Supporting Information

Iodine-Catalyzed Convergent Aerobic Dehydro-Aromatization toward Benzazoles and Benzazines

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1. General information.

All reactions were carried out under the standard conditions unless otherwise noted. Column chromatography was performed using silica gel (100-200 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (400 and 100 MHz, respectively) instrument internally referenced to tetramethylsilane (TMS) or chloroform signals. Mass spectra were measured on Agilent 5975 GC-MS instrument (EI). High-resolution mass spectra were recorded at Keecloud (Shanghai) Biotechnology co. LTD. HRMS was conducted using electrospraying ionization (ESI) and was performed on a Thermo Scientific LTQ Orbitrap XL. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and MS data with those of literature. All reagents were obtained from commercial suppliers and used without further purification.

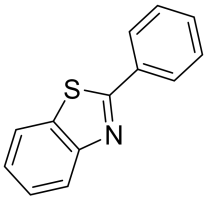
2. General procedure for the 2-phenylbenzo[*d*]thiazole synthesis

2-phenyl-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1a**, 43.0 μL, 0.2 mmol), I_2 (20 mol%, 10.2 mg), *o*-DCB (0.8 mL), toluene (0.2 mL) were added to a 10 mL reaction vessel. The sealed reaction vessel under oxygen atmosphere was stirred at 160 ^{o}C for 30 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **4a** as white solid (31.6 mg, 75% yield).

6 mmol scale: 2-phenyl-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1a**, 1290.0 mg, 6 mmol), I_2 (304.6 mg, 1.2 mmol), *o*-DCB (8 mL), toluene (2 mL), were added to a 50 mL reaction vessel. The sealed reaction vessel under oxygen atmosphere was stirred at 160 ^{o}C for 30 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product as white solid (860.8 mg, 68% yield).

3. Characterization data of products

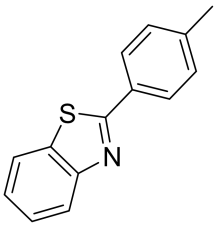
2-Phenylbenzo[*d*]thiazole (4a, CAS: 833-93-2)[1]



The reaction was conducted with 2-phenyl-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1a**, 43.0 μL, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **4a** as white solid (31.6 mg, 75% yield), mp 113-116 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.11-8.06 (m, 3H), 7.87 (d, J = 8.4 Hz, 1H), 7.51-7.46 (m, 4H), 7.39-7.34 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 168.0, 154.1, 135.0, 133.5, 130.9, 129.0, 127.5, 126.3, 125.1, 123.1, 121.6.

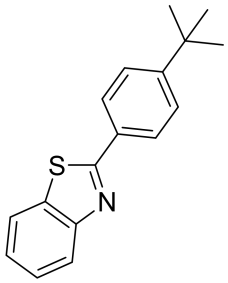
2-(*p*-Tolyl)benzo[*d*]thiazole (4b, CAS: 16112-21-3)[1]



The reaction was conducted with 2-(*p*-tolyl)-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1b**, 45.8 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **4b** as pale white solid (33.3 mg, 74% yield), mp 84-86 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.05 (d, J = 8.4 Hz, 1H), 7.98 (d, J = 8.0 Hz, 2H), 7.88 (d, J = 8.0 Hz, 1H), 7.50-7.46 (m, 1H), 7.39-7.35 (m, 1H), 7.29 (d, J = 8.0 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 168.3, 154.2, 141.5, 135.0, 131.0, 129.8, 127.5, 126.3, 125.0, 123.1, 121.6, 21.6.

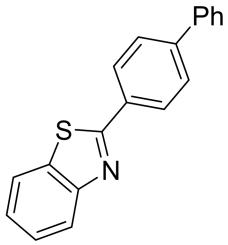
2-(4-(*t*-Butyl)phenyl)benzo[*d*]thiazole (4c, CAS: 1242329-99-2)[1]



The reaction was conducted with 2-(4-(*t*-butyl)phenyl)-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1c**, 57.2 μL, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **4c** as pale yellow solid (37.9 mg, 71% yield), mp 106-107 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (d, J = 8.0 Hz, 1H), 8.04-8.00 (m, 2H), 7.87 (d, J = 8.0 Hz, 1H), 7.52-7.45 (m, 3H), 7.38-7.34 (m, 1H), 1.36 (s, 9H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 168.1, 154.5, 154.2, 135.0, 130.9, 127.3, 126.2, 126.0, 125.0, 123.0, 121.6, 35.0, 31.1.

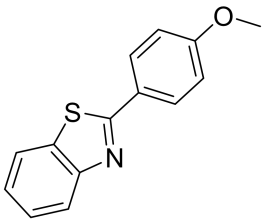
2-([1,1'-Biphenyl]-4-yl)benzo[*d*]thiazole (4d, CAS: 67362-98-5)[1]



The reaction was conducted with 2-([1,1'-biphenyl]-4-yl)-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1d**, 58.2 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **4d** as pale yellow solid (36.7 mg, 64% yield), mp 191-192 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (d, J = 8.4 Hz, 2H), 8.09 (d, J = 8.4 Hz, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 9.6 Hz, 2H), 7.68-7.66 (m, 2H), 7.53-7.47 (m, 3H), 7.42-7.38 (m, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.7, 154.2, 143.7, 140.1, 135.1, 132.5, 128.9, 128.0, 128.0, 127.6, 127.1, 126.3, 125.2, 123.2, 121.6.

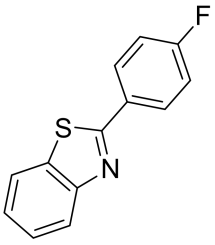
2-(4-Methox yphenyl)benzo[*d*]thiazole (4e, CAS: 6265-92-5)[1]



The reaction was conducted with 2-(4-methoxyphenyl)-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1e**, 49.0 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 60:1) to yield the desired product **4e** as pale white solid (29.4 mg, 61% yield), mp 122-124 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 (d, J = 8.8 Hz, 3H), 7.86 (d, J = 8.0 Hz, 1H), 7.49-7.44 (m, 1H), 7.36-7.34 (m, 1H), 7.01-6.97 (m, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 161.9, 154.1, 134.8, 129.0, 126.3, 126.2, 124.7, 122.8, 121.5, 114.3, 55.4.

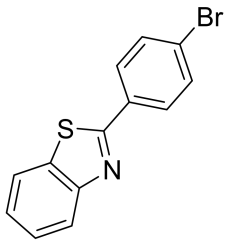
2-(4-Fluorophenyl)benzo[*d*]thiazole (4f, CAS: 1629-26-1)[2]



The reaction was conducted with 2-(4-fluorophenyl)-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1f**, 46.6 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **4f** as pale yellow solid (27.0 mg, 59% yield), mp 99-100 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09-8.05 (m, 3H), 7.88 (d, J = 8.0 Hz, 1H), 7.51-7.47 (m, 1H), 7.40-7.36 (m, 1H), 7.19-7.15 (m, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.2 (d, J = 105.6 Hz), 163.2, 153.9, 134.9, 129.8 (d, J = 13.2 Hz), 129.5 (d, J = 8.6 Hz) , 126.4, 125.2, 123.1, 121.6, 116.1 (d, J = 22.1 Hz).

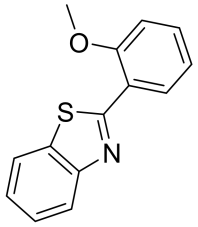
2-(4-Bromophenyl)benzo[*d*]thiazole (4g, CAS: 19654-19-4)[2]



The reaction was conducted with 2-(4-bromophenyl)-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1g**, 58.8 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **4g** as pale yellow solid (33.6 mg, 58% yield), mp 125-127 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.8 Hz, 2H), 7.90 (d, J = 7.6 Hz, 1H), 7.63 (d, J = 8.8 Hz, 2H), 7.53-7.50 (m, 1H), 7.44-7.40 (m, 1H) ; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.7, 154.0, 135.0, 132.6, 132.3, 128.9, 126.5, 125.4, 125.4, 123.3, 121.6.

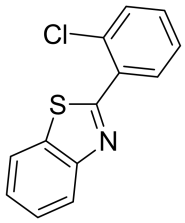
2-(2-Methoxyphenyl)benzo[*d*]thiazole (4h, CAS: 6269-47-2)[2]



The reaction was conducted with 2-(2-methoxyphenyl)-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1h**, 49.0 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **4h** as white solid (28.4 mg, 59% yield), mp 90-91 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.07 (d, J = 8.4 Hz, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.68-7.62 (m, 2H), 7.51-7.46 (m, 1H), 7.40-7.36 (m, 2H), 7.03 (d, J = 8.4 Hz, 1H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.9, 160.0, 154.0, 135.0, 134.8, 130.0, 126.3, 125.2, 123.2, 121.6, 120.2, 117.3, 111.9, 55.5.

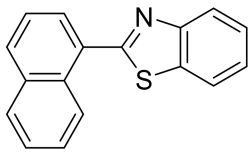
2-(2-Chlorophenyl)benzo[*d*]thiazole (4i, CAS: 6269-46-1)[2]



The reaction was conducted with 2-(2-chlorophenyl)-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1i**, 49.8 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **4i** as pale white solid (27.4 mg, 56% yield), mp 85-86 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23-8.21 (m, 1H), 8.14 (d, J = 8.0 Hz, 1H), 7.96 (d, J = 8.0 Hz, 1H), 7.56-7.52 (m, 2H), 7.46-7.41 (m, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 164.1, 152.5, 136.1, 132.6, 132.2, 131.7, 131.1, 130.8, 127.1, 126.3, 125.4, 123.4, 121.3.

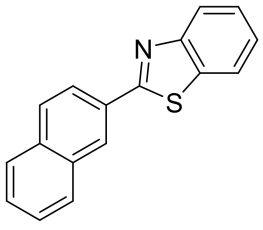
2-(Naphthalen-1-yl)benzo[*d*]thiazole (4j, CAS: 56048-50-1)[3]



The reaction was conducted with 2-(4-methoxyphenyl)-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1j**, 53.0 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 80:1) to yield the desired product **4j** as pale white solid (37.0 mg, 71% yield), mp 123-126 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.96 (d, J = 8.8 Hz, 1H), 8.22 (d, J = 8.4 Hz, 1H), 8.02-7.92 (m, 4H), 7.66-7.55 (m, 4H), 7.46-7.42 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.6, 154.2, 135.5, 134.0, 131.1, 130.8, 130.6, 129.4, 128.4, 127.7, 126.5, 126.3, 125.9, 125.3, 125.0, 123.7, 121.4.

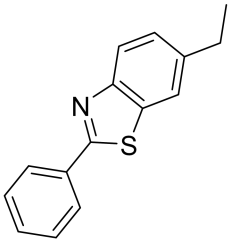
2-(Naphthalen-2-yl)benzo[*d*]thiazole (4k, CAS: 56048-51-2)[3]



The reaction was conducted with 2-(naphthalen-2-yl)-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1k**, 53.0 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 80:1) to yield the desired product **4k** as pale white solid (34.4 mg, 66% yield), mp 98-100 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.55 (s, 1H), 8.19 (d, J = 8.4 Hz, 1H), 8.10 (d, J = 8.0 Hz, 1H), 7.95-7.84 (m, 4H), 7.54-7.48 (m, 3H), 7.38 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 168.1, 154.2, 135.1, 134.6, 133.1, 131.0, 128.8, 128.8, 127.8, 127.5, 127.4, 126.8, 126.4, 125.2, 124.4, 123.2, 121.6.

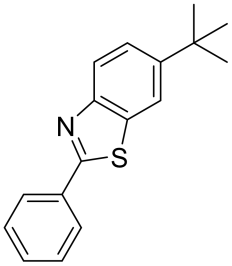
6-Ethyl-2-phenylbenzo[*d*]thiazole (4l, CAS: 124-303-5)[3]



The reaction was conducted with 6-ethyl-2-phenyl-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1l**, 48.6 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **4l** as pale white solid (29.6 mg, 62% yield), mp 58-60 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09-8.06 (m, 2H), 7.97 (d, J = 8.4 Hz, 1H), 7.71 (s, 1H), 7.50-7.47 (m, 3H), 7.34-7.32 (m, 1H), 2.78 (q, J = 7.6 Hz, 2H), 1.31 (t, J = 7.8 Hz, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.1, 152.4, 141.2, 135.2, 133.8, 130.7, 128.9, 127.4, 126.8, 122.8, 120.1, 28.9, 15.8.

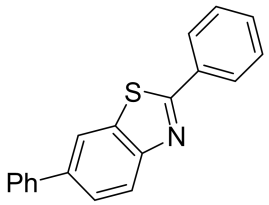
6-(*t*-Butyl)-2-phenylbenzo[*d*]thiazole (4m, CAS: 1242329-99-2)[3]



The reaction was conducted with 6-(*t*-butyl)-2-phenyl-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1m**, 54.2 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **4m** as pale white solid (35.7 mg, 67% yield), mp 105-106 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09-8.06 (m, 2H), 8.00 (d, J = 8.8 Hz, 1H), 7.89 (d, J = 2.0 Hz, 1H), 7.56-7.53 (m, 1H), 7.49-7.47 (m, 3H), 1.40 (s, 9H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.4, 152.1, 148.7, 135.1, 133.8, 130.7, 129.0, 127.4, 124.6, 122.5, 117.7, 35.0, 31.5.

