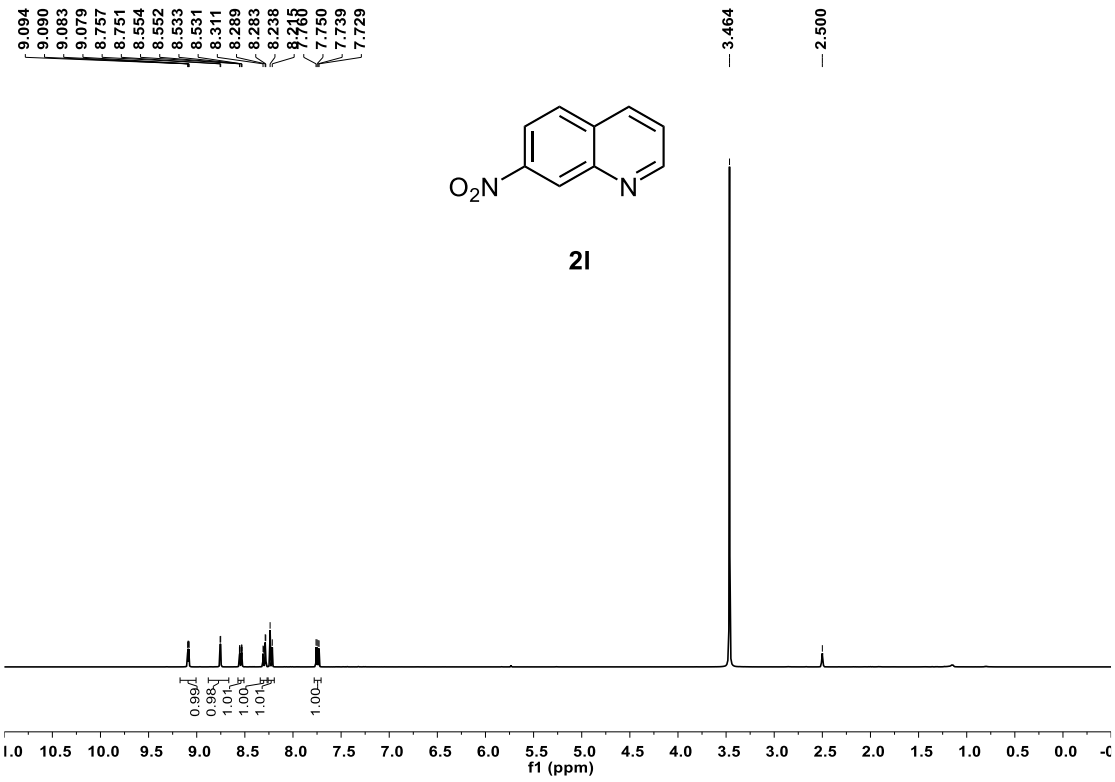

148.880
147.007
136.679
135.923
129.297
127.904
125.955
125.564
120.476
77.320
77.000
76.683
17.928
f1 (ppm)


8.257
8.254
7.963
7.961
7.942
7.940
7.717
7.713
7.484
7.482
7.475
7.472
7.337
7.334
7.324
7.321
7.211
7.190
7.121
7.112
7.108
7.099
2.723
-0.000
N
S

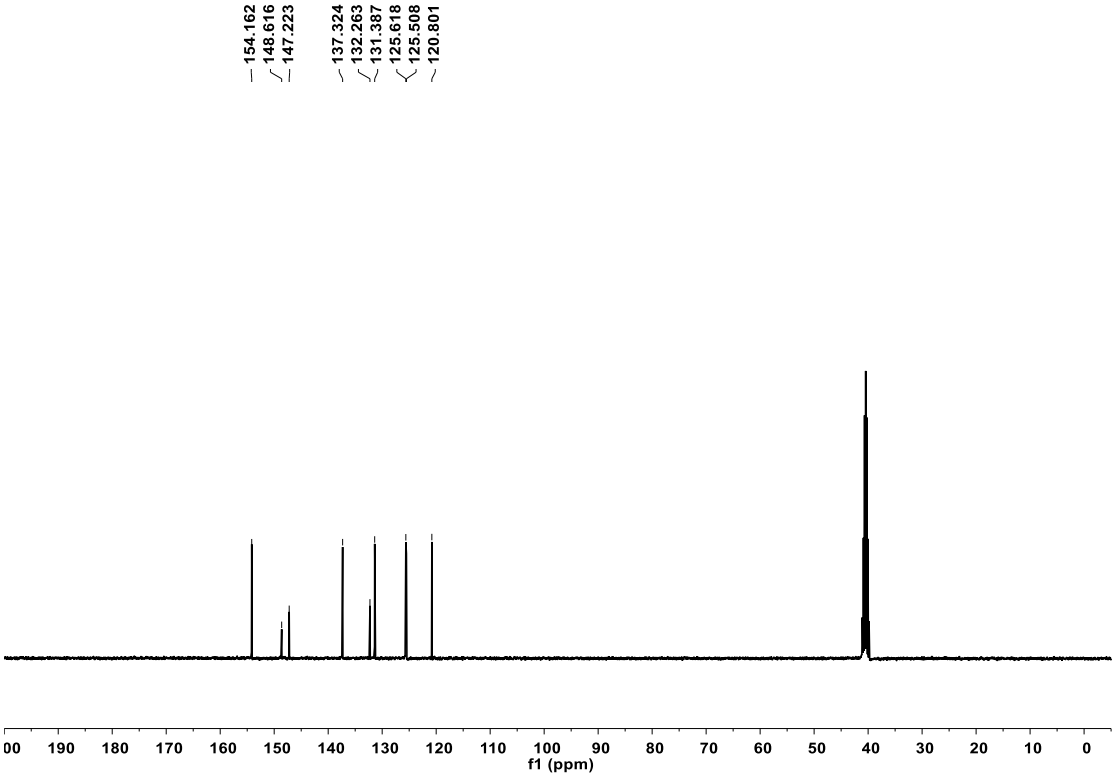
2k

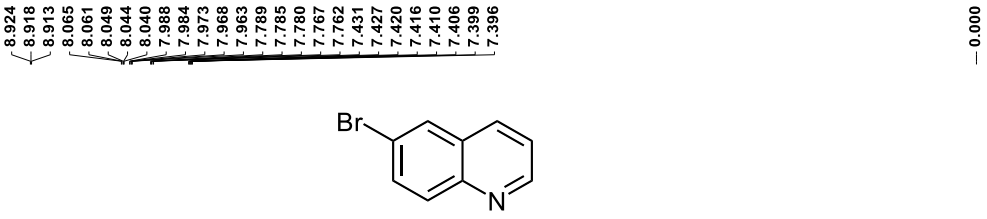

1.00
1.10
2.01
1.08
1.01
1.05
1.04
3.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


159.595
147.996
143.684
135.719
135.149
128.174
127.925
125.692
125.590
124.400
123.952
123.888
121.734
77.317
77.000
76.682
25.293
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.094
9.090
9.083
9.079
8.757
8.751
8.554
8.552
8.533
8.531
8.311
8.289
8.283
8.238
8.215
7.760
7.750
7.739
7.729
3.464
2.500
O2N
N
0.99
0.98
1.01
1.00
1.01
1.00
f1 (ppm)

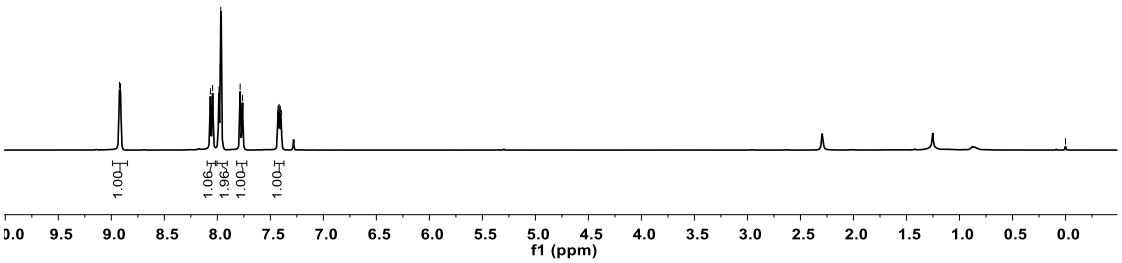
2l

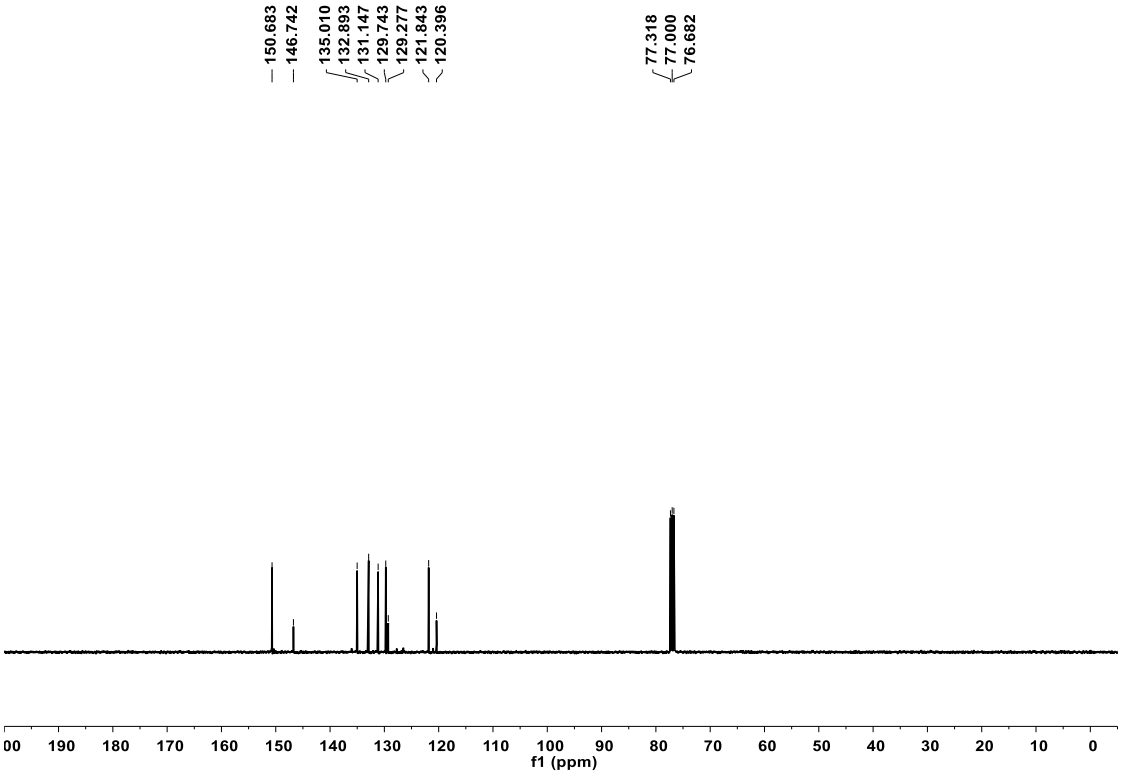

154.162
148.616
147.223
137.324
132.263
131.387
125.618
125.508
120.801
f1 (ppm)

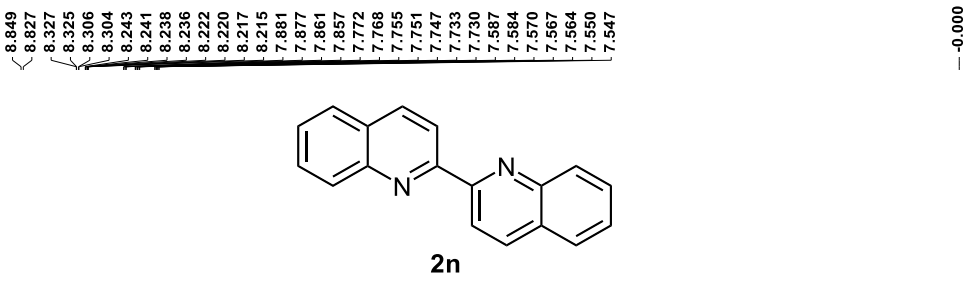

8.924
8.918
8.913
8.065
8.061
8.049
8.044
8.040
7.988
7.984
7.973
7.968
7.963
7.789
7.785
7.780
7.767
7.762
7.431
7.427
7.420
7.416
7.410
7.406
7.399
7.396
0.000

Br
N

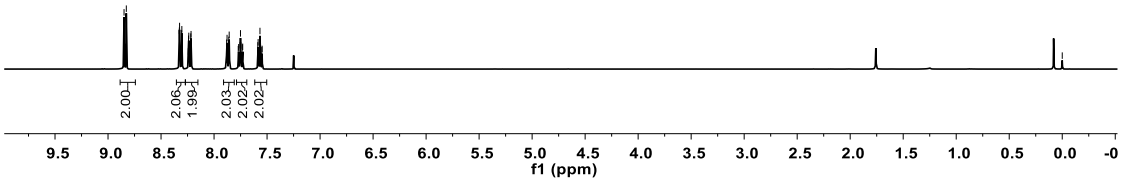
2m

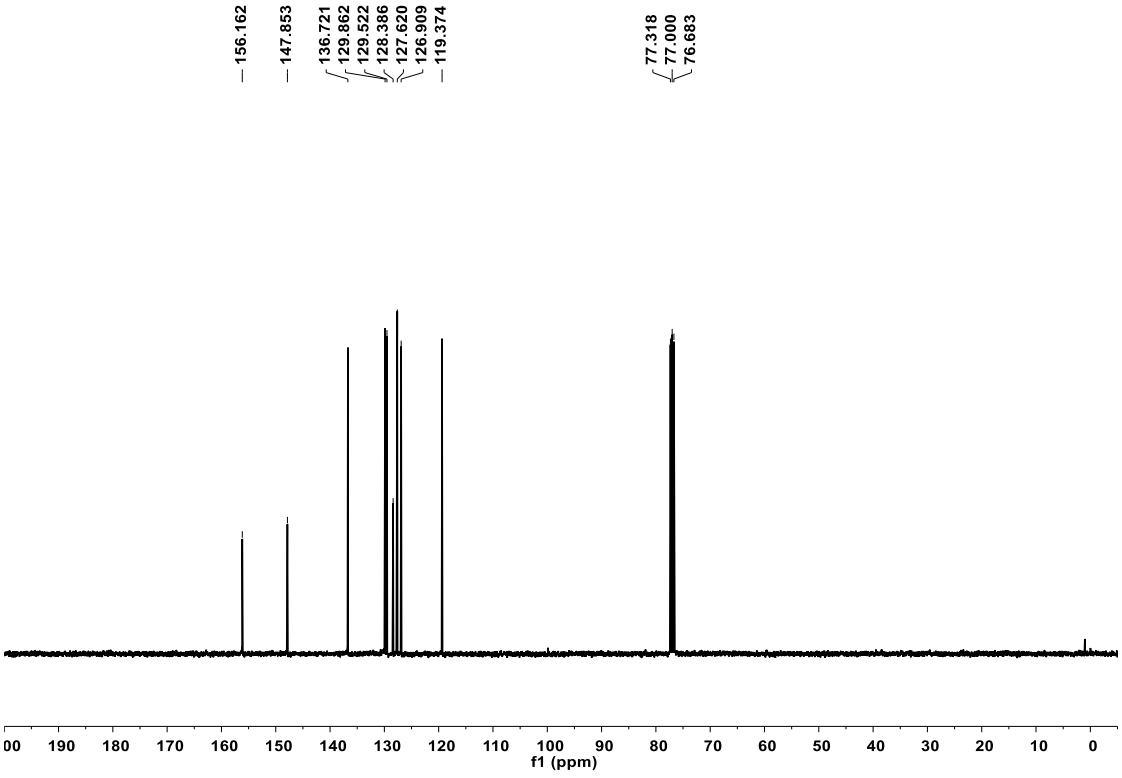

1.00
1.06
1.96
1.00
1.00
f1 (ppm)

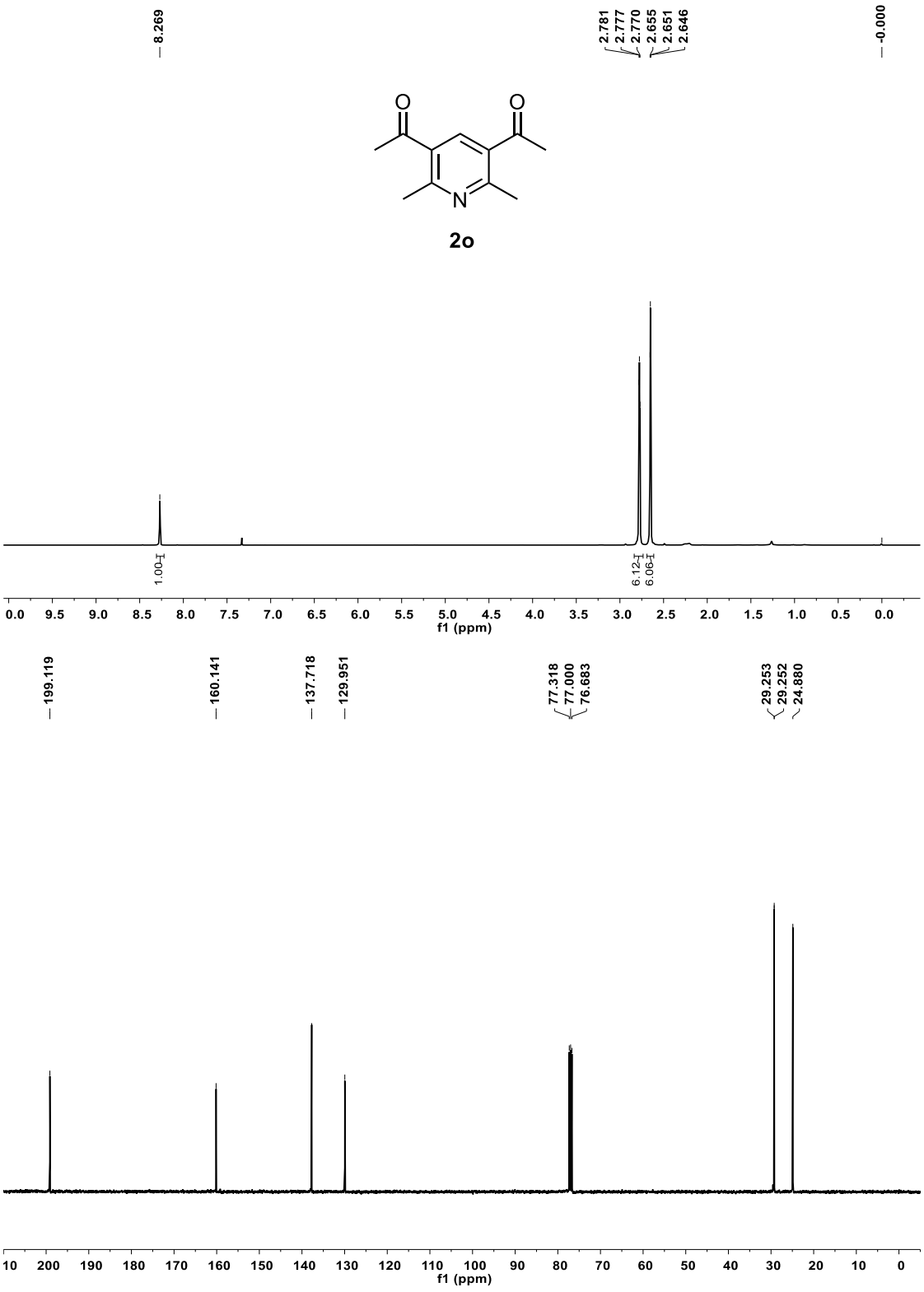

150.683
146.742
135.010
132.893
131.147
129.743
129.277
121.843
120.396
77.318
77.000
76.682
f1 (ppm)

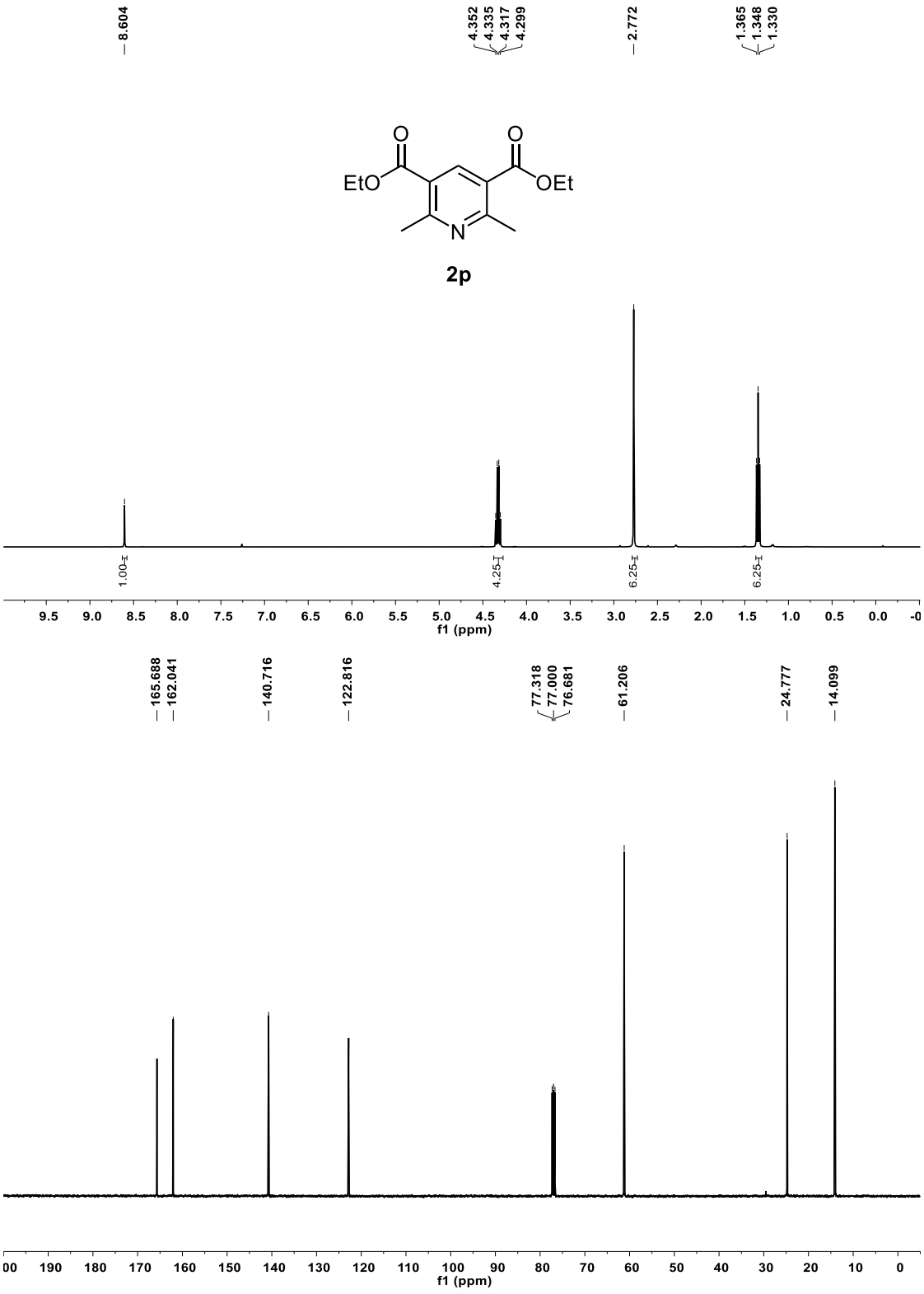

8.849
8.827
8.327
8.325
8.306
8.304
8.243
8.241
8.238
8.236
8.222
8.220
8.217
8.215
7.881
7.877
7.861
7.857
7.772
7.768
7.755
7.751
7.747
7.733
7.730
7.587
7.584
7.570
7.567
7.564
7.550
7.547
-0.000
N
N

2n

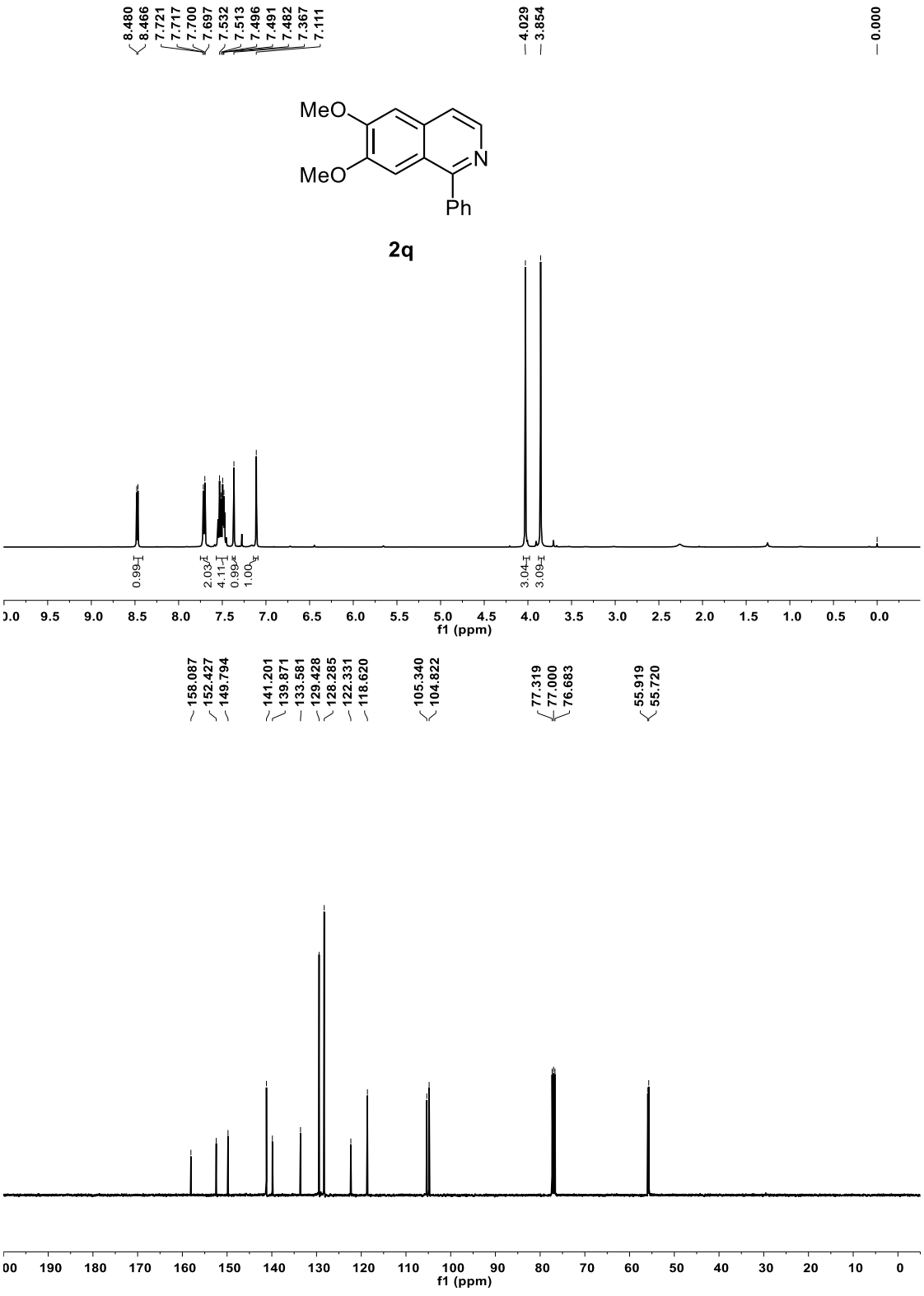

2.00
2.06
1.99
2.03
2.02
2.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

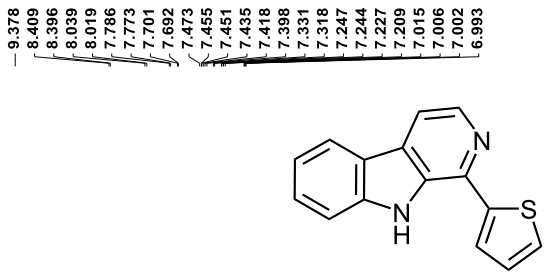

156.162
147.853
136.721
129.862
129.522
128.386
127.620
126.909
119.374
77.318
77.000
76.683
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.269
2.781
2.777
2.770
2.655
2.651
2.646
-0.000
O
O
N
2o
1.00
6.12
6.06
f1 (ppm)
199.119
160.141
137.718
129.951
77.318
77.000
76.683
29.253
29.252
24.880
f1 (ppm)


8.604
4.352
4.335
4.317
4.299
2.772
1.365
1.348
1.330
O
O
EtO
OEt
N
1.00
4.25
6.25
6.25
f1 (ppm)
165.688
162.041
140.716
122.816
77.318
77.000
76.681
61.206
24.777
14.099
f1 (ppm)

2p


8.480
8.466
7.721
7.717
7.700
7.697
7.532
7.513
7.496
7.491
7.482
7.367
7.111
4.029
3.854
0.000
MeO
MeO
N
Ph
2q
0.99
2.03
4.11
0.99
1.00
3.04
3.09
f1 (ppm)
158.087
152.427
149.794
141.201
139.871
133.581
129.428
128.285
122.331
118.620
105.340
104.822
77.319
77.000
76.683
55.919
55.720
f1 (ppm)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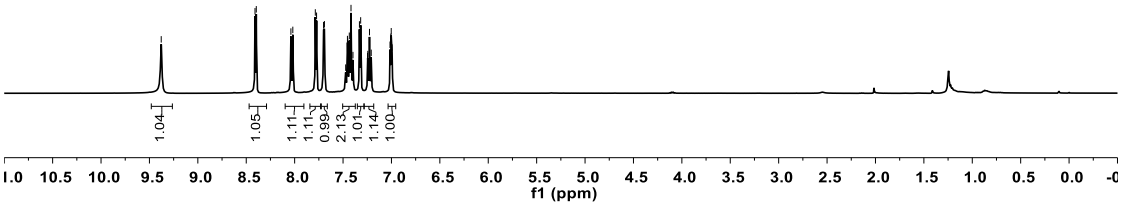
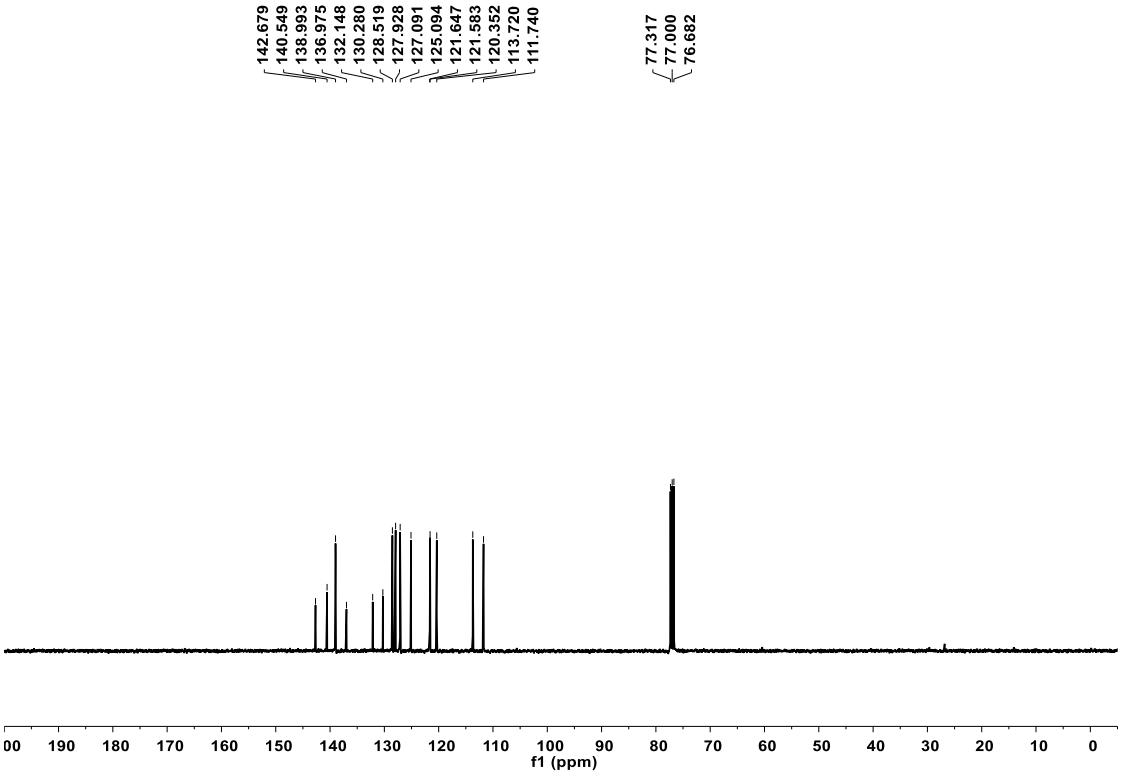
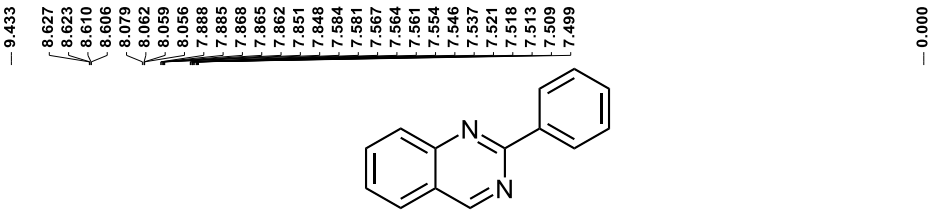
8.409
8.396
8.039
8.019
7.786
7.773
7.701
7.692
7.473
7.455
7.451
7.435
7.418
7.398
7.331
7.318
7.247
7.244
7.227
7.209
7.015
7.006
7.002
6.993
N
N
H
S