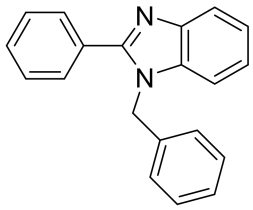
2,6-Diphenylbenzo[*d*]thiazole(4n)[4]



The reaction was conducted with 2,6-diphenyl-4,5,6,7-tetrahydrobenzo[*d*]thiazole (**1n**, 58.2 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to yield the desired product **4n** as pale white solid (42.5 mg, 74% yield), mp 185-186 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13-8.10 (m, 4H), 7.75-7.72 (m, 1H), 7.68-7.66 (m, 2H), 7.53-7.46 (m, 5H), 7.41-7.36 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 168.2, 153.5, 140.6, 138.6, 135.8, 133.6, 131.0, 129.0, 128.9, 127.5, 127.3, 127.4, 126.0, 123.3, 119.9.

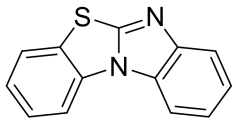
1-benzyl-2-phenyl-1H-benzo[*d*]imidazole (4o, CAS: 739-88-8)[5]



The reaction was conducted with 1-benzyl-2-phenyl-4,5,6,7-tetrahydro-1H-benzo[*d*]imidazole (**1o**, 57.6 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 5:1) to yield the desired product **4o** as white solid (31.8 mg, 56% yield), mp 133-135 ^{o}C.

H NMR (400 MHz, Chloroform-*d*) δ 7.87 (d, J = 8.0 Hz, 1H), 7.70-7.68 (m, 2H), 7.48-7.42 (m, 3H),7.35-7.29 (m, 4H), 7.25-7.20 (m, 2H), 7.10 (d, J = 6.8 Hz, 2H), 5.46 (s, 2H); ^{13}CNMR(100 MHz, Chloroform-*d*) δ 154.1, 143.2, 136.4, 136.0, 130.0, 129.9, 129.2, 129.0, 128.7, 127.7, 126.0, 123.0, 122.6, 119.9, 110.5, 48.3.

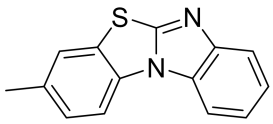
Benzo[*d*]benzo[4,5]imidazo[2,1-*b*]thiazole (5a, CAS: 206-80-4)[6]



The reaction was conducted with 7,8,9,10-tetrahydrobenzo[*d*]benzo[4,5]imidazo[2,1-b]thiazole (**2a**, 45.6 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (eluent = dichloromethane) to yield the desired product **5a** as white solid (31.8 mg, 71% yield), mp 138-139 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, J = 8.4 Hz, 2H), 7.84 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 8.0 Hz, 1H), 7.56-7.51 (m, 1H), 7.45-7.36 (m, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 155.4, 148.2, 133.3, 130.5, 129.0, 126.7, 124.4, 124.3, 123.6, 122.0, 119.5, 112.4, 110.6.

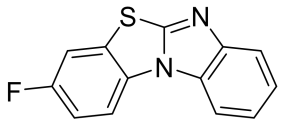
3-Methylbenzo[*d*]benzo[4,5]imidazo[2,1-*b*]thiazole (5b, CAS: 1611489-26-9)[6]



The reaction was conducted with 3-methyl-7,8,9,10-tetrahydrobenzo[*d*]benzo[4,5]Imidazo[2,1-*b*] thiazole (**2b**, 48.4 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (eluent = dichloromethane) to yield the desired product **5b** as white solid (29.9 mg, 63% yield), mp 140-142 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93-7.71 (m, 1H), 7.82 (t, J = 7.2 Hz, 2H), 7.53 (s, 1H), 7.43-7.31 (m, 3H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 155.3, 148.1, 134.4, 131.0, 130.4, 129.0, 127.5, 124.4, 123.3, 121.7, 119.4, 111.9, 110.4, 21.3.

3-Fluorobenzo[*d*]benzo[4,5]imidazo[2,1-*b*]thiazole (5c, CAS: 1611489-29-0)[6]

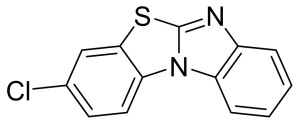


The reaction was conducted with 3-fluoro-7,8,9,10-tetrahydrobenzo[*d*]benzo[4,5]imidazo[2,1-*b*] thiazole (**2c**, 49.2 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (eluent = dichloromethane) to yield the desired product **5c** as white solid (33.8 mg, 70% yield), mp 145-146 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92-7.90 (m, 2H), 7.84-7.82 (m, 1H), 7.63 (d, J = 8.4 Hz,

1H), 7.45-7.33 (m, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 159.4 (d, J = 245.4 Hz), 155.0, 148.0, 130.5, 130.4 (d, J = 9.4 Hz), 129.7, 123.6, 122.2, 119.7, 114.1 (d, J = 24.5 Hz), 112.8 (d, J = 8.9 Hz), 111.6 (d, J = 27.3 Hz), 110.2.

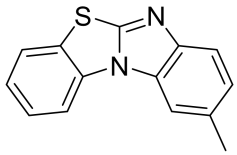
3-Chlorobenzo[*d*]benzo[4,5]imidazo[2,1-*b*]thiazole (5d, CAS: 1403604-83-0)[6]



The reaction was conducted with 3-chloro-7,8,9,10-tetrahydrobenzo[*d*]benzo[4,5]imidazo[2,1-*b*] thiazole (**2d**, 52.4 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (eluent = dichloromethane) to yield the desired product **5d** as white solid (35.1 mg, 68% yield), mp 206-208 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 (m, 2H), 7.80 (m, 1H), 7.64 (d, J = 8.0 Hz, 1H), 7.42-7.34 (m, 2H), 7.31 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 155.5, 148.2, 133.8, 132.7, 130.2, 127.3, 124.9, 124.5, 123.9, 122.3, 119.6, 112.7, 110.5.

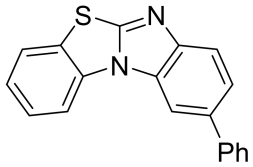
9-Methylbenzo[*d*]benzo[4,5]imidazo[2,1-*b*]thiazole (5e, CAS: 1611489-29-2)[6]



The reaction was conducted with 9-methyl-7,8,9,10-tetrahydrobenzo[*d*]benzo[4,5]imidazo[2,1-*b*] thiazole (**2e**, 48.4 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (eluent = dichloromethane) to yield the desired product **5e** as white solid (30.4 mg, 64% yield), mp 212- 213 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, J = 8.0 Hz, 1H), 7.73-7.69 (m, 3H), 7.52 (t, J = 7.8 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H), 7.22 (d, J = 7.6 Hz, 1H), 2.58 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 154.7, 154.6，146.3, 133.2, 131.9, 129.0, 126.6, 124.9, 124.2, 124.2, 118.9, 112.3, 110.7, 21.8.

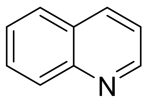
9-Phenylbenzo[*d*]benzo[4,5]imidazo[2,1-*b*]thiazole (5f)



The reaction was conducted with9-phenyl-7,8,9,10-tetrahydrobenzo[*d*]benzo[4,5]imidazo[2,1-*b*] thiazole (**2f**, 60.8 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (eluent = dichloromethane) to yield the desired product **5f** as pale white solid (42.6 mg, 71% yield), mp 175-177 ^oC.

^1H NMR (400 MHz, Chloroform-*d*) δ 8.12 (d, J = 1.2 Hz 1H), 8.01 (d, J = 8.0 Hz, 1H), 7.88 (d, J = 8.4 Hz 1H), 7.75 (d, J = 7.6 Hz, 1H), 7.73-7.70 (m, 2H), 7.67-7.65 (m, 1H), 7.58-7.56 (m, 1H), 7.55-7.53 (m, 1H), 7.50 (d, J = 7.8 Hz, 1H), 7.42-7.37 (m, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 155.7, 147.7, 141.5, 135.8, 133.2, 131.1, 129.0, 128.9, 127.6, 127.2, 126.7, 124.5, 124.4, 123.3, 119.5, 112.4, 109.2. HRMS calcd. for. $C_{19}H_{13}N_2S^+$ $(M+H)^+$ 301.0794, found 301.0799.

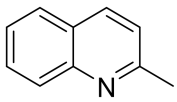
Quinoline (6a, CAS: 91-22-5)[7]



The reaction was conducted with 1,2,3,4-tetrahydroquinoline (**3a**, 26.8 μL, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc =20 :1) to yield the desired product **6a** as colourless liquid (17.2 mg, 67% yield).

^1H NMR (400 MHz, Chloroform-*d*) δ 8.93-8.92 (m, 1H), 8.14 (q, J = 8.0 Hz, 2H), 7.82 (d, J = 4.2 Hz, 1 H), 7.74-7.70 (m, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.40 (q, J = 4.1 Hz, 1H); ^{13}C NMR (100 MHz, Chlorofo rm-*d*) δ 150.4, 148.3, 136.0, 129.5, 129.5, 128.3,127.8, 126.6, 121.1.

2-Methylquinoline (6b, CAS: 91-62-4)[7]

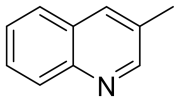


The reaction was conducted with 2-methyl-1,2,3,4-tetrahydroquinoline (**3b**, 29.4 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) to yield the desired product **6b** as colourless oil (20.3 mg, 71%

yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 (t, J = 8.4 Hz, 2H), 7.77 (d, J = 8.0 Hz, 1H), 7.70-7.66 (m, 1H), 7.48 (t, J = 7.4 Hz, 1H), 7.29 (d, J = 8.4 Hz, 1H), 2.75 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 158.9, 147.7, 136.1, 129.3, 128.5, 127.4, 126.4, 125.6, 121.9, 25.3.

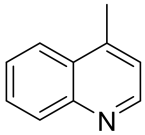
3-Methylquinoline (6c, CAS: 612-58-8)[7]



The reaction was conducted with 3-methyl-1,2,3,4-tetrahydroquinoline (**3c**, 29.4 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) to yield the desired product **6c** as pale colourless oil (19.7 mg, 69% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.76 (d, J = 2.0 Hz, 1H), 8.07 (d, J = 8.4 Hz, 1H), 7.91 (s, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.66-7.62 (m, 1H), 7.53-7.49 (m, 1H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 152.2, 146.3, 134.5, 130.3, 128.9, 128.3, 127.9, 127.0, 126.4, 18.5.

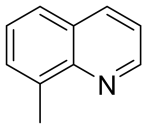
4-Methylquinoline (6d, CAS: 491-35-0)[7]



The reaction was conducted with 4-methyl-1,2,3,4-tetrahydroquinoline (**3d**, 29.4 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) to yield the desired product **6d** as colourless oil (20.3 mg, 71% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.77 (d, J = 4.0 Hz, 1H), 8.11 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.4 Hz, 1H), 7.70 (t, J = 7.6 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.20 (d, J = 4.0 Hz, 1H), 2.68 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 150.1, 147.9, 144.2, 129.8, 129.0, 128.2, 126.2, 123.7, 121.8, 18.6.

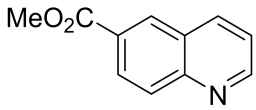
8-Methylquinoline (6e, CAS: 611-32-5)[7]



The reaction was conducted with 8-methyl-1,2,3,4-tetrahydroquinoline (**3e**, 29.4 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) to yield the desired product **6e** as pale yellow liquid (21.1 mg, 74% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.93 (d, J = 2.8 Hz, 1H), 8.09 (d, J = 8.0 Hz 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.54 (d, J = 6.8 Hz, 1H), 7.42-7.34 (m, 2H), 2.82 (s, 3H); ^{13}C NMR (100 MHz, Chloro- form-*d*) δ 149.1, 147.2, 137.0, 136.2, 129.5, 128.2, 126.2, 125.8, 120.7, 18.1.

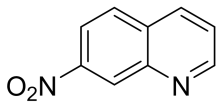
Methyl quinoline-6-carboxylate (6f, CAS: 6931-19-7)[7]



The reaction was conducted with methyl 1,2,3,4-tetrahydroquinoline-6-carboxylate (**3f**, 38.2 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) to yield the desired product **6f** as pale yellow liquid (27.3 mg, 73% yield), mp 141-143 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.01 (d, J = 4..0 Hz, 1H), 8.60 (s, 1H), 8.32-8.26 (m, 2H), 8.15 (d, J = 8.8 Hz, 1H), 7.48 (q, J = 4.3 Hz, 1H), 4.00 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.6, 152.5, 150.0, 137.3, 131.0, 129.8, 128.9, 128.1, 127.4, 121.8, 52.4.

7-Nitroquinoline (6g, CAS: 91-22-5)[8]

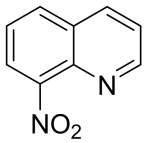


The reaction was conducted with 7-nitro-1,2,3,4-tetrahydroquinoline (**3g**, 35.6 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) to yield the desired product **6g** as pale yellow solid (25.7 mg, 74% yield), mp 127-129 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.10 (d, J = 3.6 Hz, 1H), 9.01 (s, 1H), 8.35-8.32 (m, 1H), 8.29 (d, J = 8.0 Hz, 1H), 8.00 (d, J = 8.8 Hz, 1H), 7.61 (q, J = 4.1 Hz, 1H); ^{13}C NMR (100 MHz,

Chloroform-*d*) δ 152.7, 148.0, 147.1, 136.0, 131.3, 129.5, 125.8, 123.9, 120.1.

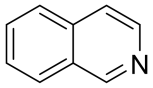
8-Nitroquinoline (6h, CAS: 607-35-2)[9]



The reaction was conducted with 8-nitro-1,2,3,4-tetrahydroquinoline (**3h**, 35.6 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) to yield the desired product **6h** as pale yellow solid (26.8 mg, 77% yield), mp 89-91 ^{o}C .