2r


1.04
1.05
1.11
1.11
0.99
2.13
1.01
1.14
1.00
f1 (ppm)


142.679
140.549
138.993
136.975
132.148
130.280
128.519
127.928
127.091
125.094
121.647
121.583
120.352
113.720
111.740
77.317
77.000
76.682
f1 (ppm)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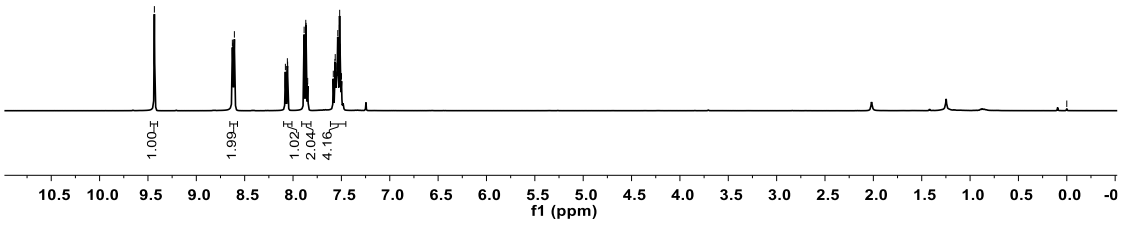
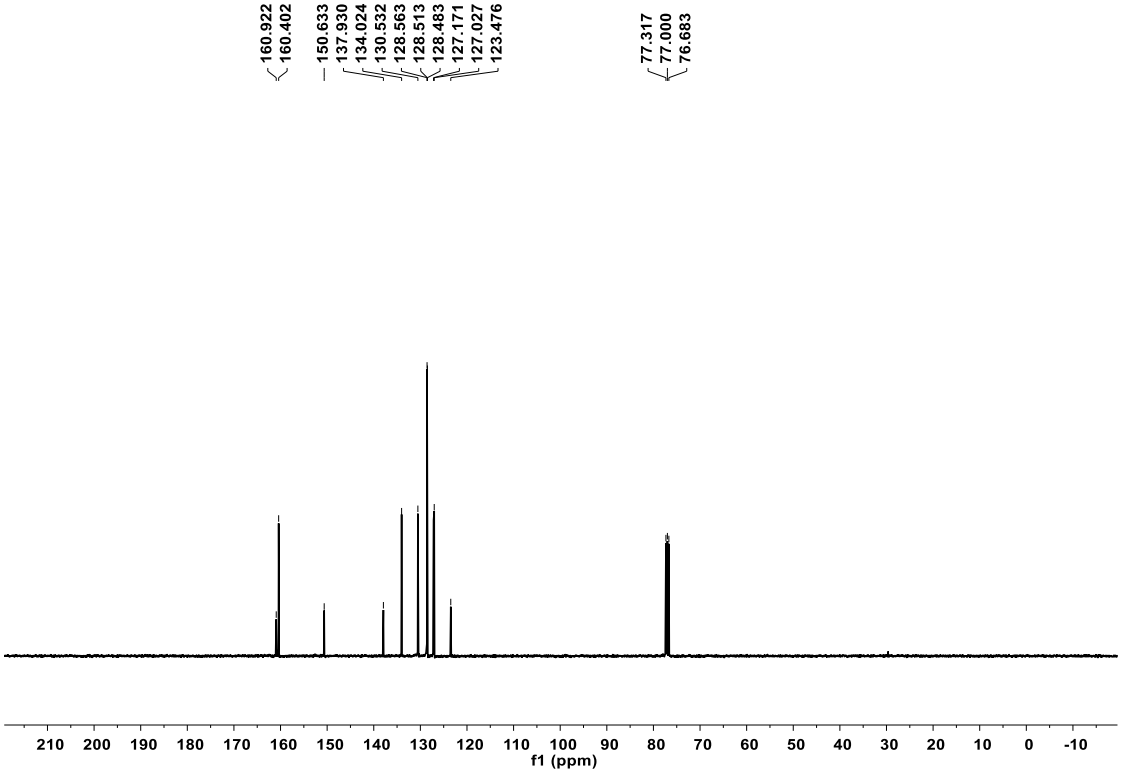
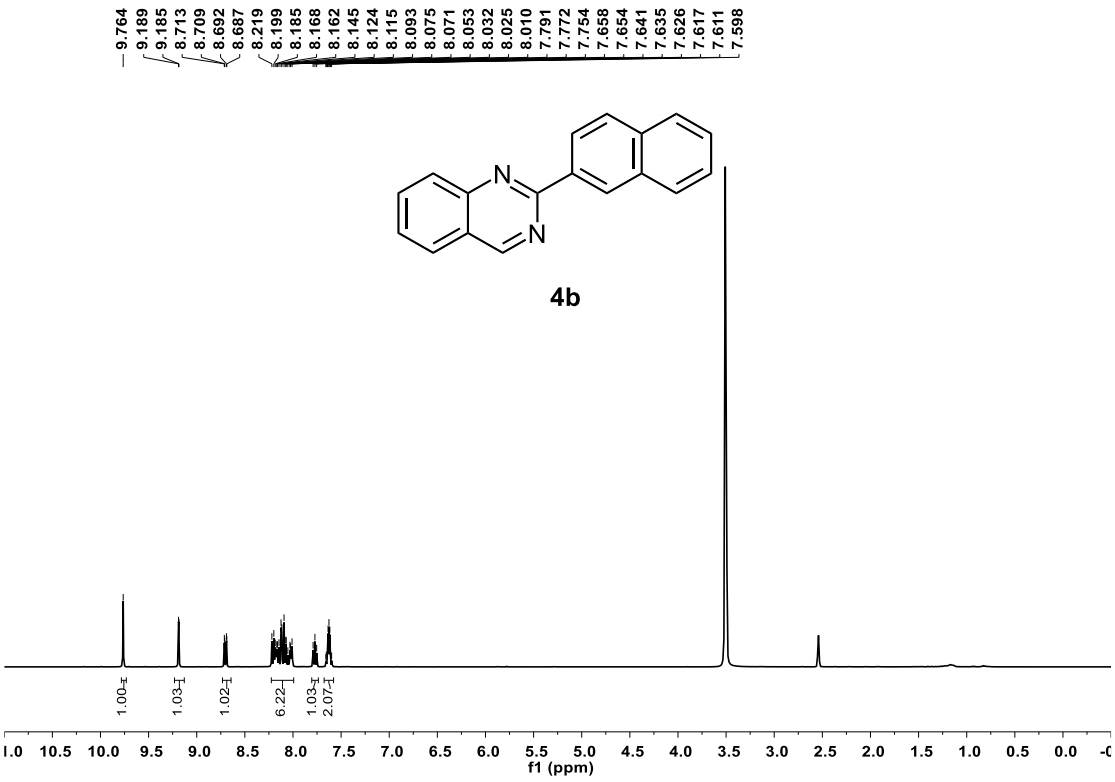
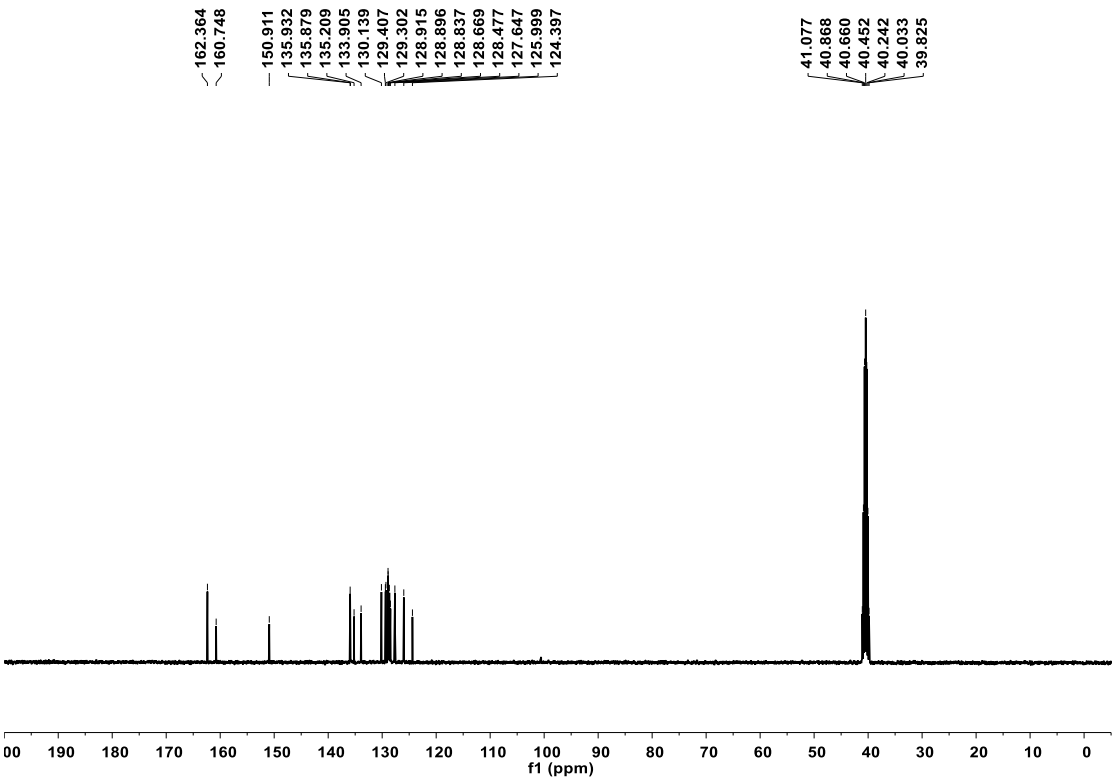
8.627
8.623
8.610
8.606
8.079
8.062
8.059
8.056
7.888
7.885
7.868
7.865
7.862
7.851
7.848
7.584
7.581
7.567
7.564
7.561
7.554
7.546
7.537
7.521
7.518
7.513
7.509
7.499
0.000
N
N

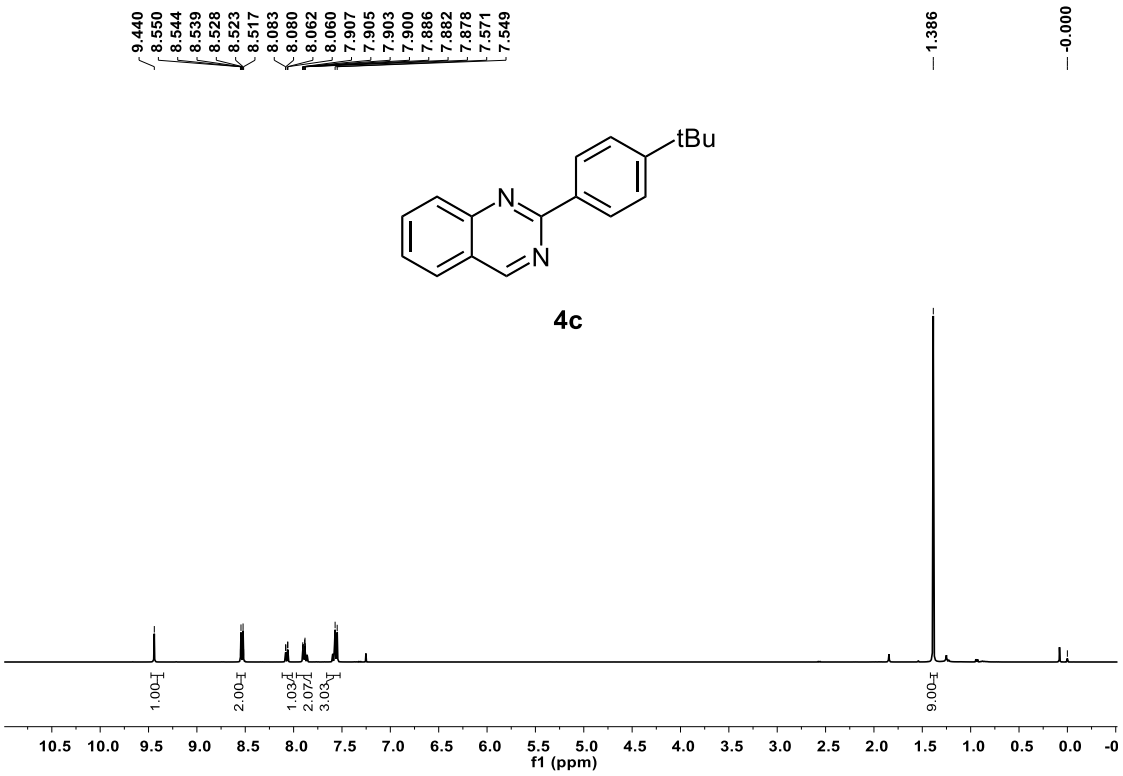
4a


1.00
1.99
1.02
2.04
4.16
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)


160.922
160.402
150.633
137.930
134.024
130.532
128.563
128.513
128.483
127.171
127.027
123.476
77.317
77.000
76.683
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)


9.764
9.189
9.185
8.713
8.709
8.692
8.687
8.219
8.199
8.185
8.168
8.162
8.145
8.124
8.115
8.093
8.075
8.071
8.053
8.032
8.025
8.010
7.791
7.772
7.754
7.658
7.654
7.641
7.635
7.626
7.617
7.611
7.598
N
N
4b
1.00
1.03
1.02
6.22
1.03
2.07
f1 (ppm)


162.364
160.748
150.911
135.932
135.879
135.209
133.905
130.139
129.407
129.302
128.915
128.896
128.837
128.669
128.477
127.647
125.999
124.397
41.077
40.868
40.660
40.452
40.242
40.033
39.825
f1 (ppm)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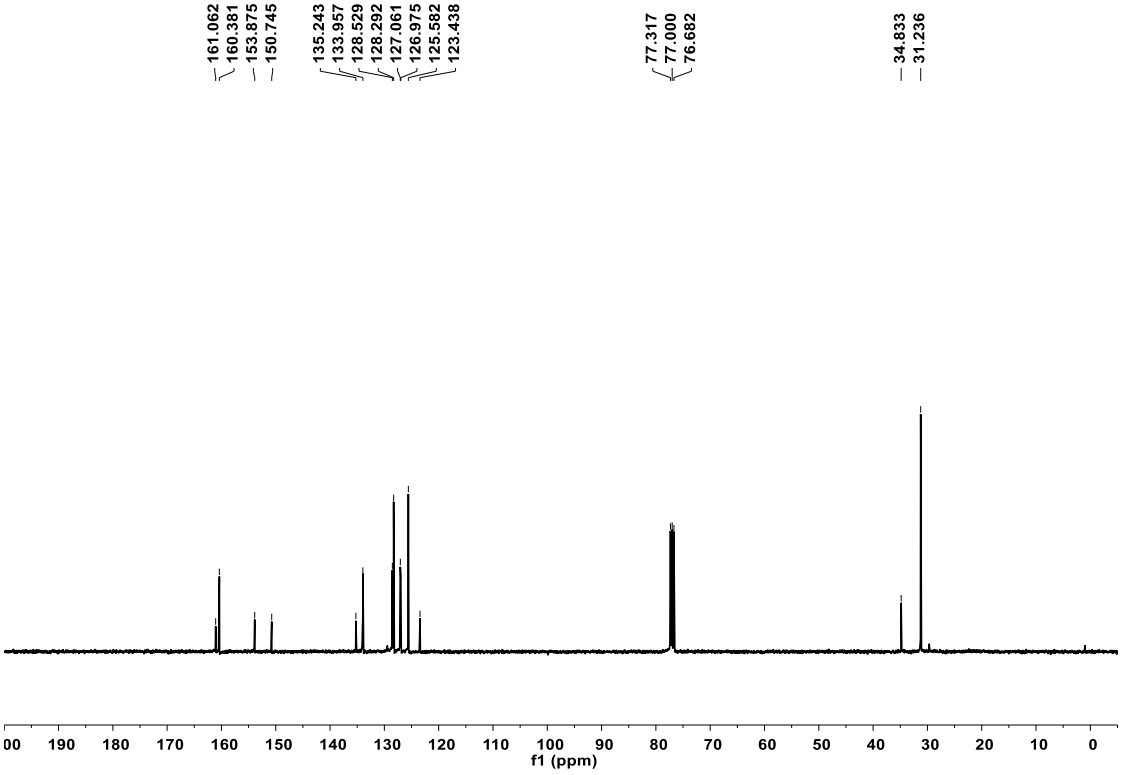
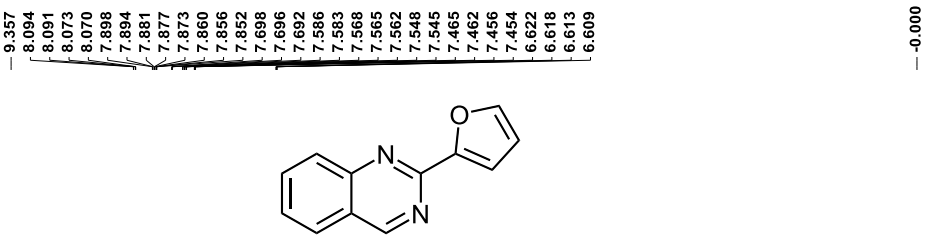
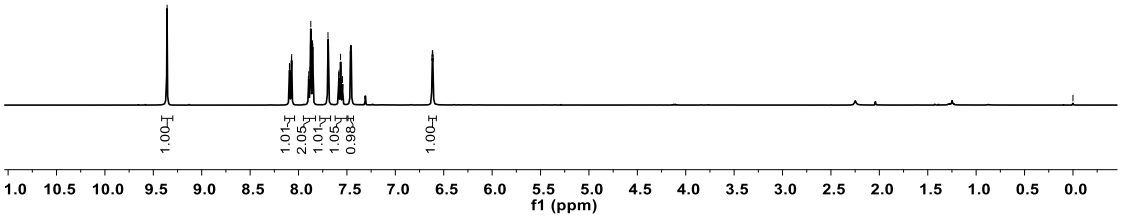
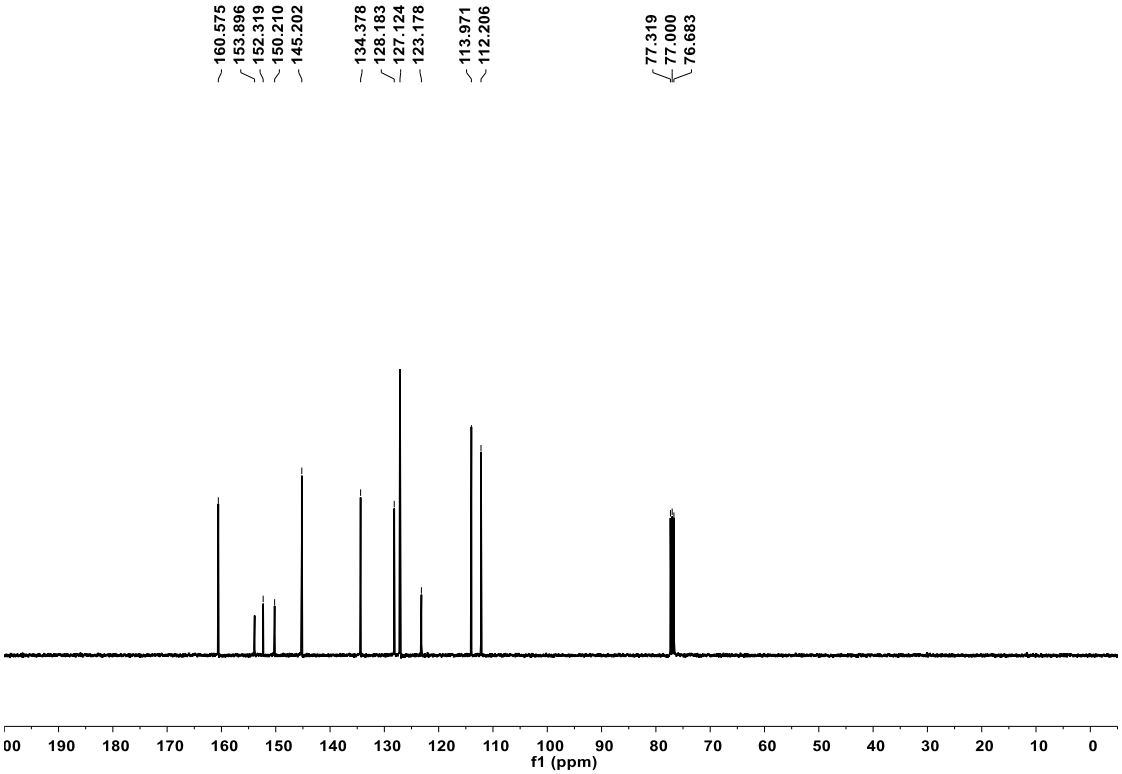
8.550
8.544
8.539
8.528
8.523
8.517
8.083
8.080
8.062
8.060
7.907
7.905
7.903
7.900
7.886
7.882
7.878
7.571
7.549
1.386
-0.000
tBu
N
N
4c
1.00
2.00
1.03
2.07
3.03
9.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

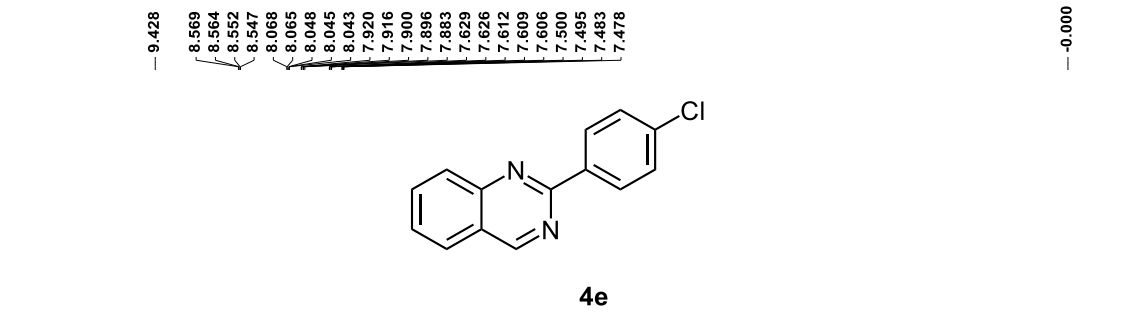

161.062
160.381
153.875
150.745
135.243
133.957
128.529
128.292
127.061
126.975
125.582
123.438
77.317
77.000
76.682
34.833
31.236
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.357
8.094
8.091
8.073
8.070
7.898
7.894
7.881
7.877
7.873
7.860
7.856
7.852
7.698
7.696
7.692
7.586
7.583
7.568
7.565
7.562
7.548
7.545
7.465
7.462
7.456
7.454
6.622
6.618
6.613
6.609
-0.000
O
N
N

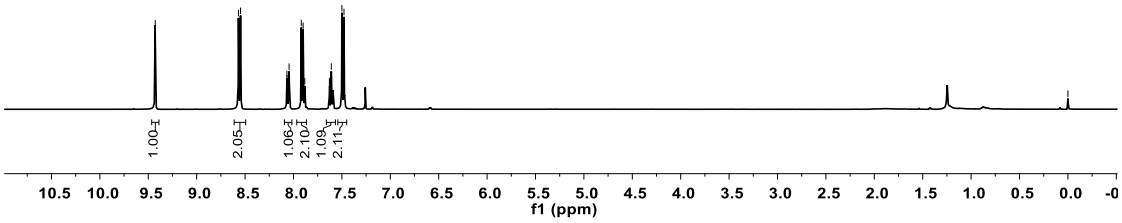
4d

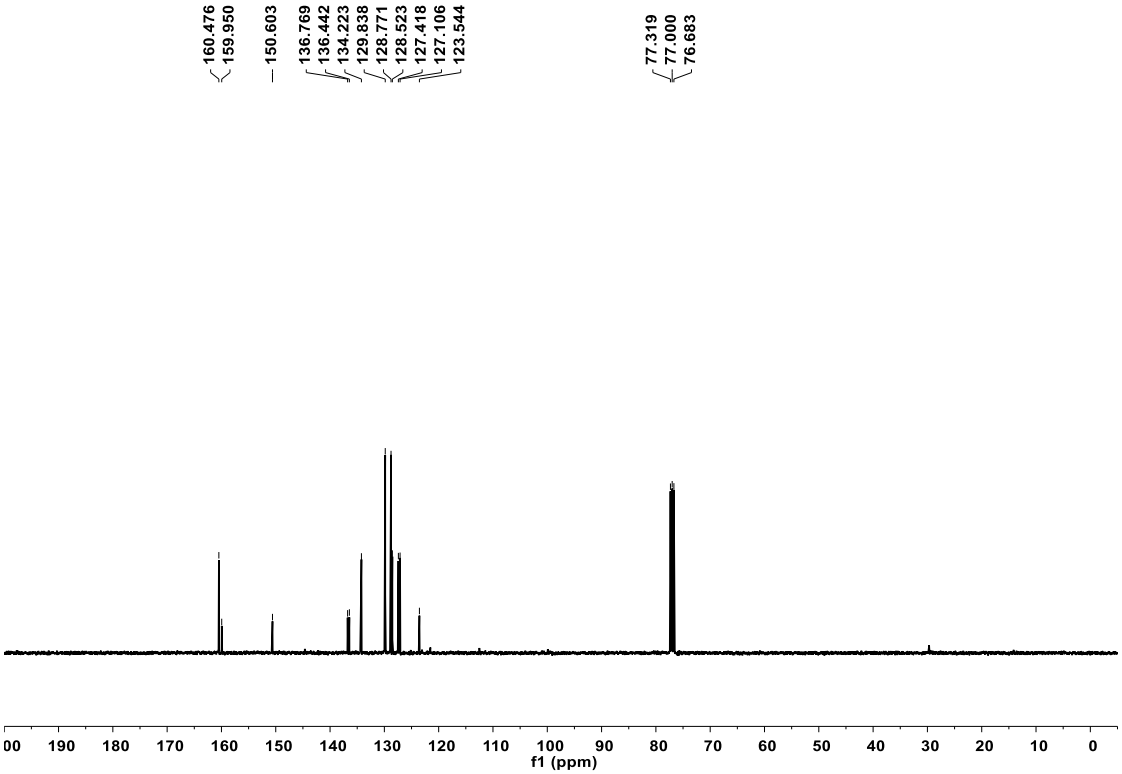

1.00
1.01
2.05
1.01
1.05
0.98
1.00
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

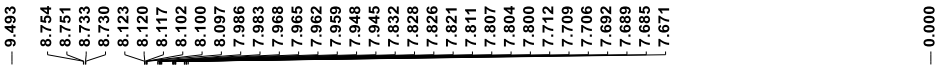

160.575
153.896
152.319
150.210
145.202
134.378
128.183
127.124
123.178
113.971
112.206
77.319
77.000
76.683
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.428
8.569
8.564
8.552
8.547
8.068
8.065
8.048
8.045
8.043
7.920
7.916
7.900
7.896
7.883
7.629
7.626
7.612
7.609
7.606
7.500
7.495
7.483
7.478
-0.000
Cl
N
N

4e


1.00
2.05
1.06
2.10
1.09
2.11
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)


160.476
159.950
150.603
136.769
136.442
134.223
129.838
128.771
128.523
127.418
127.106
123.544
77.319
77.000
76.683
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.493
8.754
8.751
8.733
8.730
8.123
8.120
8.117
8.102
8.100
8.097
7.986
7.983
7.968
7.965
7.962
7.959
7.948
7.945
7.832
7.828
7.826
7.821
7.811
7.807
7.804
7.800
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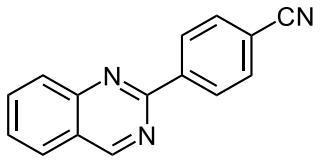
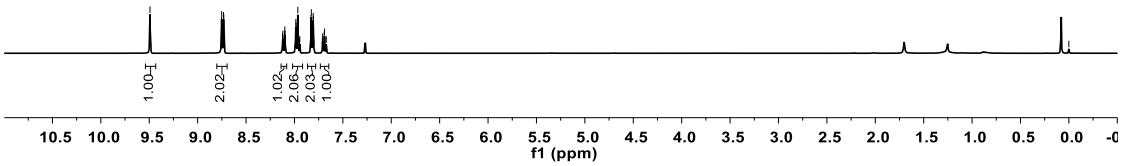
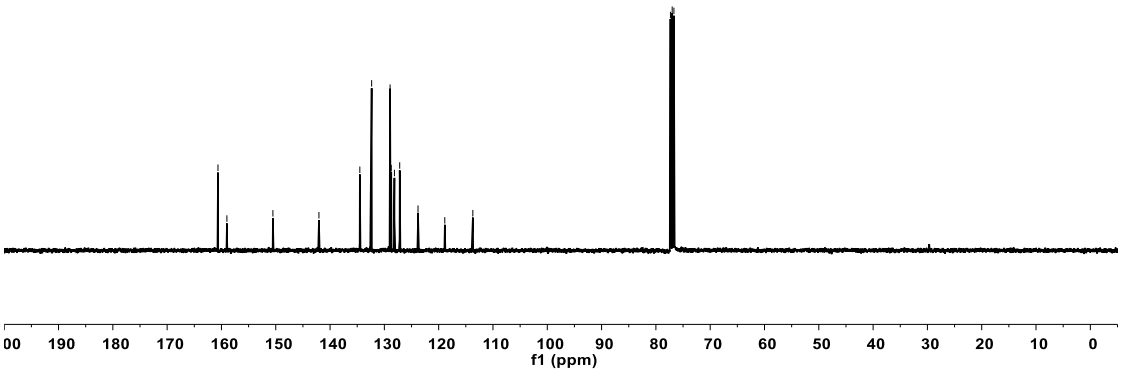
7.706
7.692
7.689
7.685
7.671
0.000