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.08 (d, J = 4.4 Hz, 1H), 8.28 (d, J = 8.4 Hz, 1H), 8.06 (d, J = 8.0 Hz, 2H), 7.64 (t, J = 7.8 Hz, 1H), 7.60 (q, J = 4.1 Hz 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 152.6, 139.5, 136.1, 132.0, 129.0, 125.3, 123.8, 122.8.

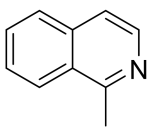
Isoquinoline (6i, CAS: 119-65-3)[9]



The reaction was conducted with 1,2,3,4-tetrahydroisoquinoline (**3i**, 26.8 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) to yield the desired product **6i** as colourless liquid (17.3 mg, 67% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.26 (s, 1H), 8.53 (d, J = 6.0 Hz, 1H), 7.96 (d, J = 8.0 Hz, 1H), 7.82 (d, J = 8.0 Hz, 1H), 7.71-7.58 (m, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 152.4, 142.9, 135.7, 130.2, 128.6, 127.5, 127.1, 126.4, 120.4.

1-Methylisoquinoline (6j, CAS: 1721-93-3)[9]

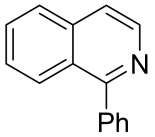


The reaction was conducted with 1-methyl-1,2,3,4-tetrahydroisoquinoline (**3j**, 29.4 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel

(petroleum ether/EtOAc = 10:1) to yield the desired product **6j** as pale yellow liquid (21.7 mg, 76% yield).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (d, J = 5.6 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.68-7.64 (m, 1H), 7.58-7.50 (m, 1H), 7.49 (d, J = 5.6 Hz, 1H), 2.96 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 149.1, 147.2, 137.0, 136.2, 129.5, 128.2, 126.2, 125.8, 120.7, 18.1.

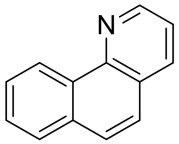
1-Phenylisoquinoline (6k, CAS: 3297-72-1)[9]



The reaction was conducted with 1-phenyl-1,2,3,4-tetrahydroisoquinoline (**3k**, 41.8 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) to yield the desired product **6k** as white solid (35.7 mg, 87% yield), mp 94-95 ^{o}C .

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.61 (d, J = 5.6 Hz, 1H), 8.11 (d, J = 8.4 Hz, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.72-7.64 (m, 4H), 7.56-7.50 (m, 4H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 160.7, 142.1, 139.4, 136.8, 130.0, 129.9, 128.6, 128.3, 127.6, 127.2, 126.9, 126.6, 120.0.

Benzo[*h*]quinoline (6l, CAS: 85-02-9)[10]

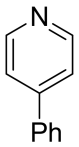


The reaction was conducted with 1,2,3,4-tetrahydrobenzo[*h*]quinoline (**3l**, 36.6 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) to yield the desired product **6l** as pale yellow solid (25.4 mg, 71% yield), mp 211-213 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.31-9.29 (m, 1H), 9.00 (q, J = 2.1 Hz, 1H), 8.18-8.15 (m, 1H), 7.92-7.89 (m, 1H), 7.81 (d, J = 8.8 Hz, 1H), 7.77-7.66 (m, 3H), 7.53-7.50 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 148.8, 146.5, 135.8, 133.6, 131.5, 128.2, 127.8, 127.7, 127.1, 126.4,

125.3, 124.3, 121.8.

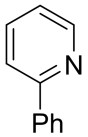
4-Phenylpyridine (6m, CAS: 939-23-1)[11]



The reaction was conducted with 4-phenylpiperidine (**3m**, 31.8 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 5:1) to yield the desired product **6m** as pale yellow solid (17.3 mg, 56% yield), mp 76-78 ^oC.

^1H NMR (400 MHz, Chloroform-*d*) δ 8.95 (d, J = 6.4 Hz, 1H), 8.09 (d, J = 2.0 Hz, 2H), 7.67 (d, J = 6.8 Hz, 1H), 7.61-7.58 (m, 1H), 7.50-7.48 (m, 1H), 7.41-7.39 (m, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 152.3, 145.0, 136.1, 133.6, 130.4, 129.5, 127.5, 127.2, 122.8.

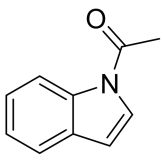
2-Phenylpyridine (6n, CAS: 1008-89-5)[11]



The reaction was conducted with 2-phenylpiperidine (**3n**, 31.8 mg, 0.2 mmol), I_2 (20 mol%1, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 5:1) to yield the desired product **6n** as pale white solid (17.0 mg, 55% yield), mp 147-149 ^oC.

^1H NMR (400 MHz, Chloroform-*d*) δ 8.68 (d, J = 4.8 Hz, 1H), 7.98 (d, J = 7.2 Hz, 2H), 7.74-7.69 (m, 2H), 7.49-7.38 (m, 3H), 7.21-7.18 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.4, 149.6, 139.3, 136.7, 128.9, 128.7, 126.8, 122.0, 120.5.

1-(5-Nitro-1*H*-indol-1-yl)ethan-1-one (6o, CAS: 576-15-8)[12]

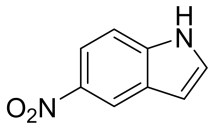


The reaction was conducted with 1-(indolin-1-yl)ethan-1-one (**3o**, 21.6 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) to yield the desired product **6o** as pale white solid (20.3 mg, 64% yield), mp

99-101 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.44 (d, J = 8.4 Hz, 1H), 7.56 (d, J = 8.0 Hz, 1H), 7.42 (d, J = 4.0 Hz, 1H), 7.36 (t, J = 8.2 Hz, 1H), 7.30-7.26 (m, 1H), 6.64 (d, J = 3.6 Hz, 1H), 2.64 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 168.6, 135.5, 130.4, 125.2, 125.1, 123.6, 120.8, 116.5, 109.2, 24.0.

5-Nitro-1*H*-indole (6p, CAS: 6146-52-7)[13]



The reaction was conducted with 5-nitroindoline (**3p**, 33.2 mg, 0.2 mmol), I_2 (20 mol%, 10.2 mg). The residue was purified by column chromatography on silica gel (petroleum ether/dichloromethane = 1:1) to yield the desired product **3p** as pale white solid (18.5 mg, 57% yield), mp 142-144 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.82 (s, 1H), 8.61 (d, J = 2.0 Hz, 1H), 8.13-8.10 (m, 1H), 7.46 (d, J = 9.2 Hz, 1H), 7.41-7.39 (m, 1H), 6.74-6.73 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 141.8, 138.9, 127.5, 127.2, 118.0, 117.6, 111.1, 105.0.

4. References

(1) Yang, Z.; Hu, R. H.; Li, X. T.; Wang, X.; Gu, R.; Han, S. Q. *Tetrahedron Lett.* **2017**, *58*, 2366-2369.

(2) Canivet, J.; Yamaguchi, J.; Ban, I.; Itami, K. *Org. Lett.* **2009**, *11*, 1733-1736.

(3) Zhang, J.; Zhao, X.; Liu, P.; Sun, P. P. *J. Org. Chem.* **2019**, *84*, 12596-12605.

(4) Heo, Y.; Song, Y. S.; Kim, B. T. Heo, J.-N. *Tetrahedron Lett.* **2006**, *47*, 3091-3094.

(5) Sun, X.; Lv, X.-H.; Ye, L.-M.; Hu, Y.; Chen, Y.-Y.; Zhang,X.-J.; Yan. M. *Org. Biomol. Chem.* **2015**, *13*, 7381-7383.

(6) Gao, J. L.; Zhu, J. Y.; Chen, L. B.; Shao, Y. Y.; Zhu, J. Q.; Huang, Y. J.; Wang, X. X.; Lv, X. *Tetrahedron Lett.* **2014**, *55*, 3367-3373.

(7) Yang, L.; Ma, F.-X.; Xu, F.; Li, D.; Su, L. M.; Xu, H.-C.; Wang, C. *Chem. Asian J.* **2019**, *14*, 3557-3560.

(8) Sahoo, M. K.; Jaiswal, G.; Rana, J.; Balaraman, E. *Chem. A Eur. J.* **2017**, *23,* 14167- 14172.

(9) Pedron, J.; Boudot, C.; Hutter, S.; Bourgeade-Delmas, S.; Stigliani, J.-L.; Sournia-Saquet, A.; Moreau, A.; Boutet-Robinet, E.; Paloque, L.; Mothes, E.; Laget, M.; Vendier, L.; Pratviel, G.; Wyllie, S.; Fairlamb, A.; Azas, N.; Courtioux, B.; Valentin, A.; Verhaeghe, P. *Eur. J. Med. Chem.* **2018**, 155, 135-152.

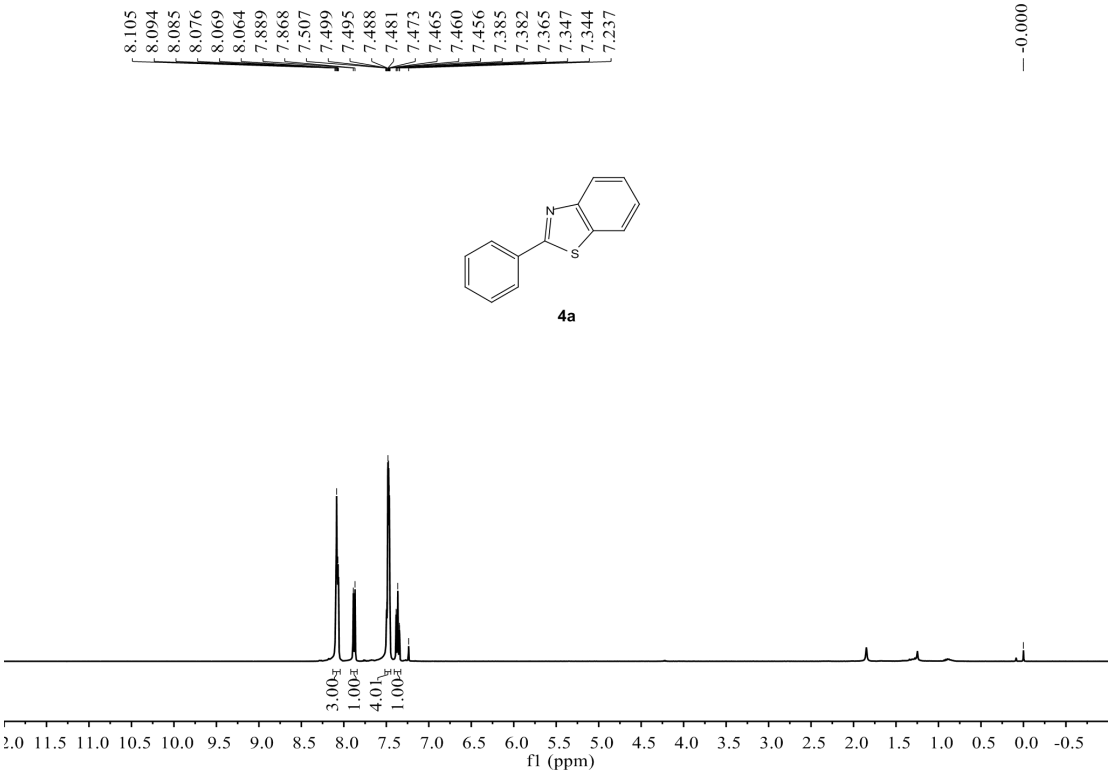
(10) Kojima, M.; Kanai, M. *Angew. Chem. Int. Ed.* **2016**, *55*, 12224-12227.

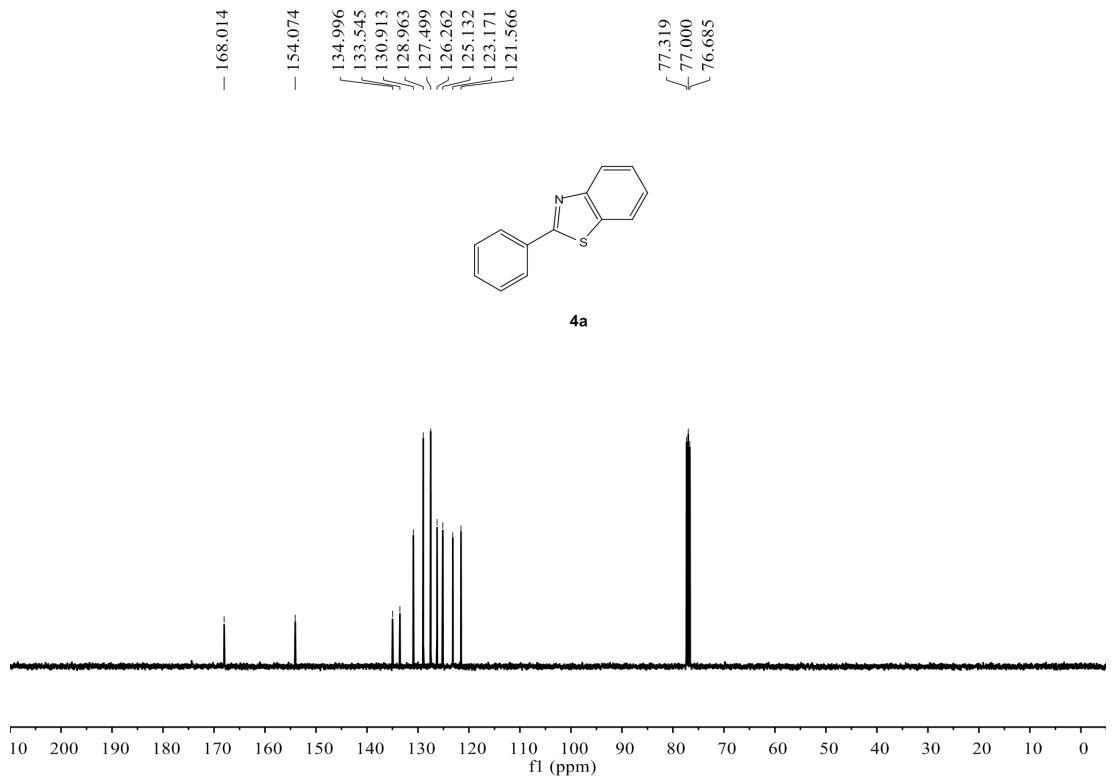
(11) Wei, J.; Liang, H. M.; Ni, C. F.; Sheng, R.; Hu, J. B. *Org. Lett.* **2019**, *21*, 937-940.