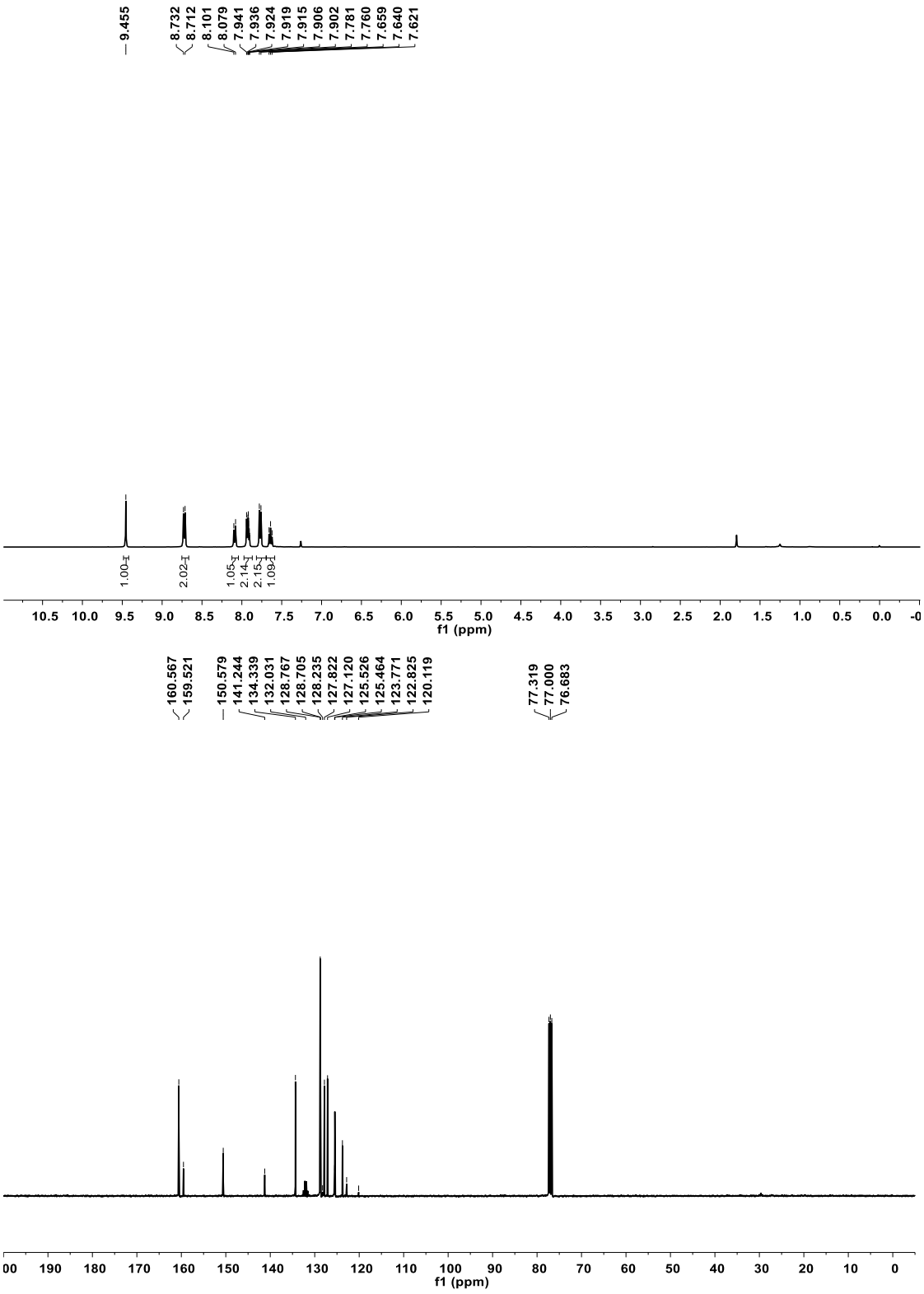

CN
N
N

4f


1.00
2.02
1.02
2.06
2.03
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


160.641
158.997
150.524
142.051
134.518
132.342
128.947
128.734
128.147
127.175
123.804
118.871
113.708
77.318
77.000
76.682


00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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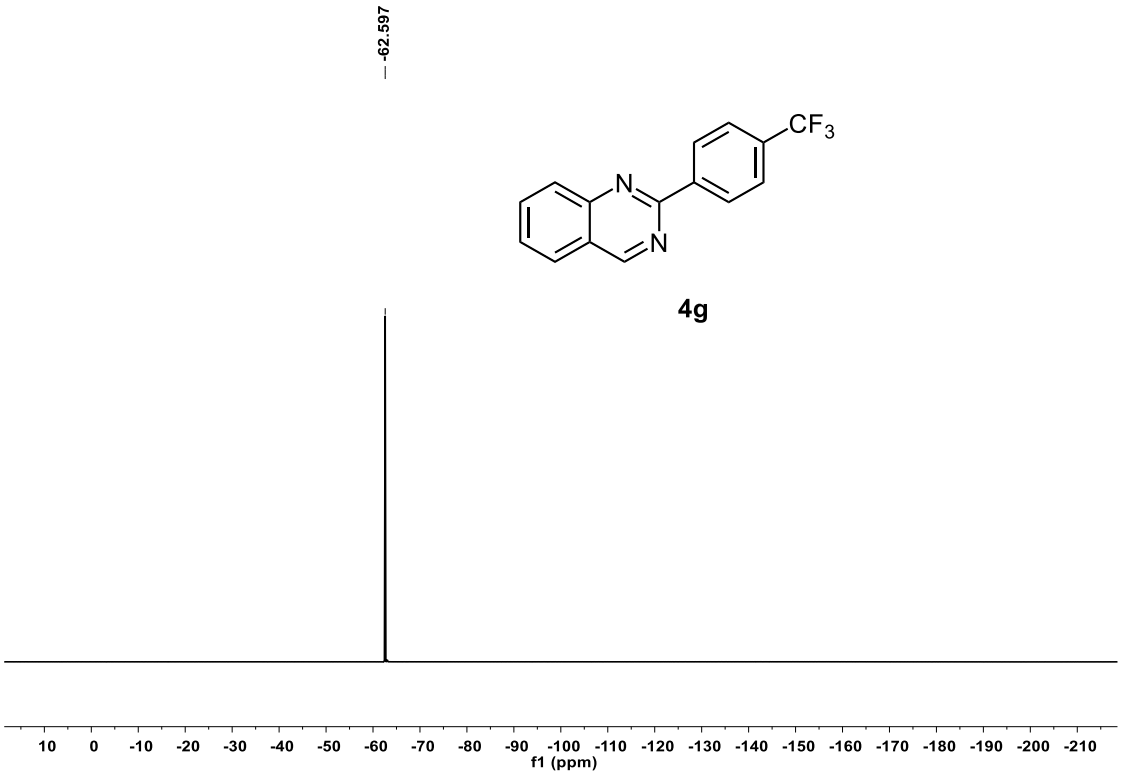
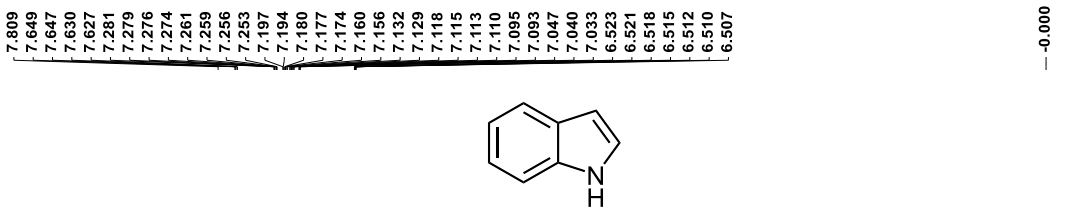
8.732
8.712
8.101
8.079
7.941
7.936
7.924
7.919
7.915
7.906
7.902
7.781
7.760
7.659
7.640
7.621
1.00
2.02
1.05
2.14
2.15
1.09
f1 (ppm)
160.567
159.521
150.579
141.244
134.339
132.031
128.767
128.705
128.235
127.822
127.120
125.526
125.464
123.771
122.825
120.119
77.319
77.000
76.683
f1 (ppm)


-62.597
CF3
N
N
4g
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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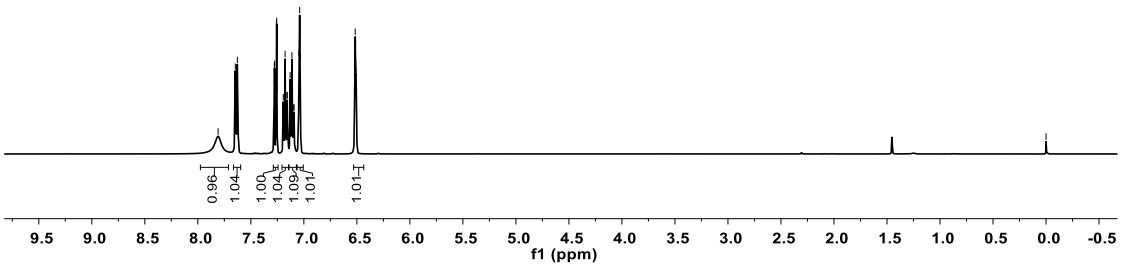
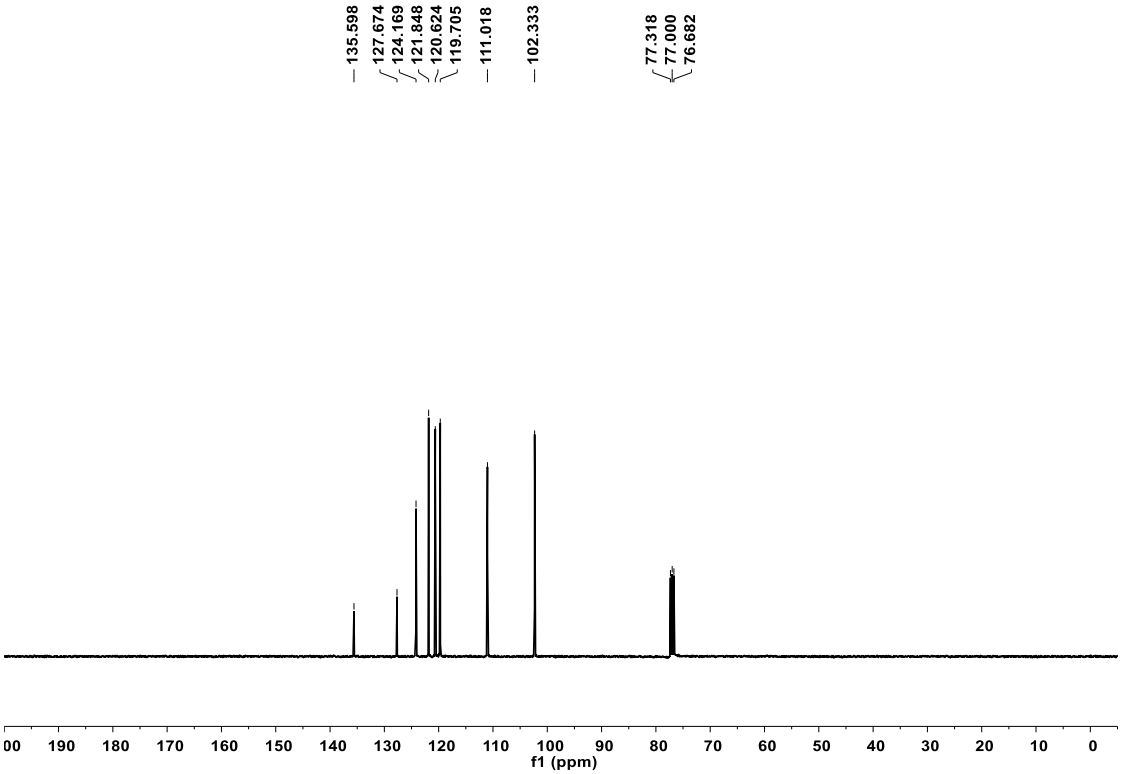
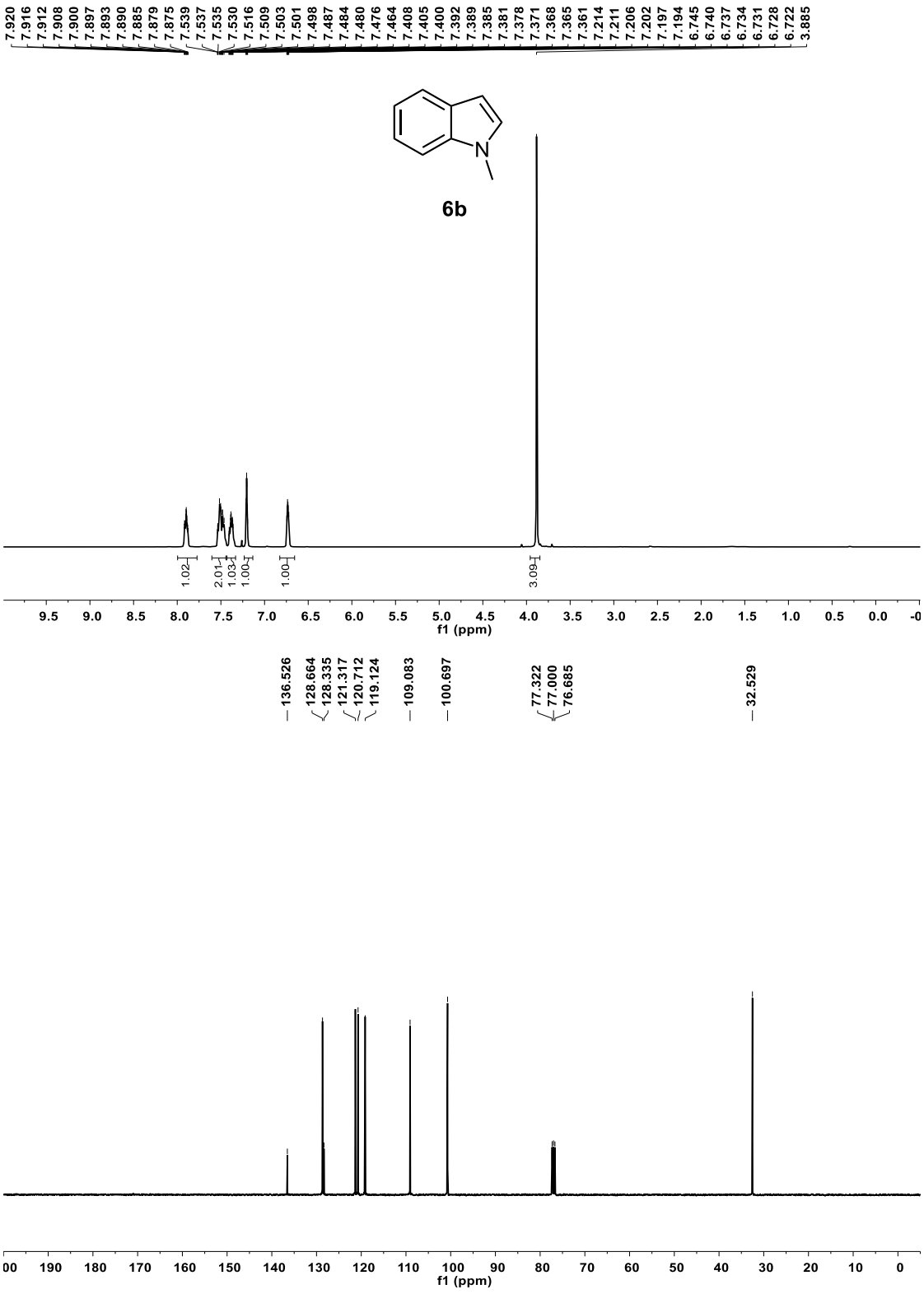
7.647
7.630
7.627
7.281
7.279
7.276
7.274
7.261
7.259
7.256
7.253
7.197
7.194
7.180
7.177
7.174
7.160
7.156
7.132
7.129
7.118
7.115
7.113
7.110
7.095
7.093
7.047
7.040
7.033
6.523
6.521
6.518
6.515
6.512
6.510
6.507
-0.000

N
H

6a


0.96
1.04
1.00
1.04
1.09
1.01
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