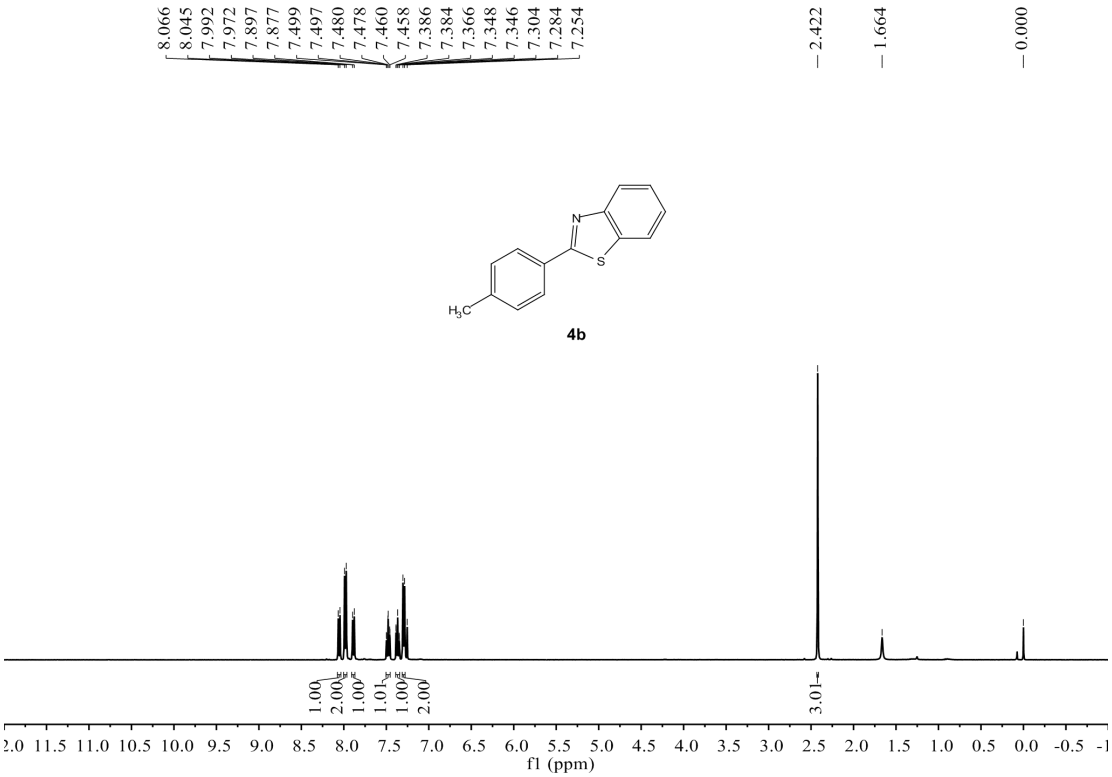
(12) Dissanayake, D. M. M. M.; Vannucci, A. K. *Org. Lett.* **2019**, *21*, 457-460.

(13) Zhang, J. Y.; Chen, S. Y.; Chen, F. F.; Xu, W. S.; Deng, G.-J.; Gong, H. *Adv. Synth. Catal.* **2017**, *359*, 2358-2363.

5. ^{1}H NMR and ^{13}C NMR spectra of products



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7.992
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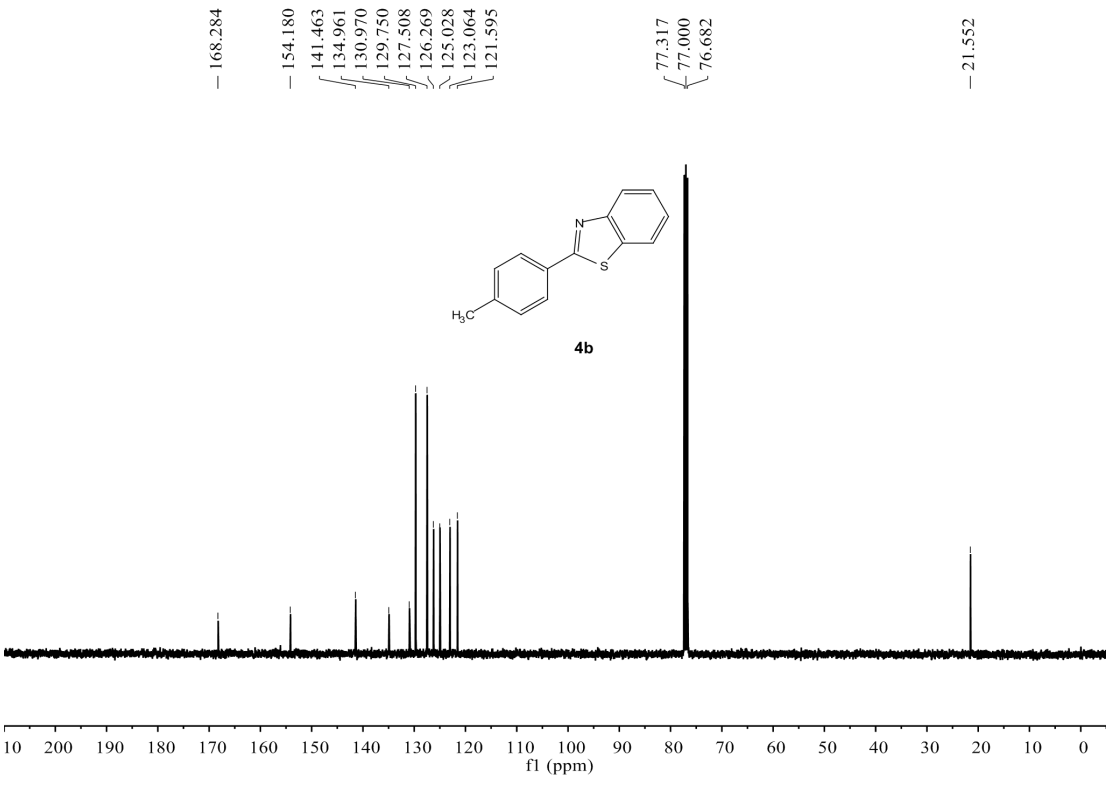
7.897
7.877
7.499
7.497
7.480
7.478
7.460
7.458
7.386
7.384
7.366
7.348
7.346
7.304
7.284
7.254
2.422
1.664
0.000
N
S
H3C
4b
1.00
2.00
1.00
1.01
1.00
2.00
3.01
f1 (ppm)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126.269
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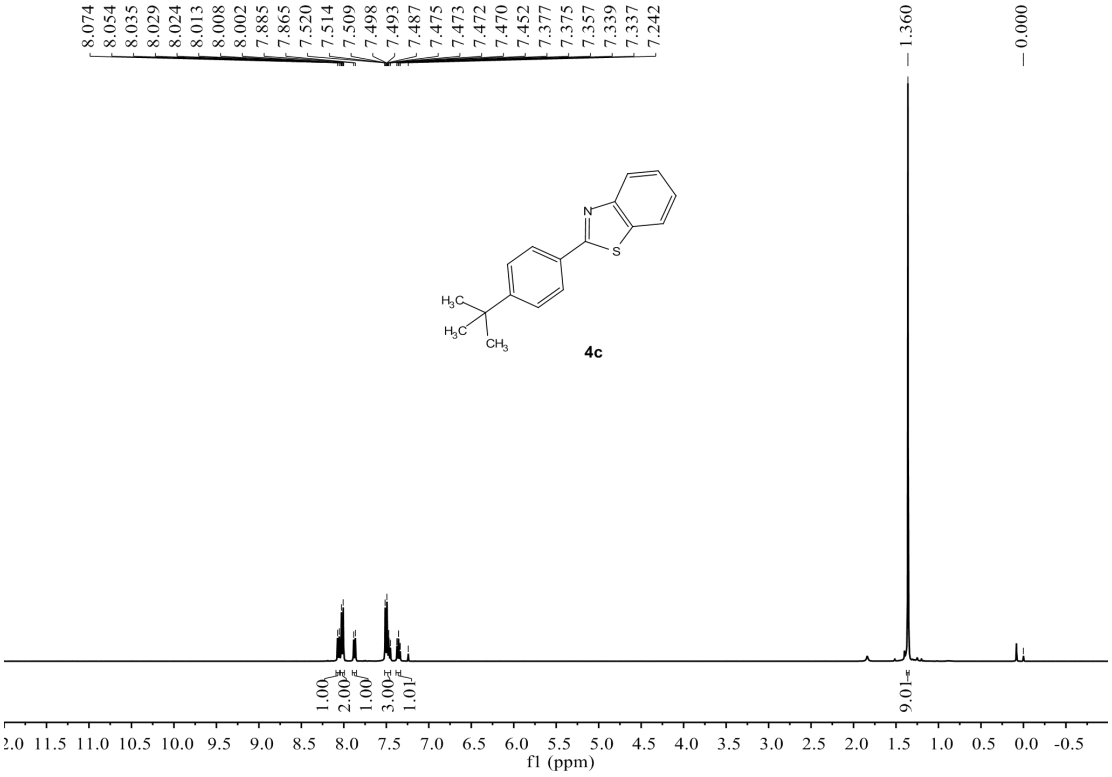
21.552
N
S
H3C
4b
f1 (ppm)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8.002
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7.475
7.473
7.472
7.470
7.452
7.377
7.375
7.357
7.339
7.337
7.242
1.360
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S
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H3C
CH3
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3.00
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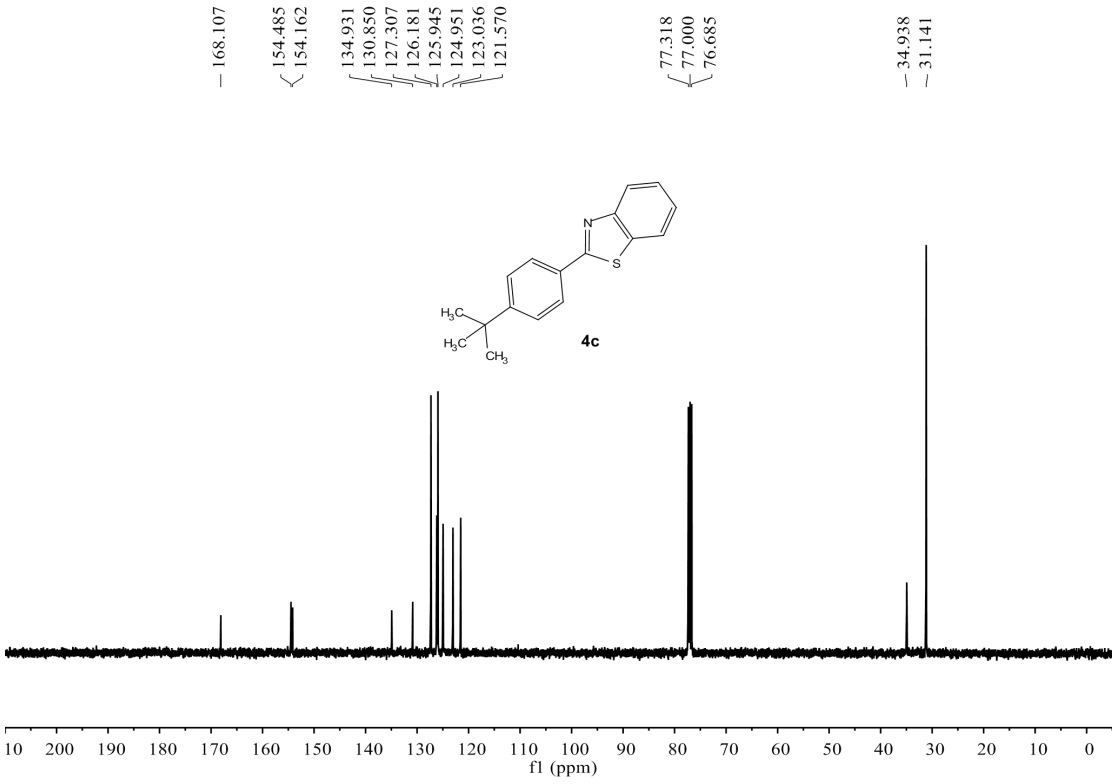
9.01
f1 (ppm)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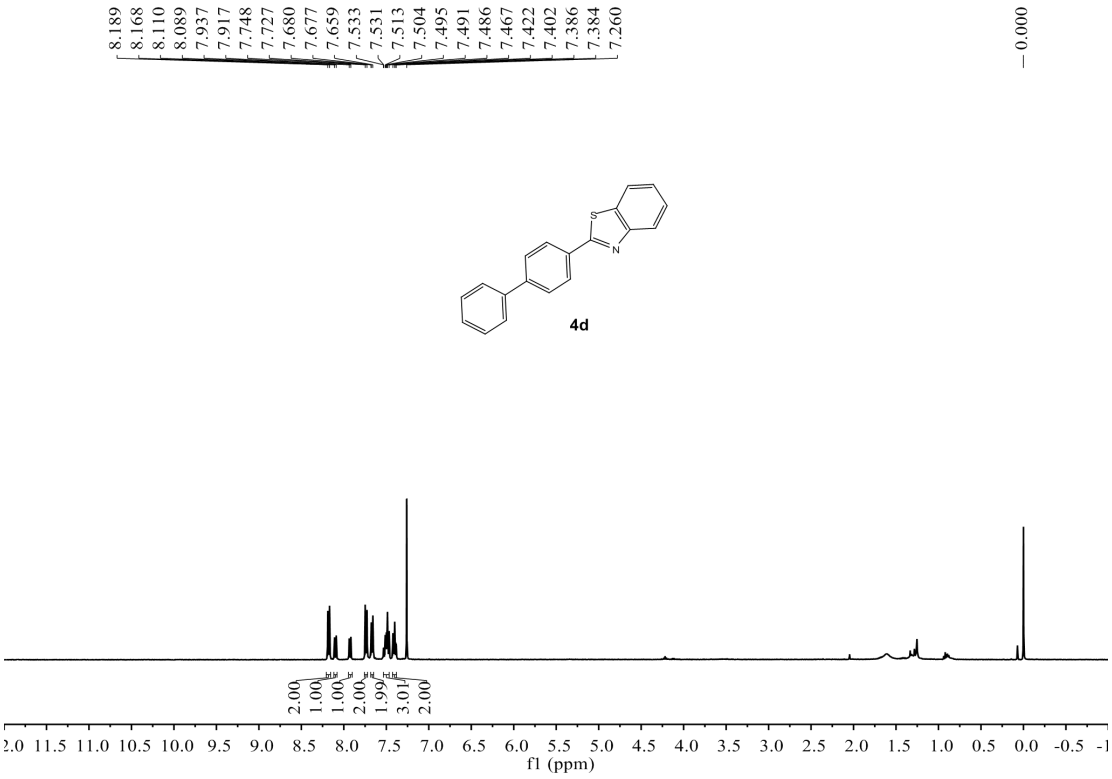
N
S
H3C
H3C
CH3
4c
f1 (ppm)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8.168
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7.677
7.659
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7.531
7.513
7.504
7.495
7.491
7.486
7.467
7.422
7.402
7.386
7.384
7.260
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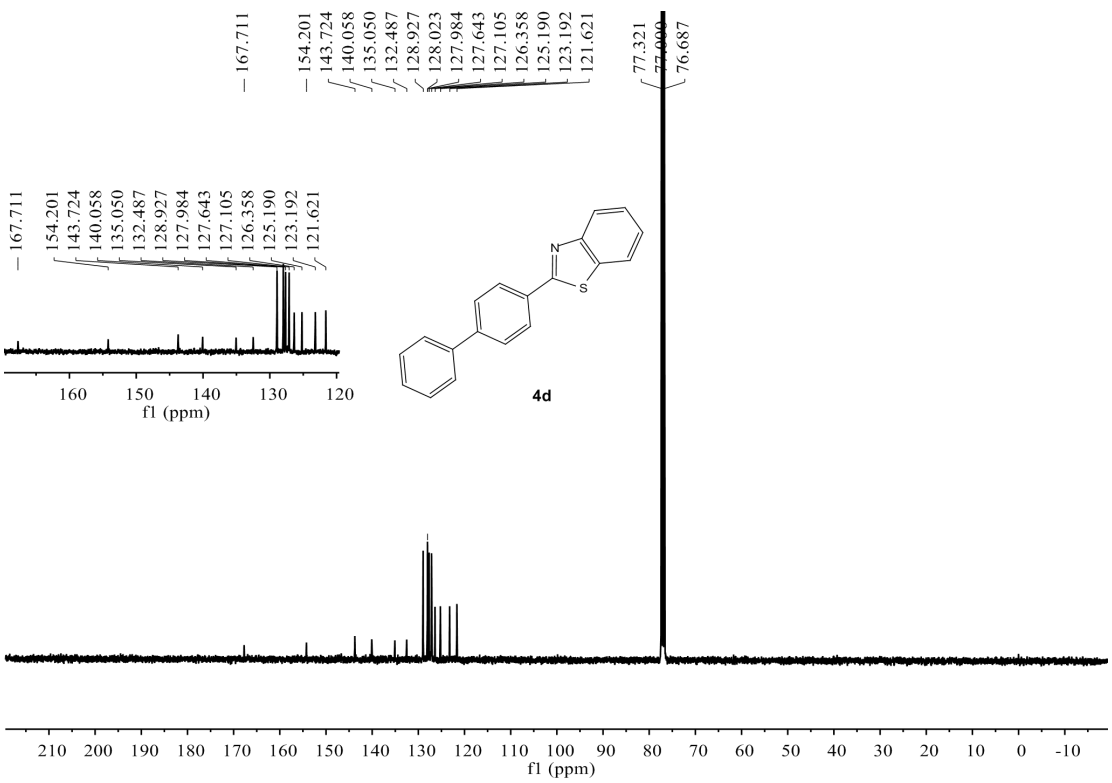
2.00
f1 (ppm)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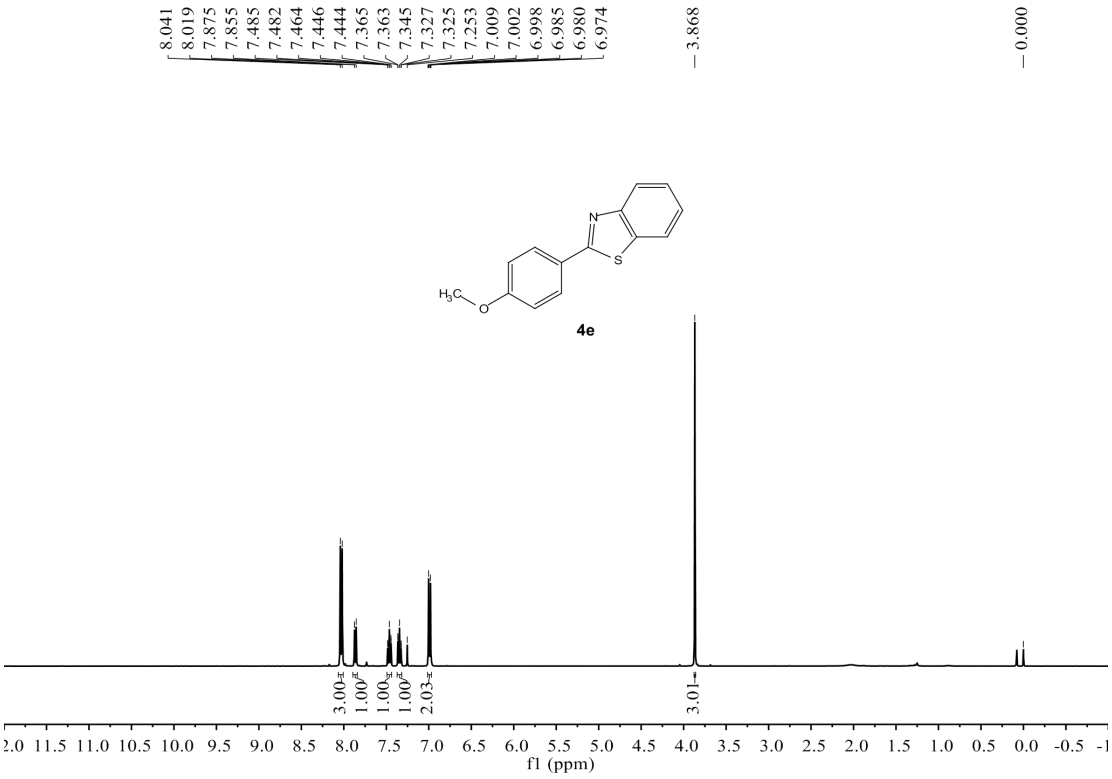
4d
f1 (ppm)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7.365
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7.327
7.325
7.253
7.009
7.002
6.998
6.985
6.980
6.974
3.868
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H3C
O
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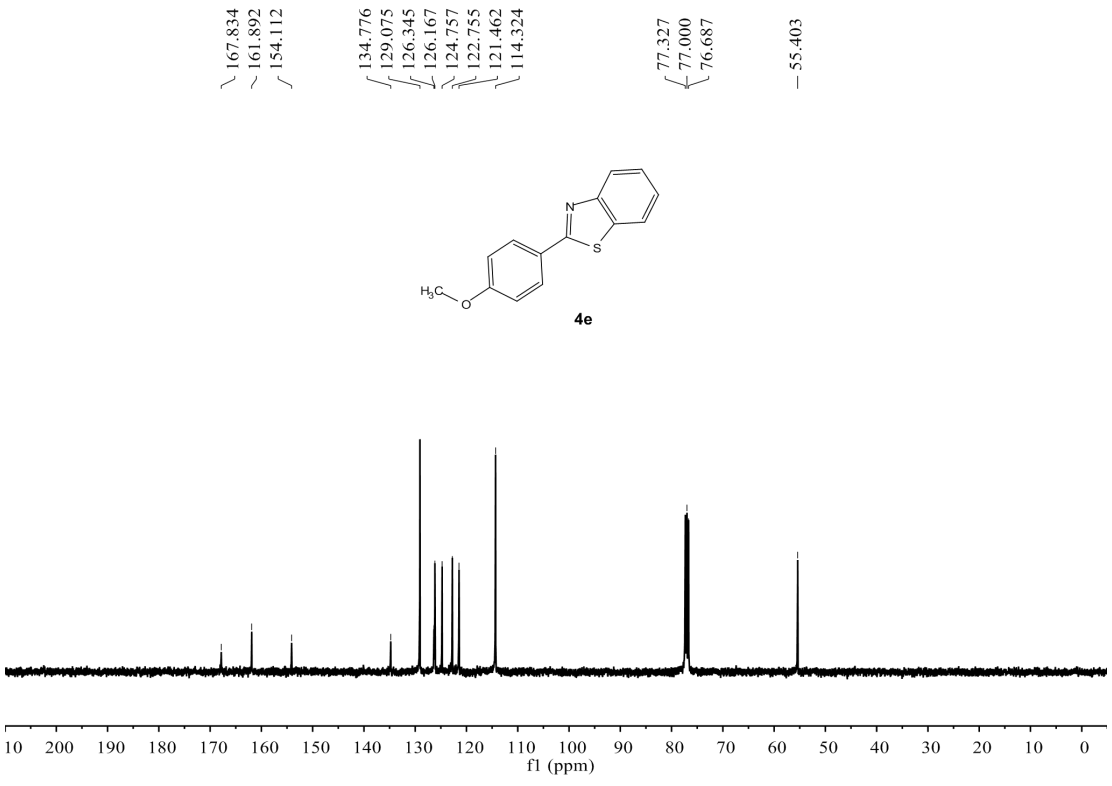
3.01
f1 (ppm)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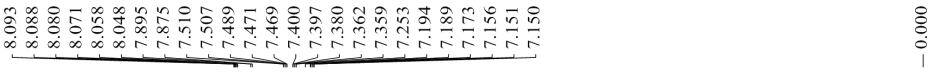
S
H3C
O
4e
f1 (ppm)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7.400
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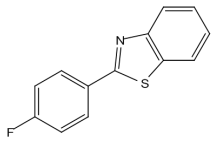
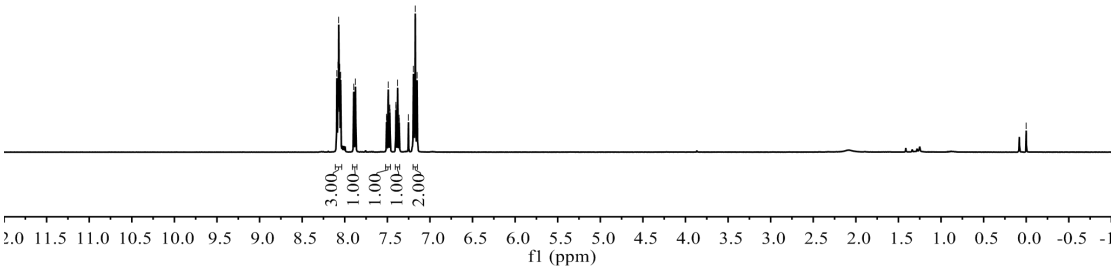