135.598
127.674
124.169
121.848
120.624
119.705
111.018
102.333
77.318
77.000
76.682
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.920
7.916
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7.908
7.900
7.897
7.893
7.890
7.885
7.879
7.875
7.539
7.537
7.535
7.530
7.516
7.509
7.503
7.501
7.498
7.487
7.484
7.480
7.476
7.464
7.408
7.405
7.400
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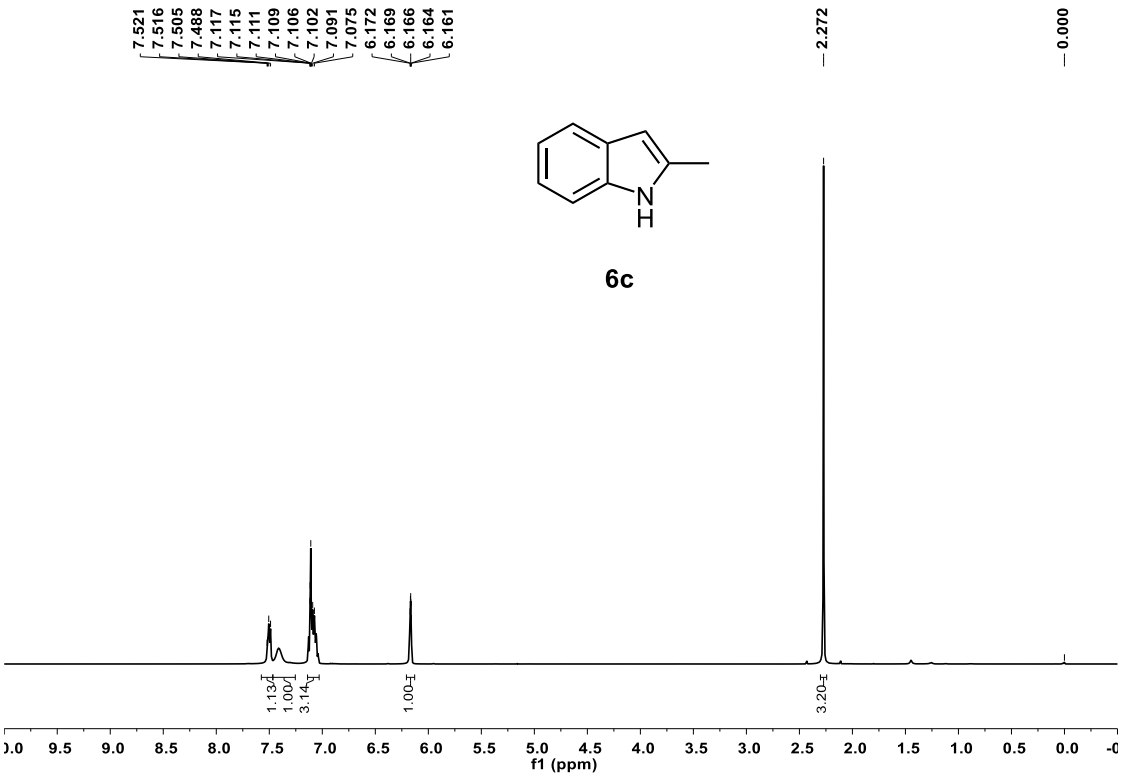
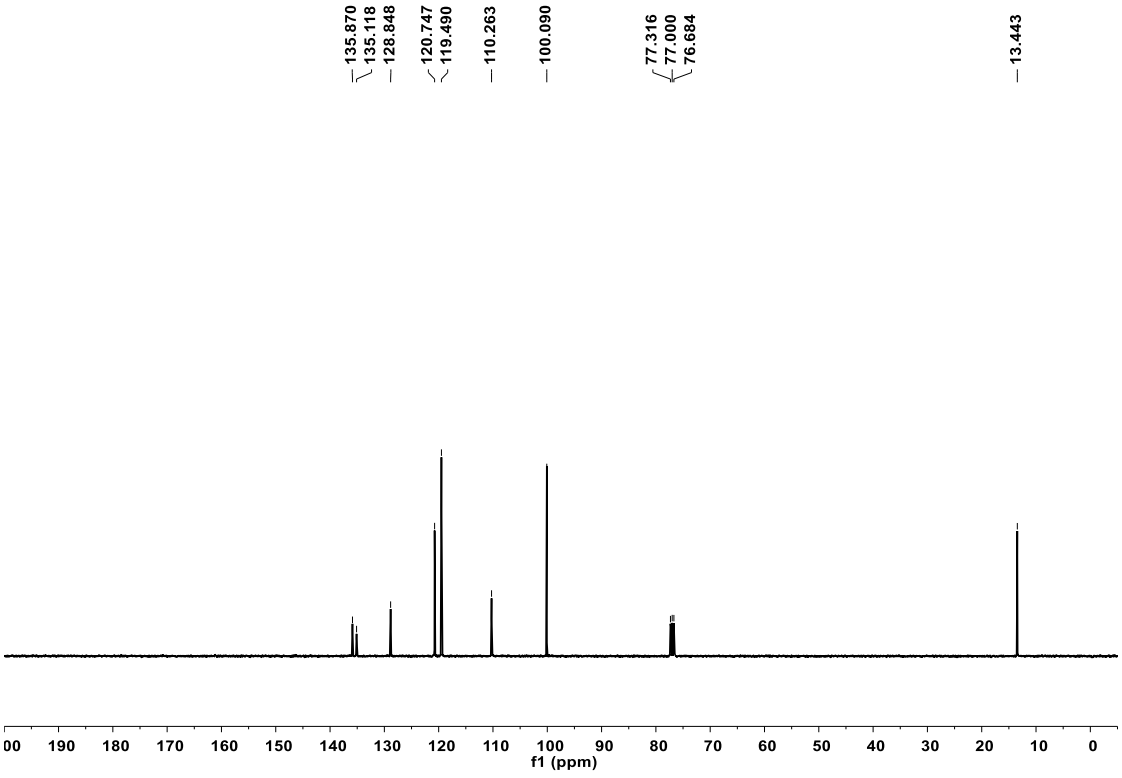
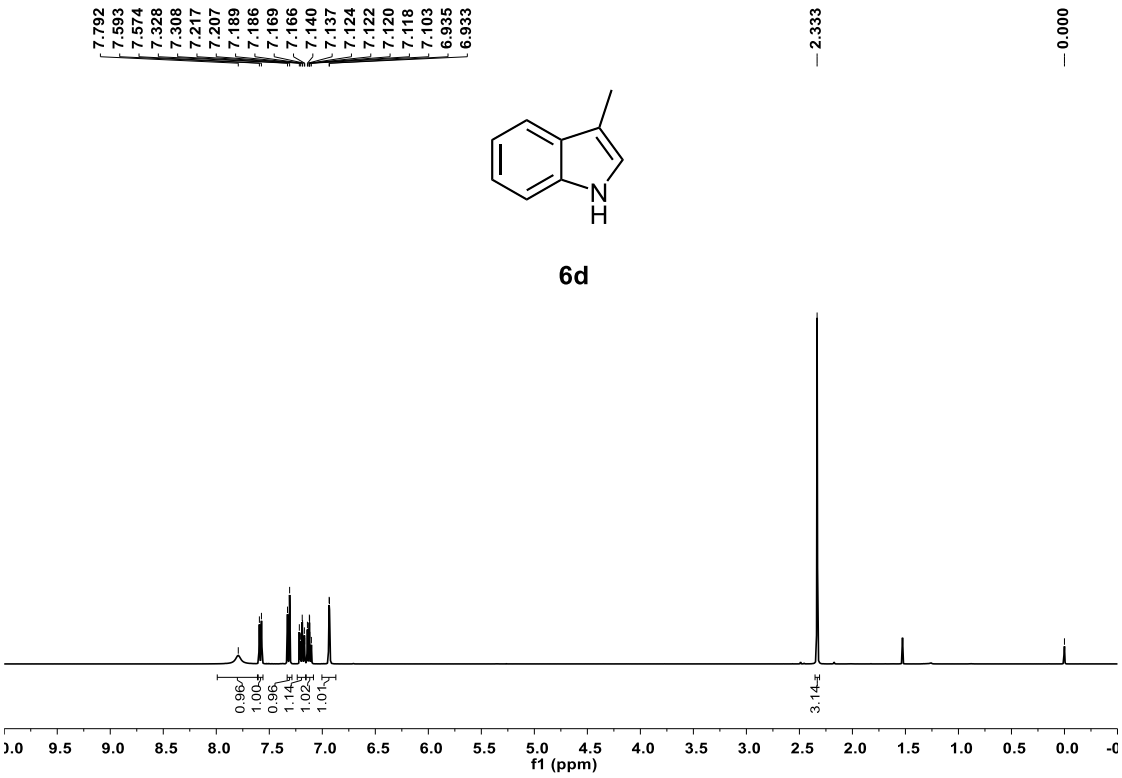
7.389
7.385
7.381
7.378
7.371
7.368
7.365
7.361
7.214
7.211
7.206
7.202
7.197
7.194
6.745
6.740
6.737
6.734
6.731
6.728
6.722
3.885
N
6b
1.02
2.01
1.03
1.00
1.00
3.09
f1 (ppm)
136.526
128.664
128.335
121.317
120.712
119.124
109.083
100.697
77.322
77.000
76.685
32.529
f1 (ppm)


7.521
7.516
7.505
7.488
7.117
7.115
7.111
7.109
7.106
7.102
7.091
7.075
6.172
6.169
6.166
6.164
6.161
2.272
0.000
1.13
1.00
3.14
1.00
3.20
f1 (ppm)

6c


135.870
135.118
128.848
120.747
119.490
110.263
100.090
77.316
77.000
76.684
13.443
f1 (ppm)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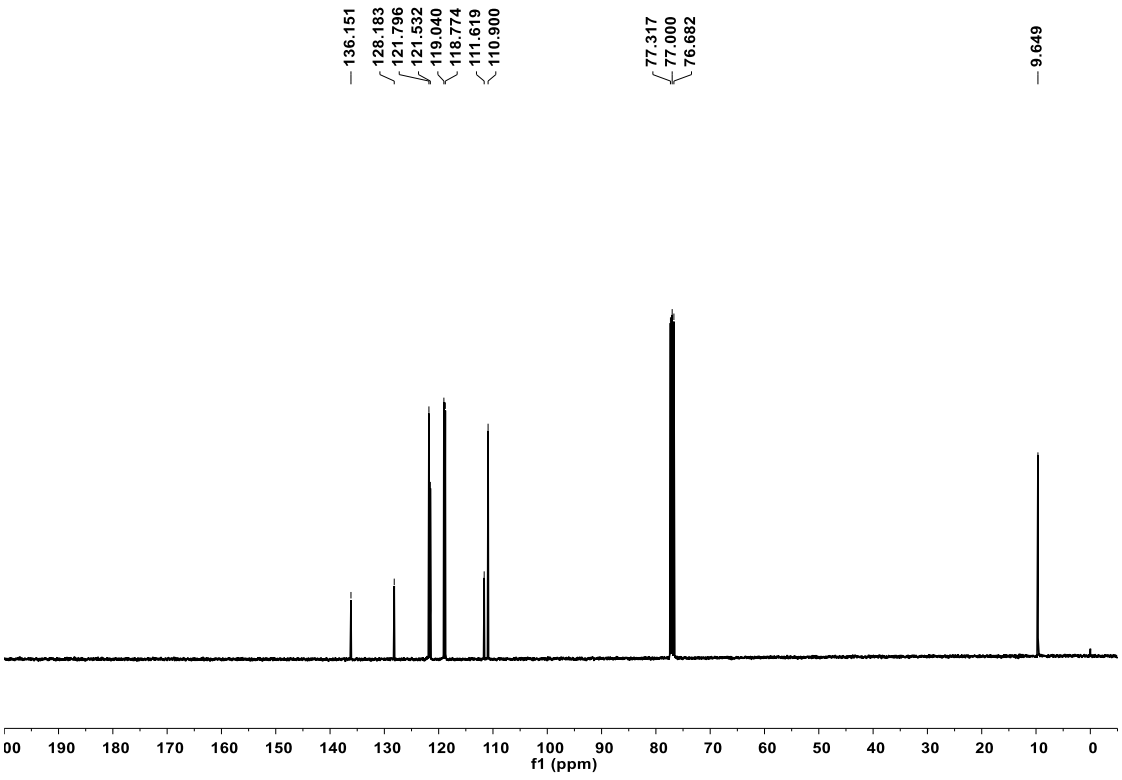
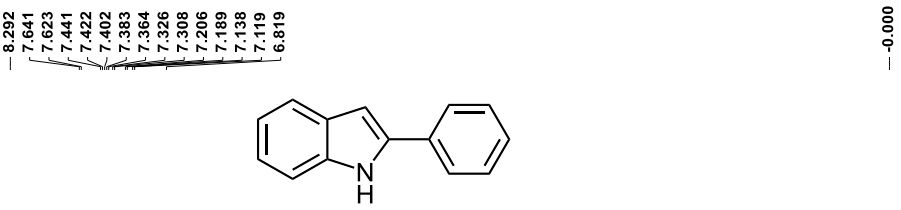
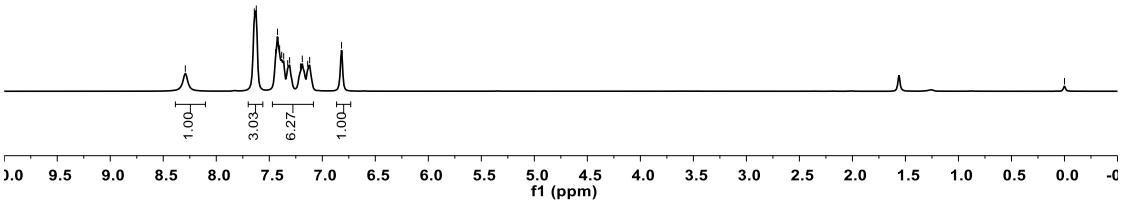
7.593
7.574
7.328
7.308
7.217
7.207
7.189
7.186
7.169
7.166
7.140
7.137
7.124
7.122
7.120
7.118
7.103
6.935
6.933
2.333
0.000
N
H
0.96
1.00
0.96
1.14
1.02
1.01
3.14
f1 (ppm)

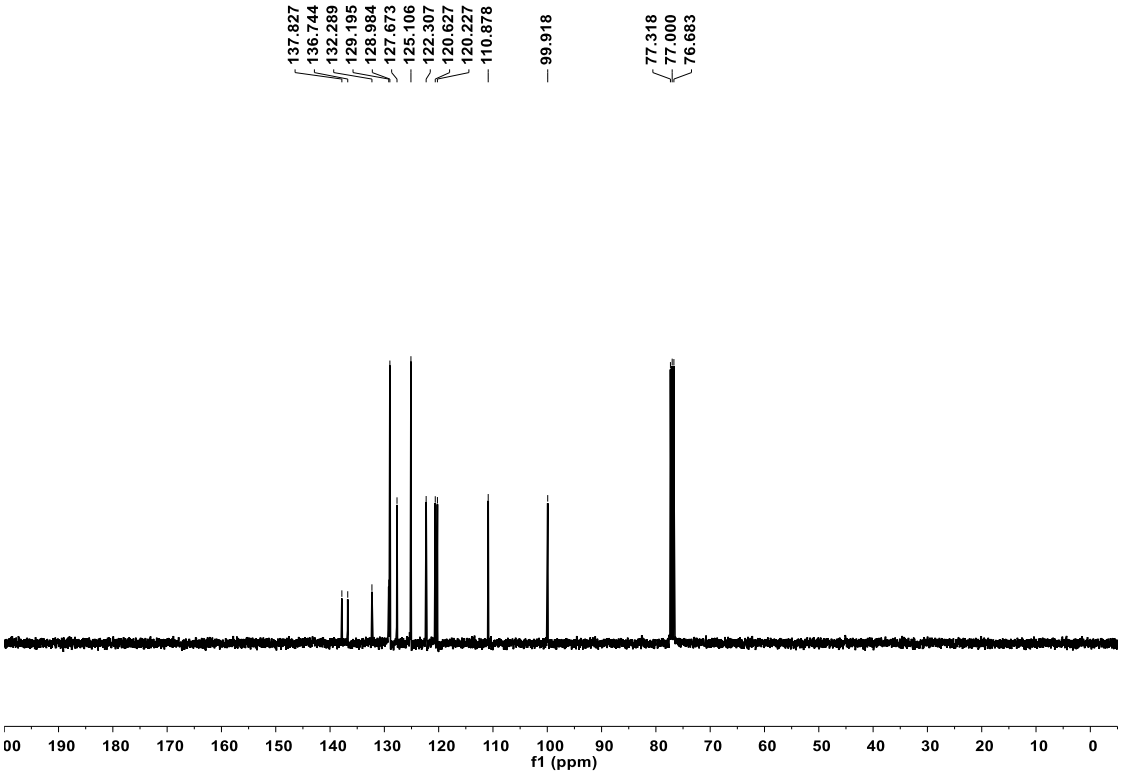
6d


136.151
128.183
121.796
121.532
119.040
118.774
111.619
110.900
77.317
77.000
76.682
9.649
f1 (ppm)

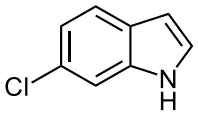

8.292
7.641
7.623
7.441
7.422
7.402
7.383
7.364
7.326
7.308
7.206
7.189
7.138
7.119
6.819
-0.000
N
H

6e

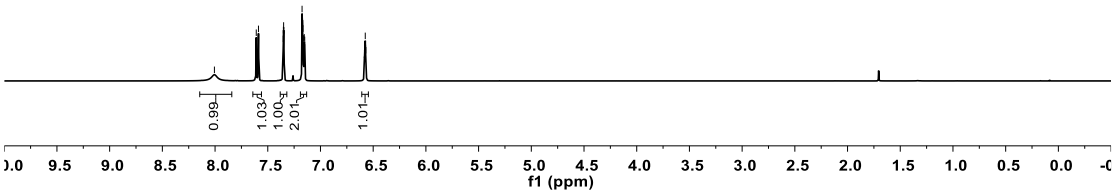

1.00
3.03
6.27
1.00
f1 (ppm)


137.827
136.744
132.289
129.195
128.984
127.673
125.106
122.307
120.627
120.227
110.878
99.918
77.318
77.000
76.683
f1 (ppm)

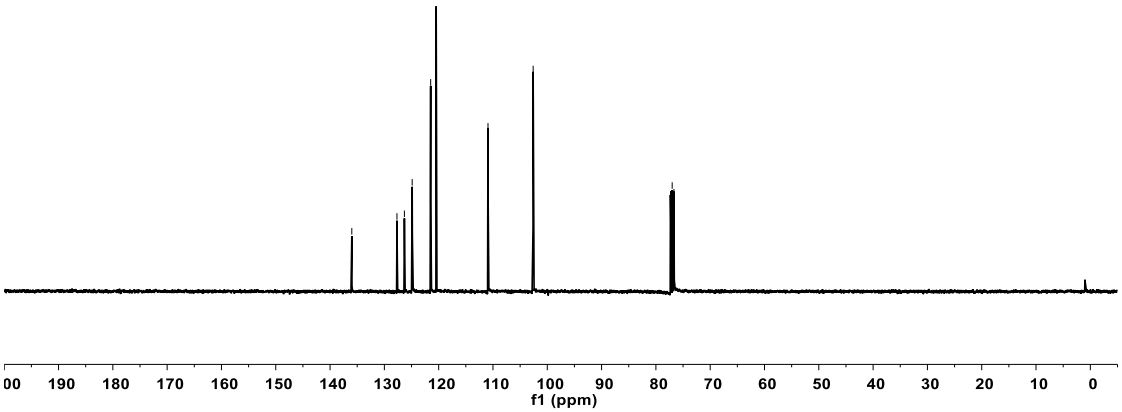

8.006
7.609
7.588
7.353
7.352
7.350
7.347
7.175
7.170
7.168
7.166
7.160
7.154
7.149
6.583
6.581
6.578
6.575
6.572
6.570

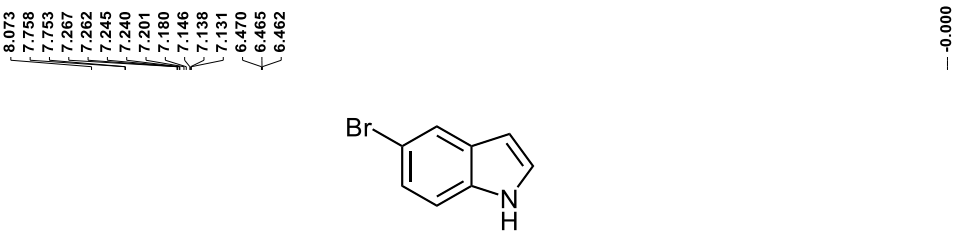

Cl
N
H

6f

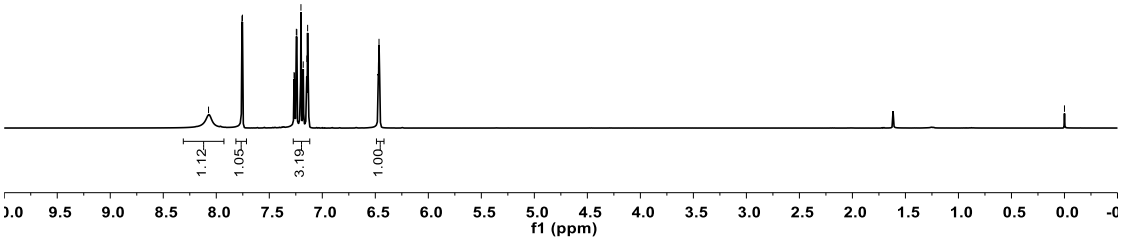

0.99
1.03
1.00
2.01
1.01
f1 (ppm)

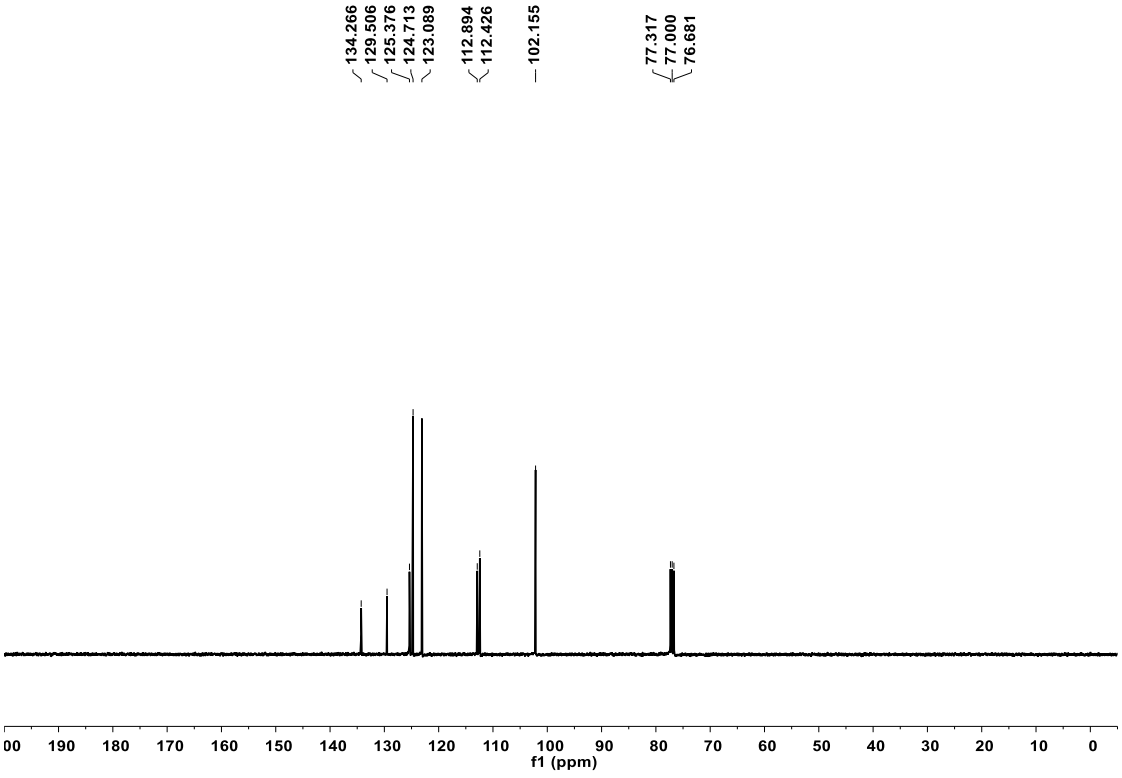

135.996
127.680
126.310
124.879
121.473
120.456
110.919
102.603
77.312
77.000
76.675

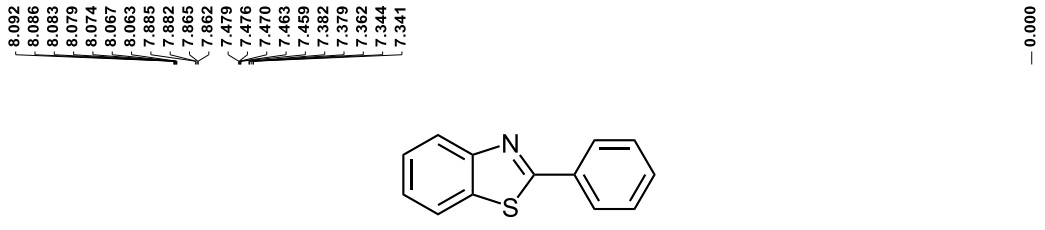

f1 (ppm)


8.073
7.758
7.753
7.267
7.262
7.245
7.240
7.201
7.180
7.146
7.138
7.131
6.470
6.465
6.462
-0.000
Br
N
H

6g

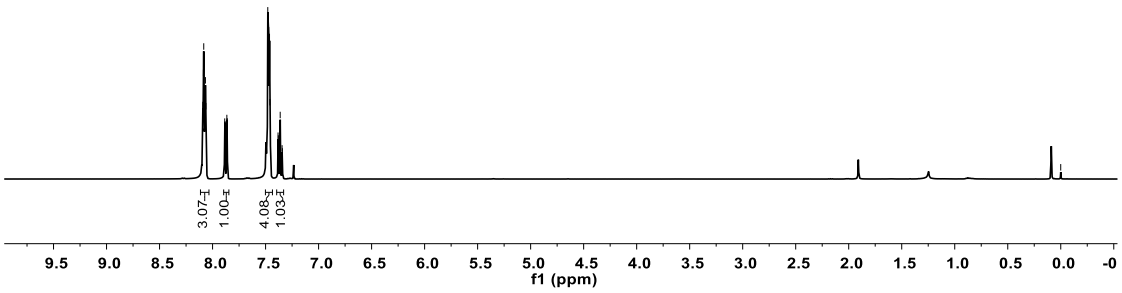

1.12
1.05
3.19
1.00
f1 (ppm)

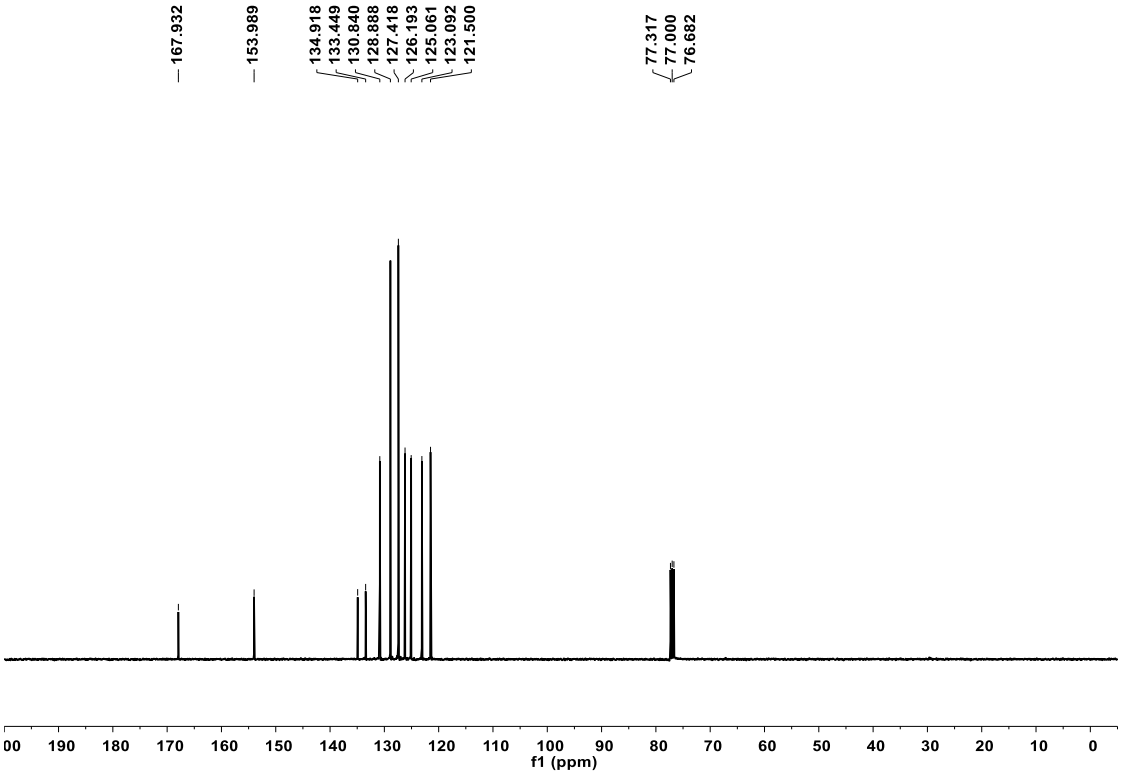

134.266
129.506
125.376
124.713
123.089
112.894
112.426
102.155
77.317
77.000
76.681
f1 (ppm)

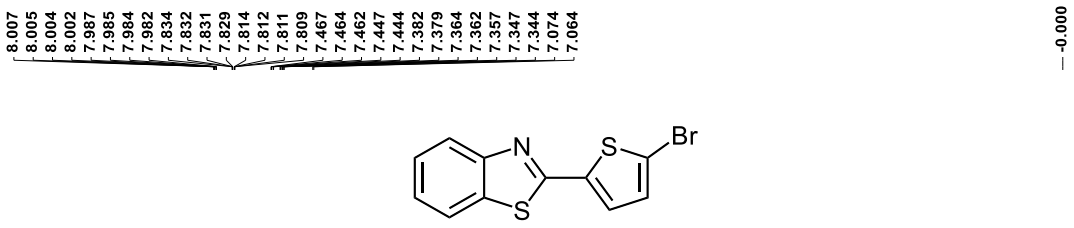

8.092
8.086
8.083
8.079
8.074
8.067
8.063
7.885
7.882
7.865
7.862
7.479
7.476
7.470
7.463
7.459
7.382
7.379
7.362
7.344
7.341
0.000

N
S

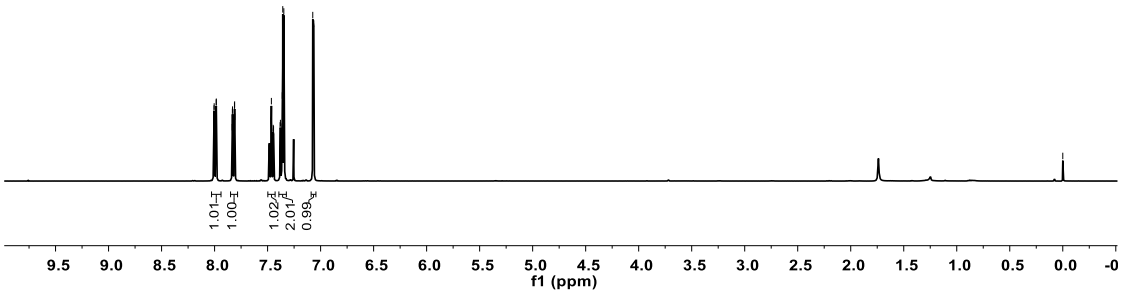
6h


3.07
1.00
4.08
1.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

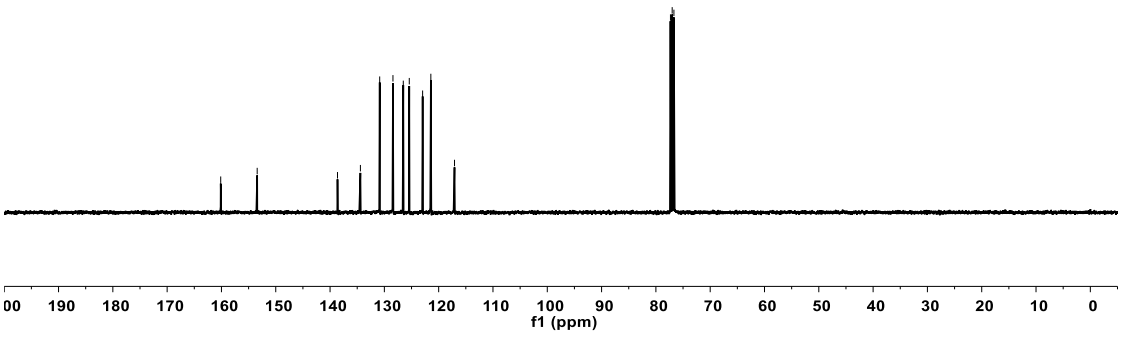

167.932
153.989
134.918
133.449
130.840
128.888
127.418
126.193
125.061
123.092
121.500
77.317
77.000
76.682
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