N
S
F

4f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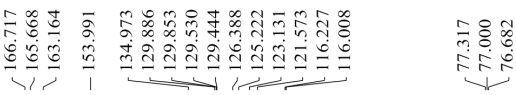
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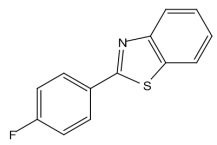
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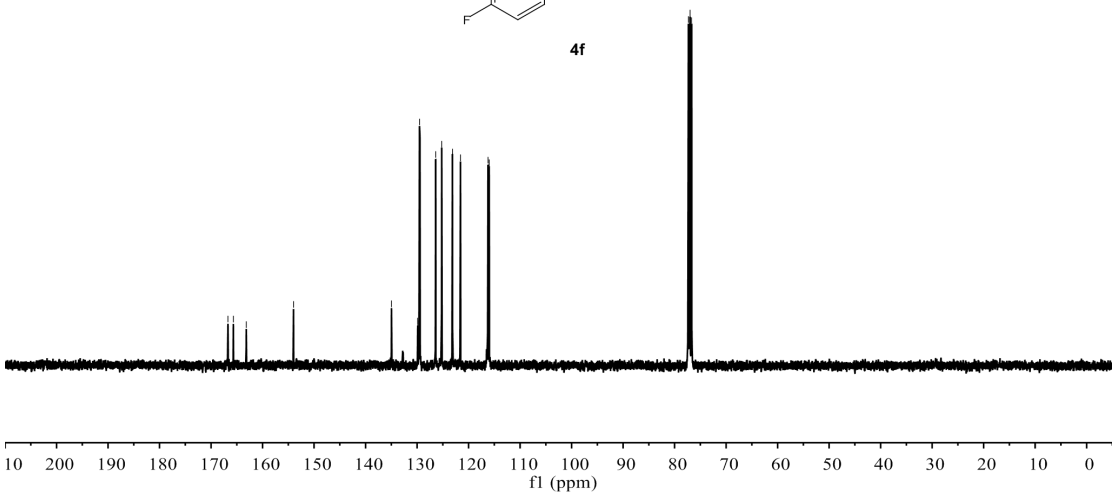
S
F

4f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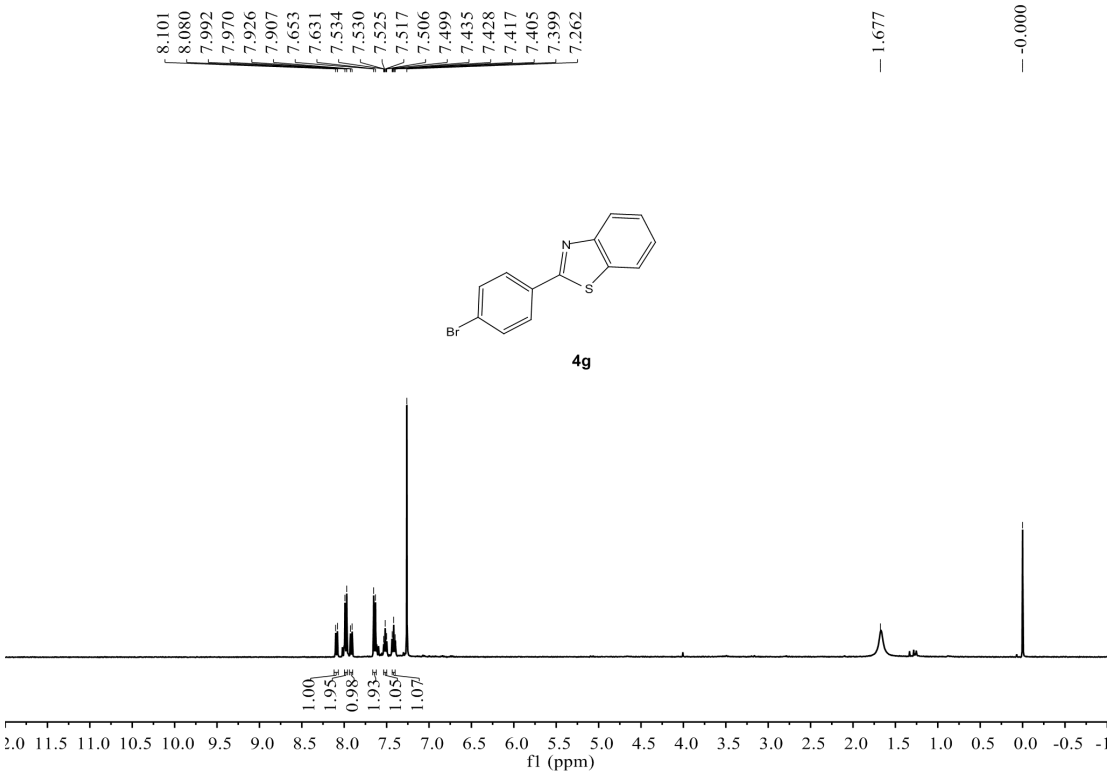
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7.499
7.435
7.428
7.417
7.405
7.399
7.262
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S
Br
4g
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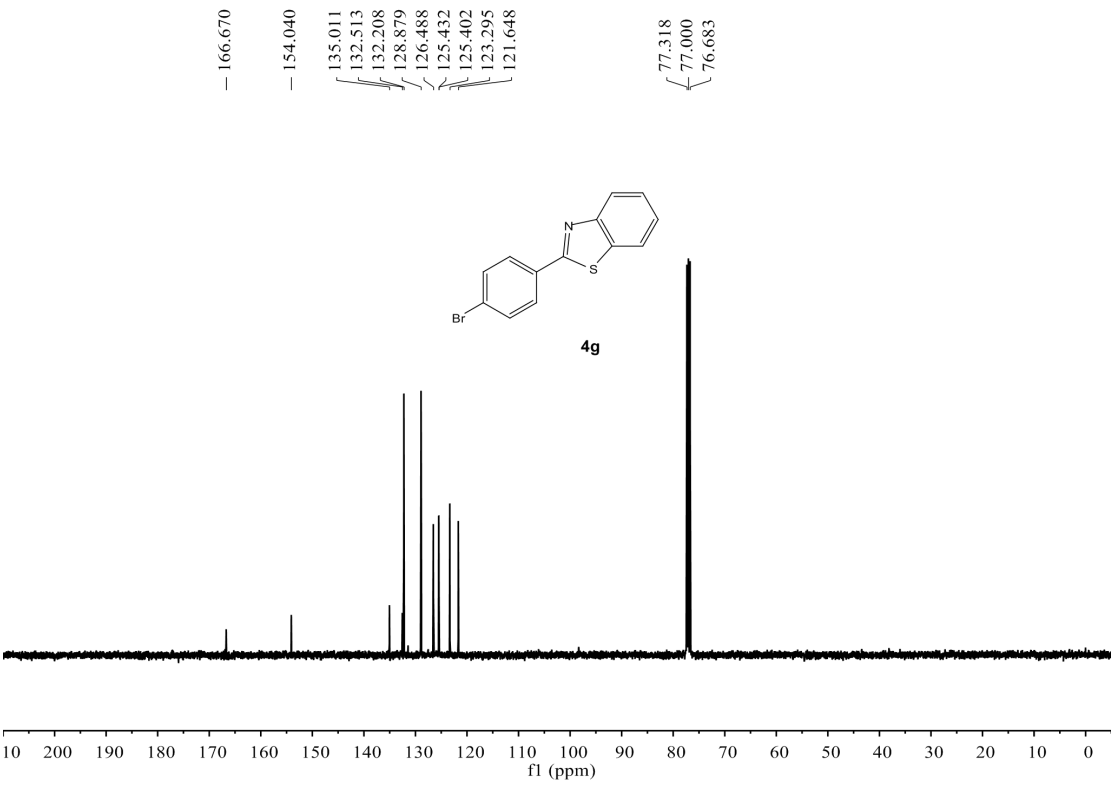
f1 (ppm)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76.683
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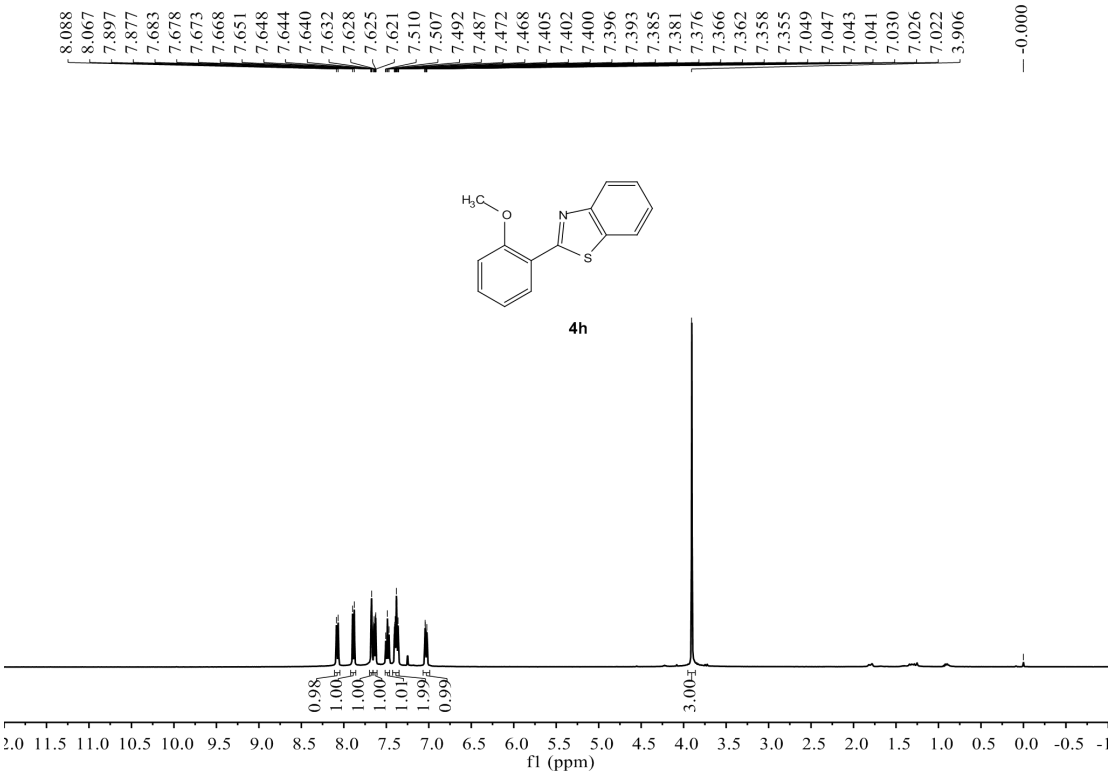
Br
4g
f1 (ppm)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7.628
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7.472
7.468
7.405
7.402
7.400
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7.393
7.385
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7.376
7.366
7.362
7.358
7.355
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7.047
7.043
7.041
7.030
7.026
7.022
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0.98
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1.00
1.00
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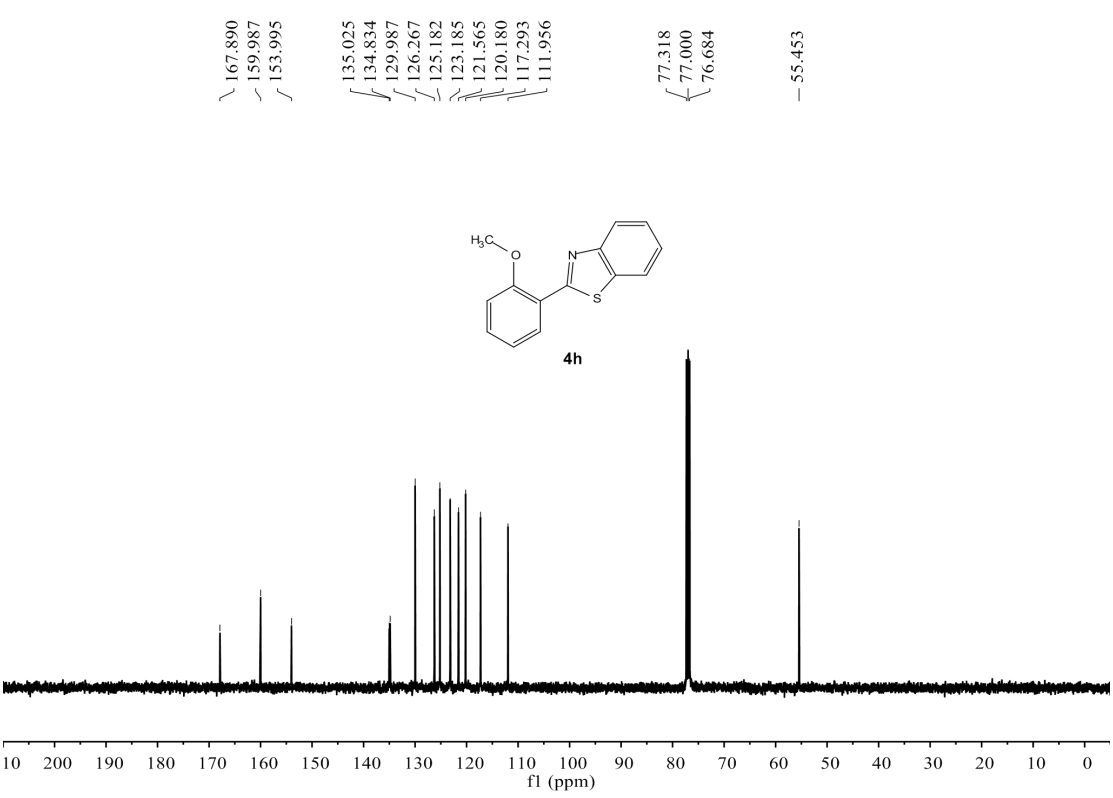
1.99
0.99
3.00
f1 (ppm)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77.000
76.684
55.453
4h
f1 (ppm)


8.229
8.220
8.214
8.205
8.154
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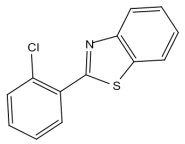
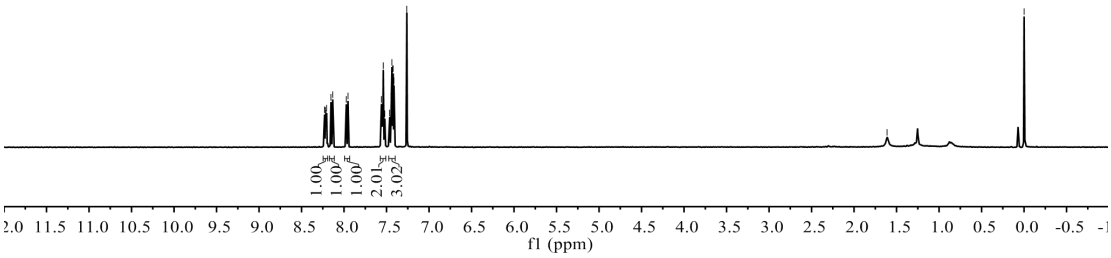