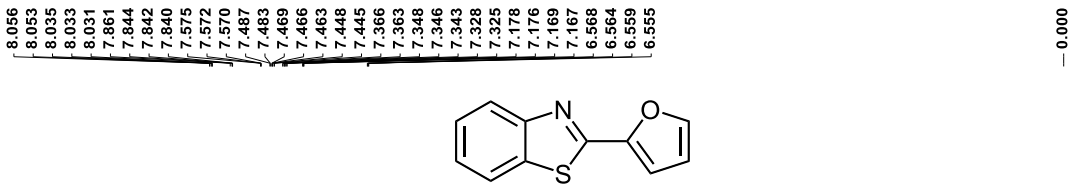

8.007
8.005
8.004
8.002
7.987
7.985
7.984
7.982
7.834
7.832
7.831
7.829
7.814
7.812
7.811
7.809
7.467
7.464
7.462
7.447
7.444
7.382
7.379
7.364
7.362
7.357
7.347
7.344
7.074
7.064
-0.000
N
S
S
Br

6i

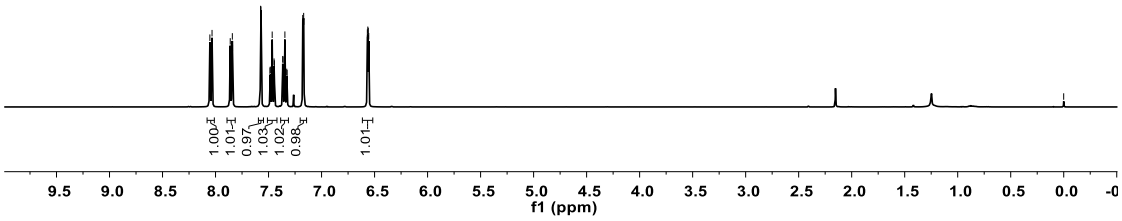

1.01
1.00
1.02
2.01
0.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

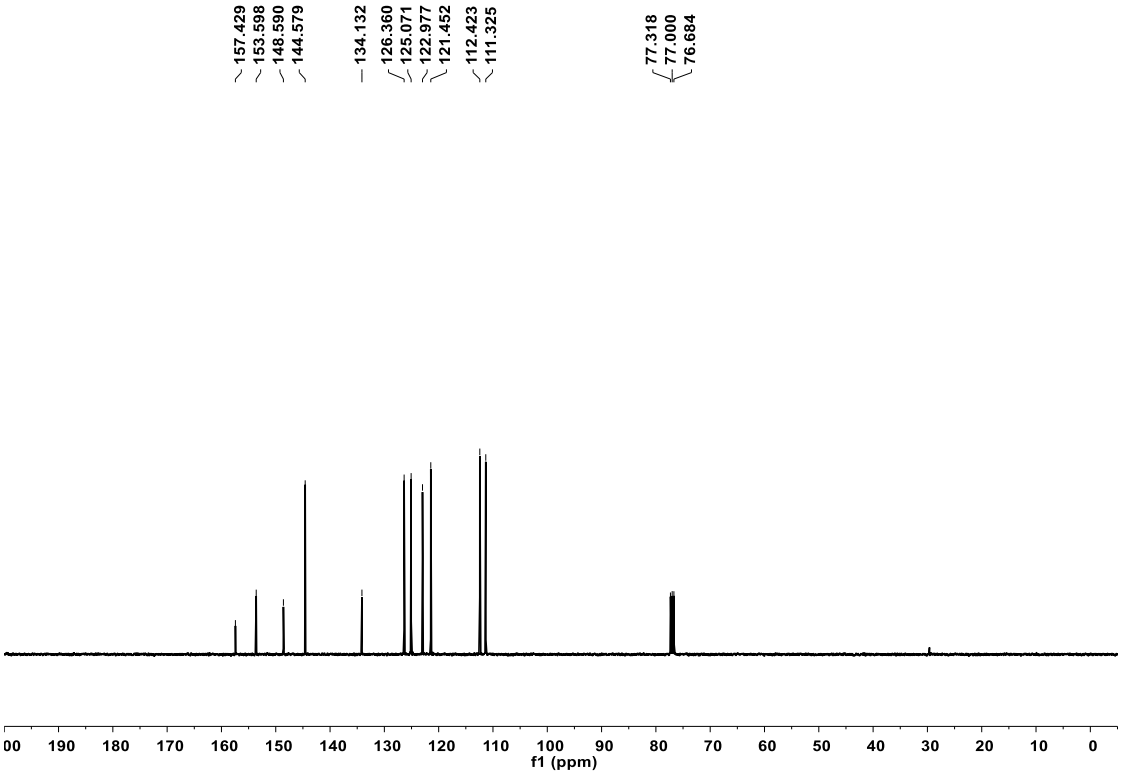

160.135
153.420
138.630
134.412
130.860
128.418
126.517
125.415
122.957
121.442
117.084
77.317
77.000
76.682

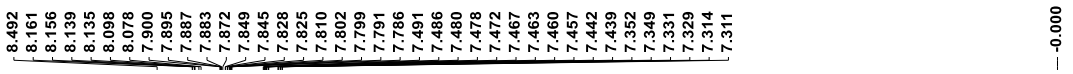

00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

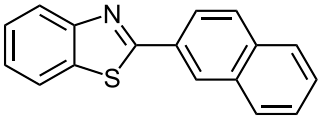

8.056
8.053
8.035
8.033
8.031
7.861
7.844
7.842
7.840
7.575
7.572
7.570
7.487
7.483
7.469
7.466
7.463
7.448
7.445
7.366
7.363
7.348
7.346
7.343
7.328
7.325
7.178
7.176
7.169
7.167
6.568
6.564
6.559
6.555
0.000
N
O
S

6j

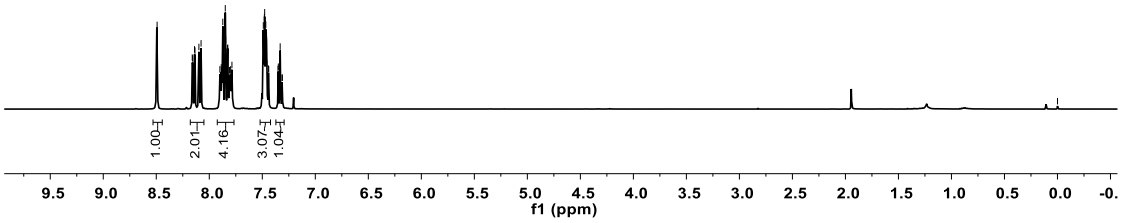

1.00
1.01
0.97
1.03
1.02
0.98
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

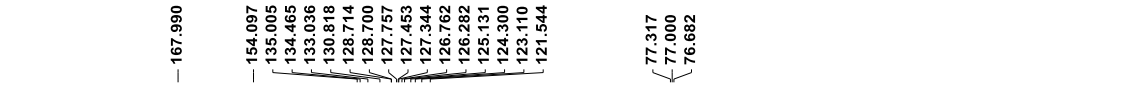

157.429
153.598
148.590
144.579
134.132
126.360
125.071
122.977
121.452
112.423
111.325
77.318
77.000
76.684
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

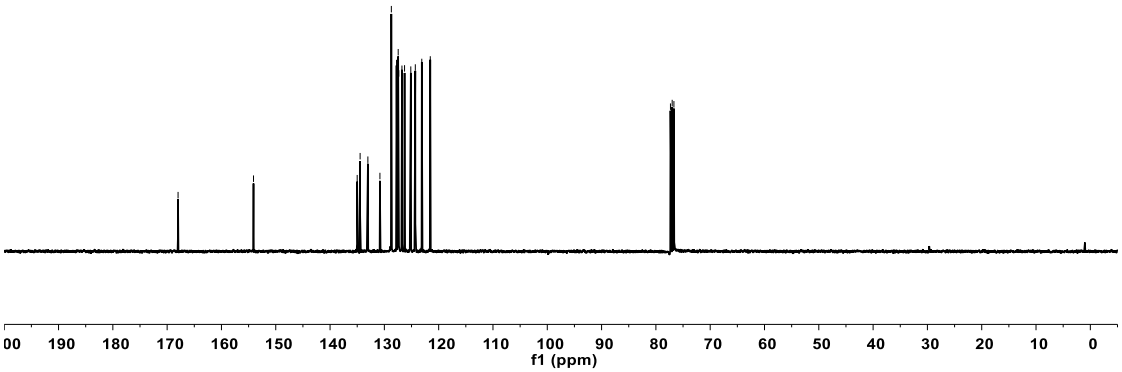

8.492
8.161
8.156
8.139
8.135
8.098
8.078
7.900
7.895
7.887
7.883
7.872
7.849
7.845
7.828
7.825
7.810
7.802
7.799
7.791
7.786
7.491
7.486
7.480
7.478
7.472
7.467
7.463
7.460
7.457
7.442
7.439
7.352
7.349
7.331
7.329
7.314
7.311
-0.000

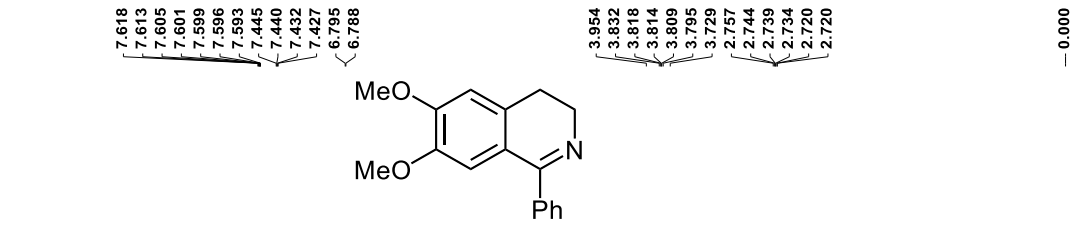

N
S

6k

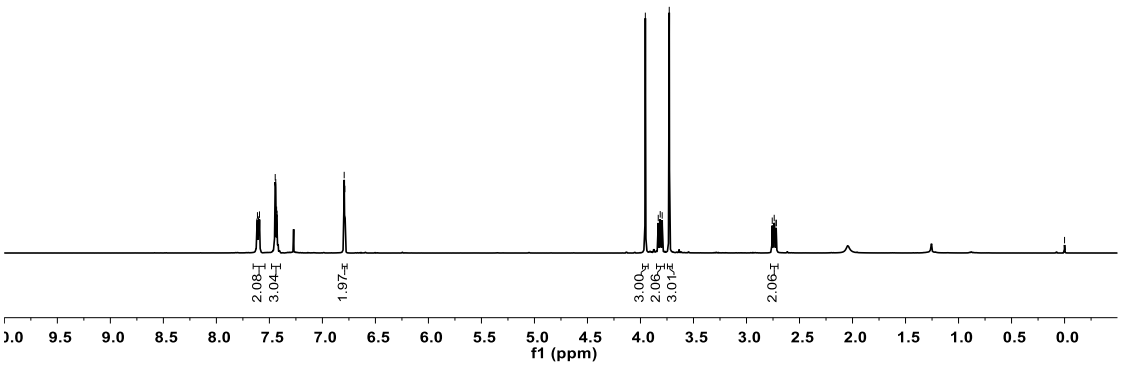

1.00
2.01
4.16
3.07
1.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

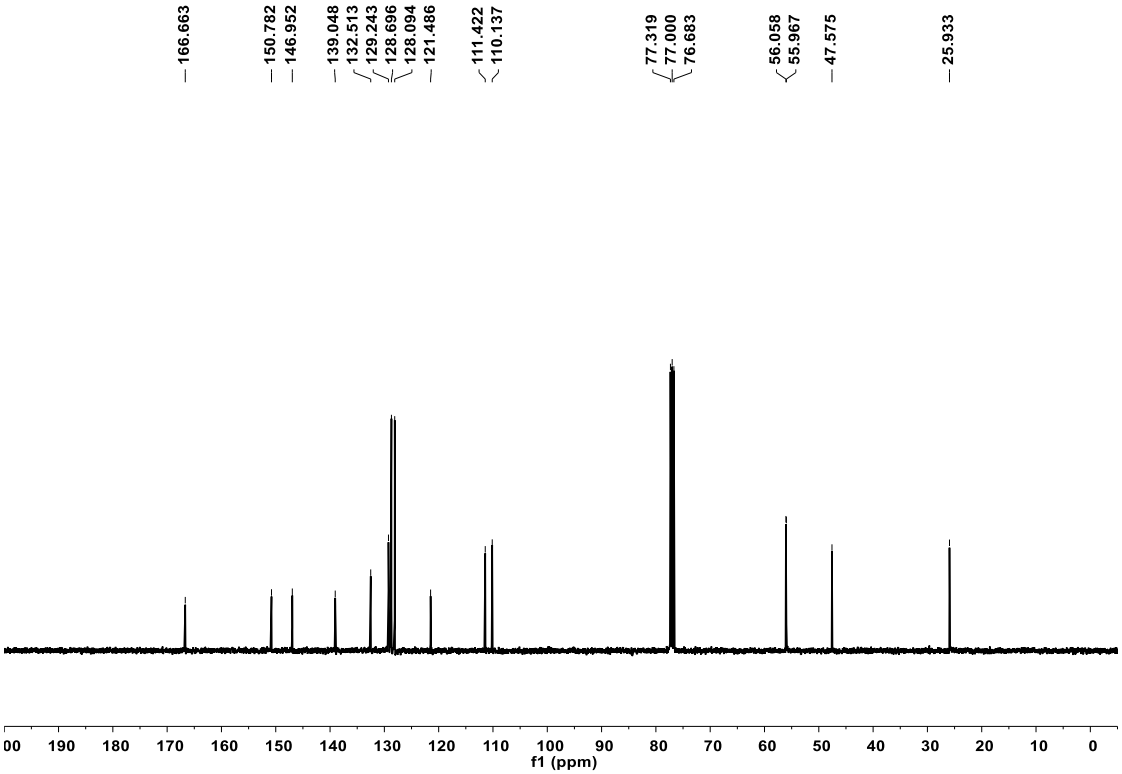

167.990
154.097
135.005
134.465
133.036
130.818
128.714
128.700
127.757
127.453
127.344
126.762
126.282
125.131
124.300
123.110
121.544
77.317
77.000
76.682


00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.618
7.613
7.605
7.601
7.599
7.596
7.593
7.445
7.440
7.432
7.427
6.795
6.788
3.954
3.832
3.818
3.814
3.809
3.795
3.729
2.757
2.744
2.739
2.734
2.720
2.720
0.000
MeO
MeO
N
Ph

7


2.08
3.04
1.97
3.00
2.06
3.01
2.06
f1 (ppm)


166.663
150.782
146.952
139.048
132.513
129.243
128.696
128.094
121.486
111.422
110.137
77.319
77.000
76.683
56.058
55.967
47.575
25.933
f1 (ppm)