Cl
N
S

4i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3.02
2.0 11.5 11.0 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 -0.5
f1 (ppm)


164.146
152.482
136.087
132.687
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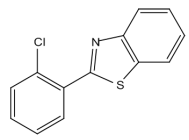
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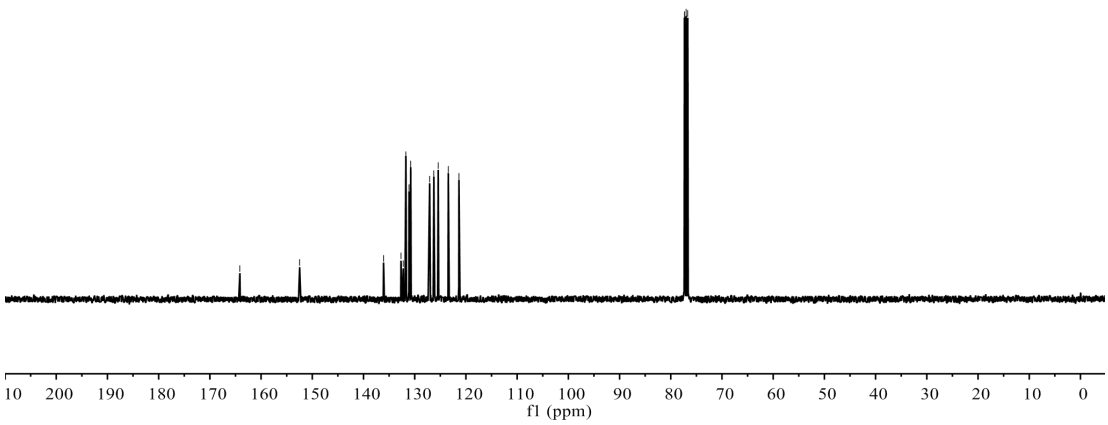
S

4i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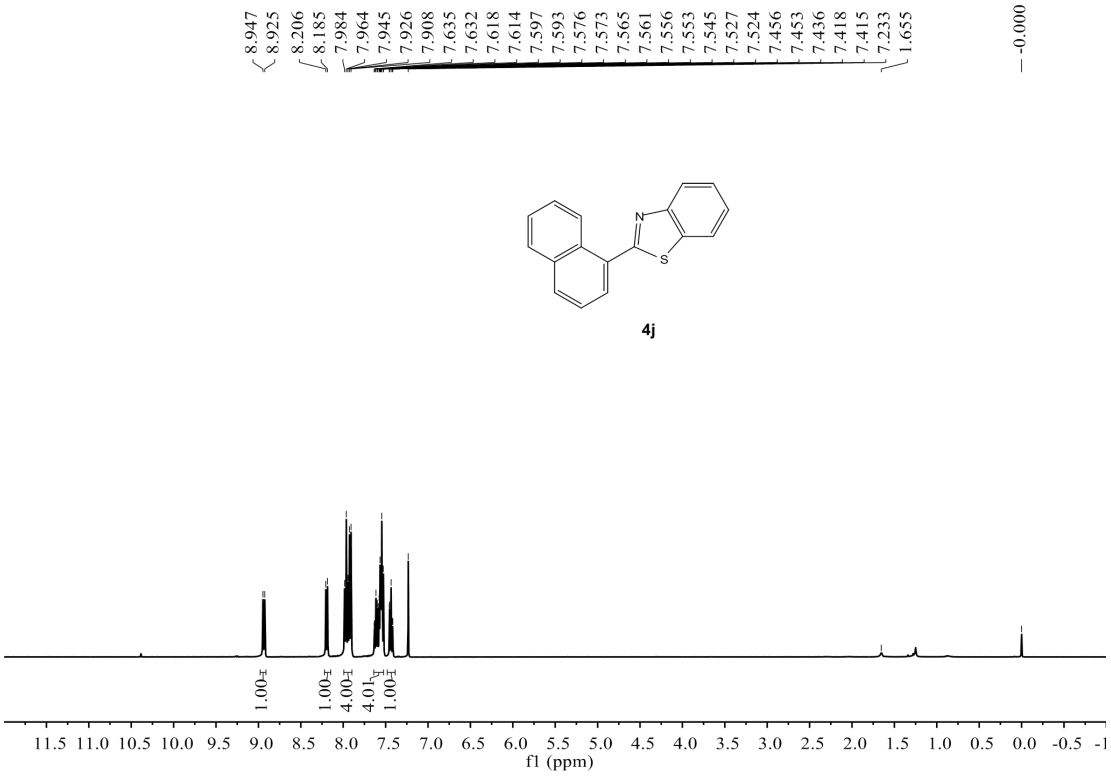
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7.556
7.553
7.545
7.527
7.524
7.456
7.453
7.436
7.418
7.415
7.233
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N
S
4j
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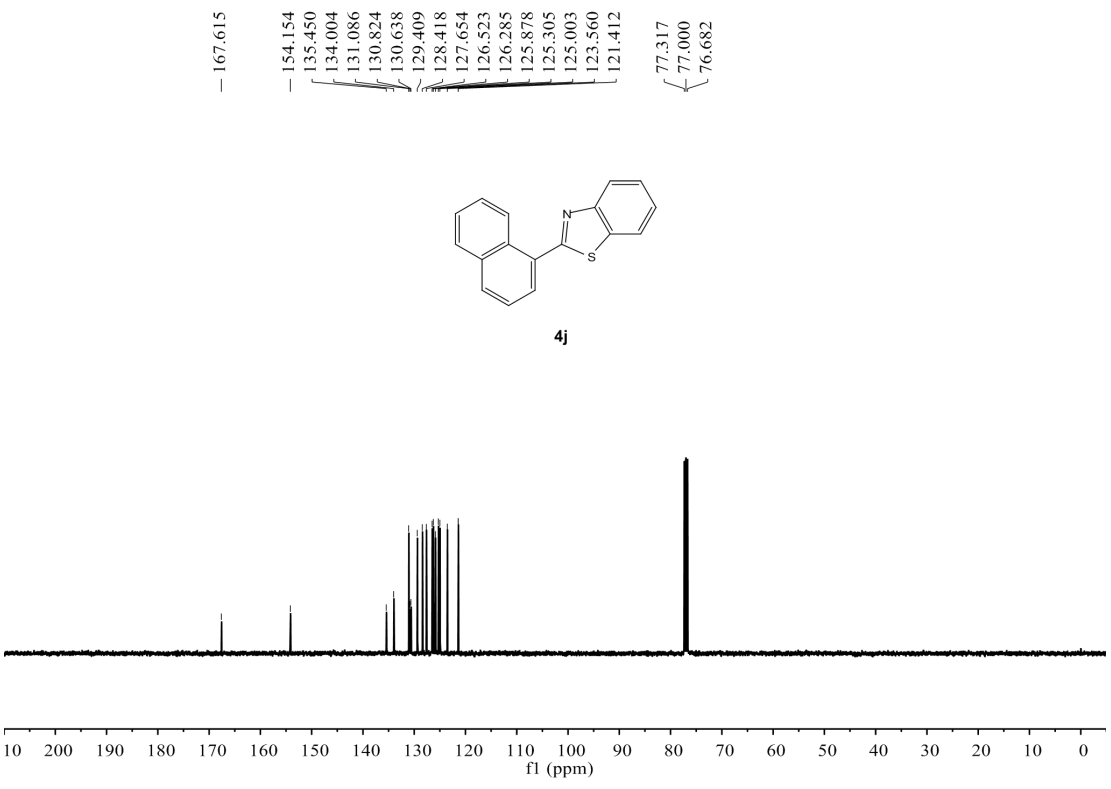
1.00
4.00
4.01
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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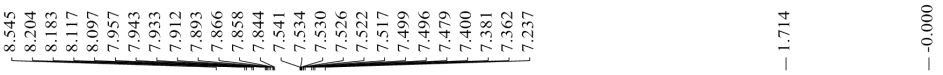
129.409
128.418
127.654
126.523
126.285
125.878
125.305
125.003
123.560
121.412
77.317
77.000
76.682
N
S
4j
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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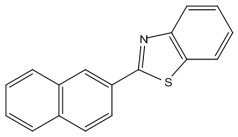
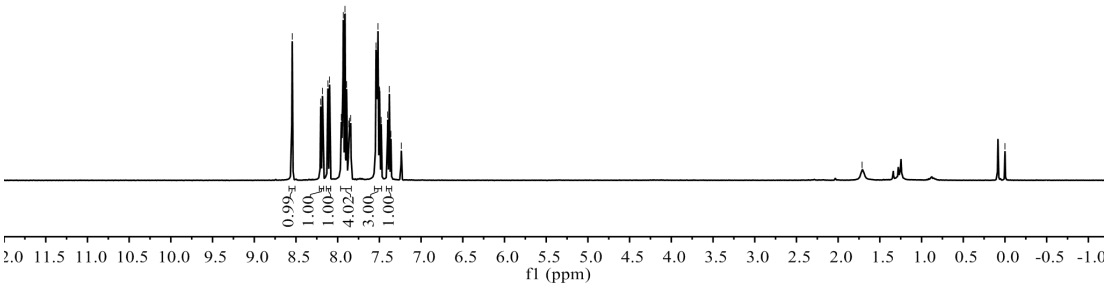
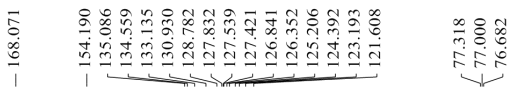
8.183
8.117
8.097
7.957
7.943
7.933
7.912
7.893
7.866
7.858
7.844
7.541
7.534
7.530
7.526
7.522
7.517
7.499
7.496
7.479
7.400
7.381
7.362
7.237
1.714
-0.000


N
S

4k


0.99
1.00
1.00
4.02
3.00
1.00
f1 (ppm)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154.190
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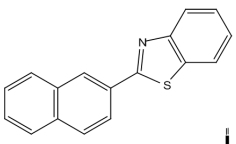
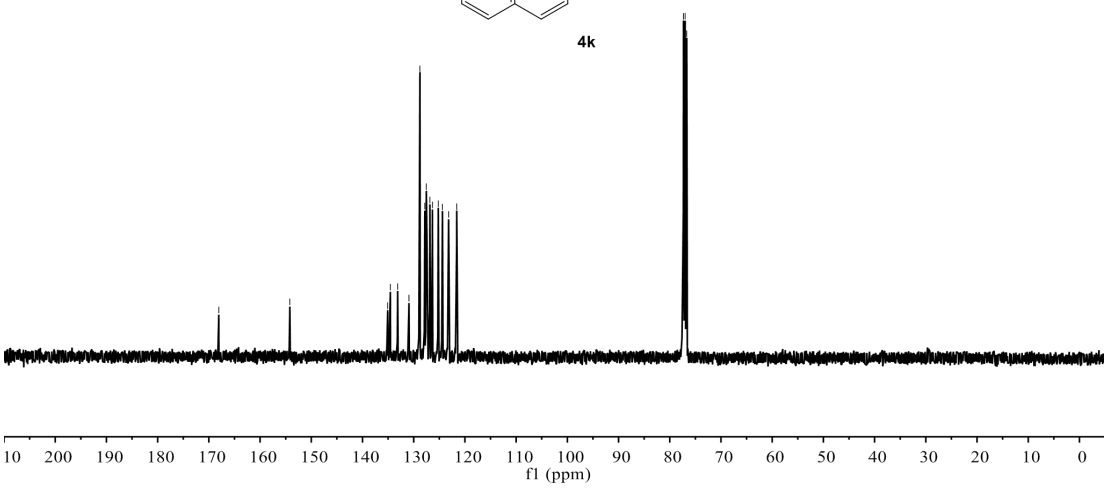
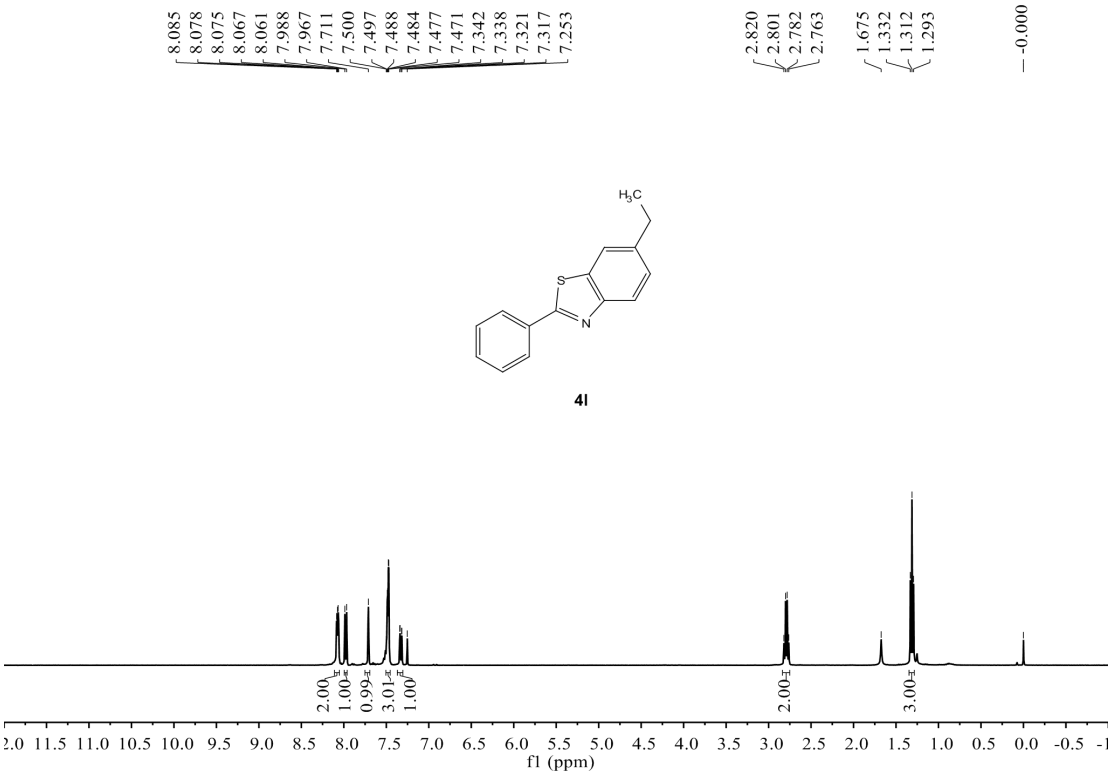
134.559
133.135
130.930
128.782
127.832
127.539
127.421
126.841
126.352
125.206
124.392
123.193
121.608
77.318
77.000
76.682


N
S

4k


f1 (ppm)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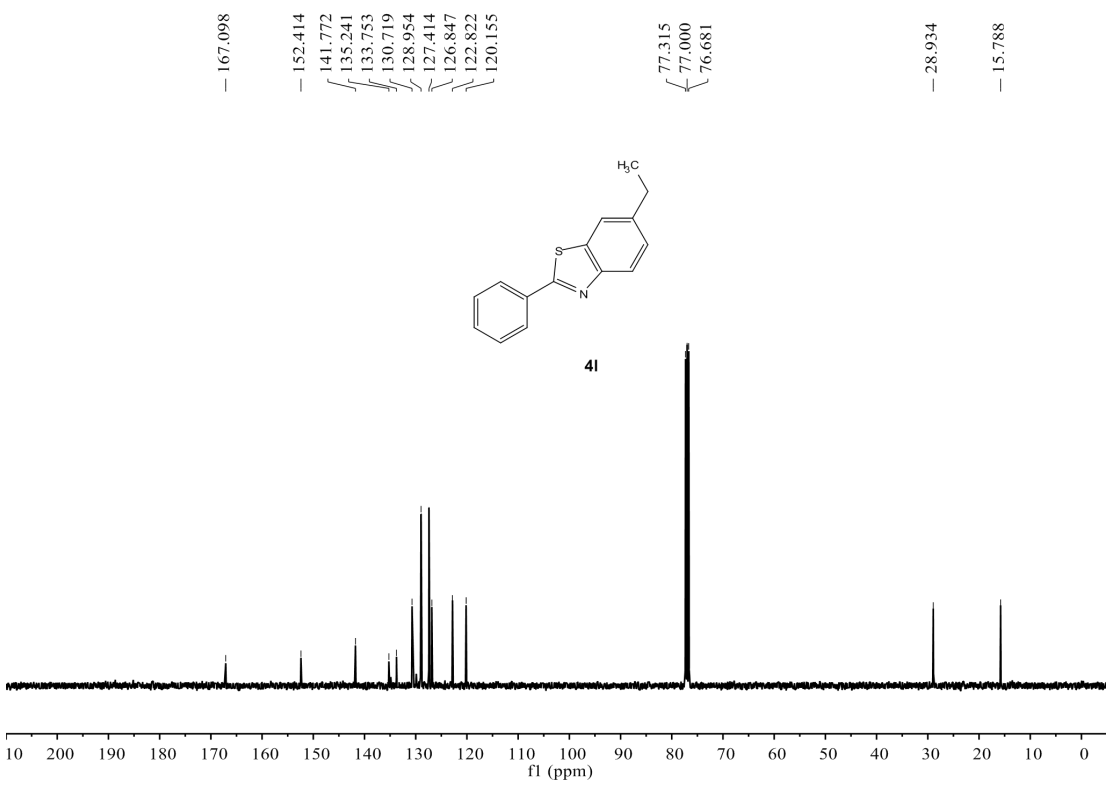
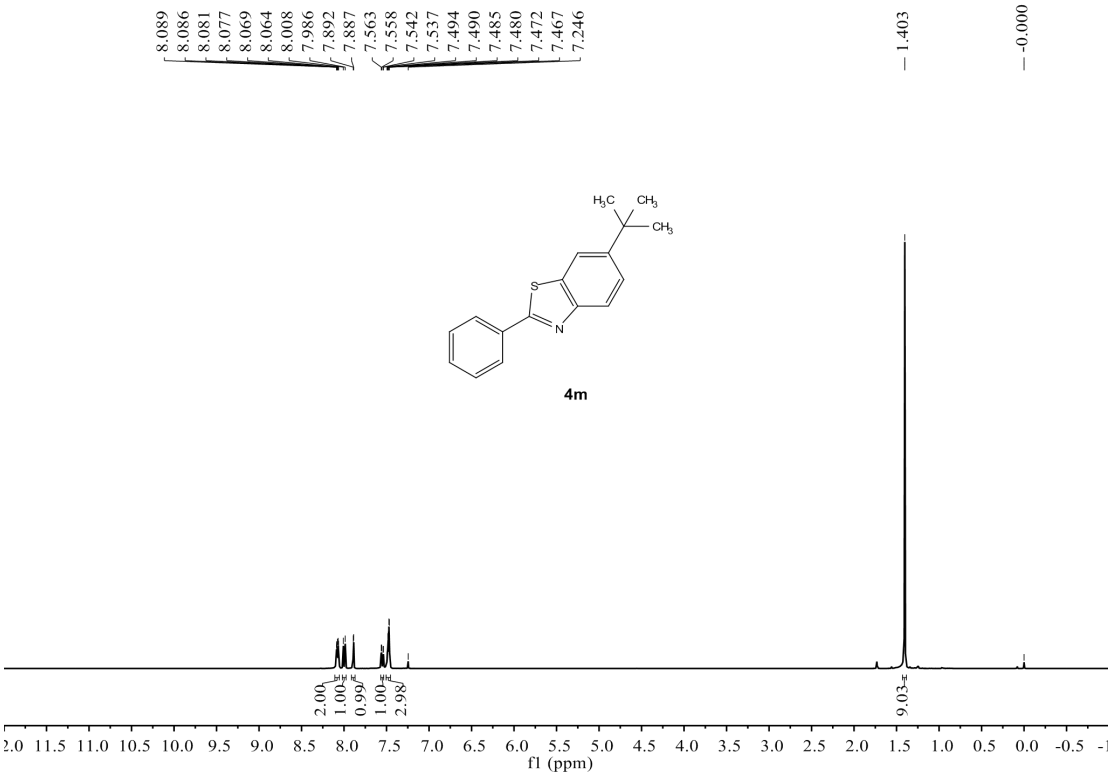
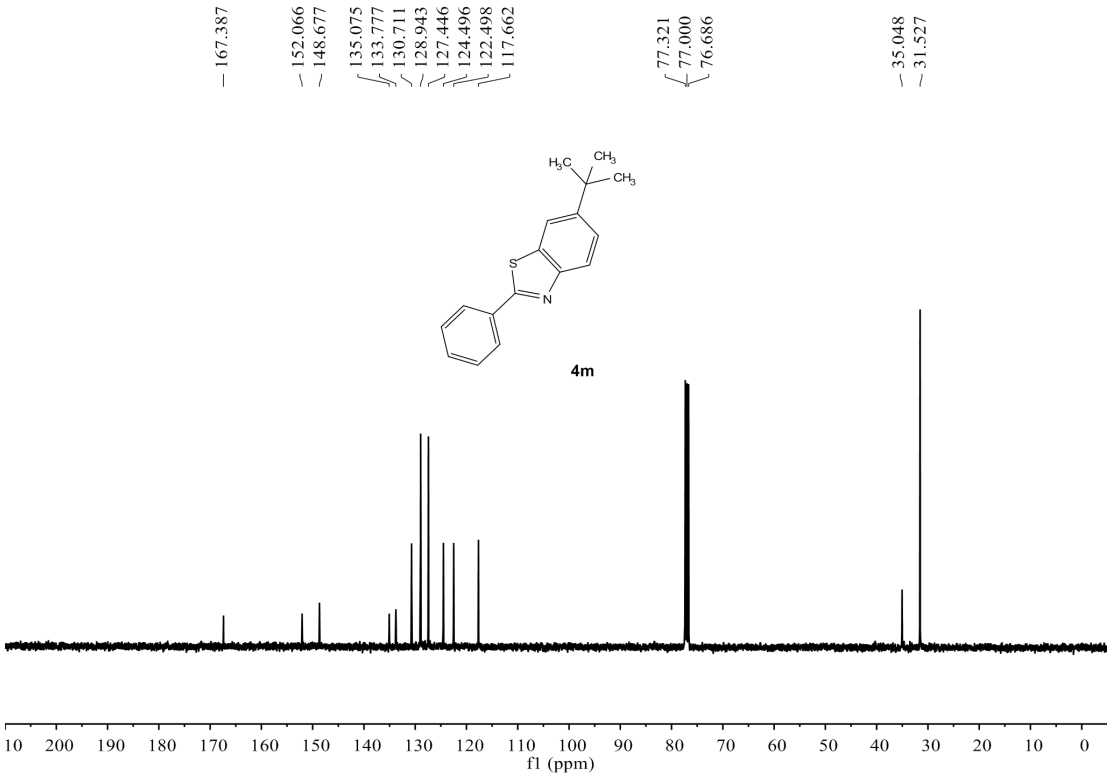
8.078
8.075
8.067
8.061
7.988
7.967
7.711
7.500
7.497
7.488
7.484
7.477
7.471
7.342
7.338
7.321
7.317
7.253
2.820
2.801
2.782
2.763
1.675
1.332
1.312
1.293
-0.000
H3C
S
N
4l
2.00
1.00
0.99
3.01
1.00
2.00
3.00
f1 (ppm)


167.098
152.414
141.772
135.241
133.753
130.719
128.954
127.414
126.847
122.822
120.155
77.315
77.000
76.681
28.934
15.788
H3C
S
N
4l
f1 (ppm)


8.089
8.086
8.081
8.077
8.069
8.064
8.008
7.986
7.892
7.887
7.563
7.558
7.542
7.537
7.494
7.490
7.485
7.480
7.472
7.467
7.246
1.403
0.000
4m
2.00
1.00
0.99
1.00
2.98
9.03
f1 (ppm)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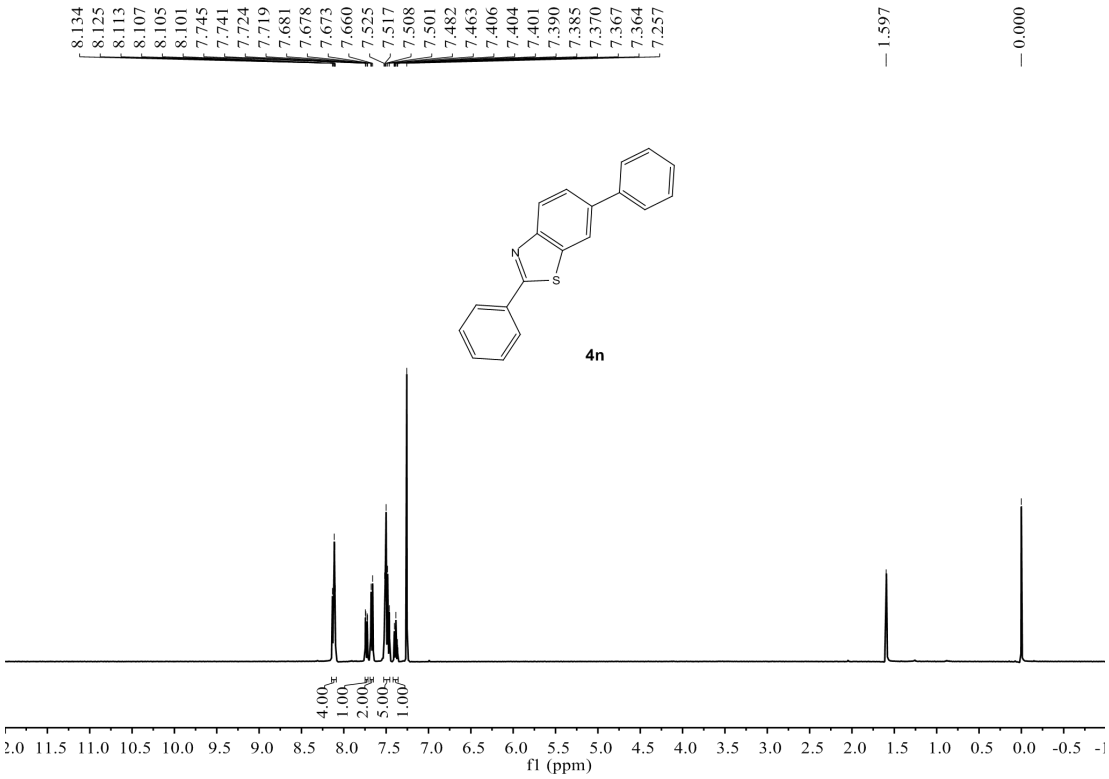
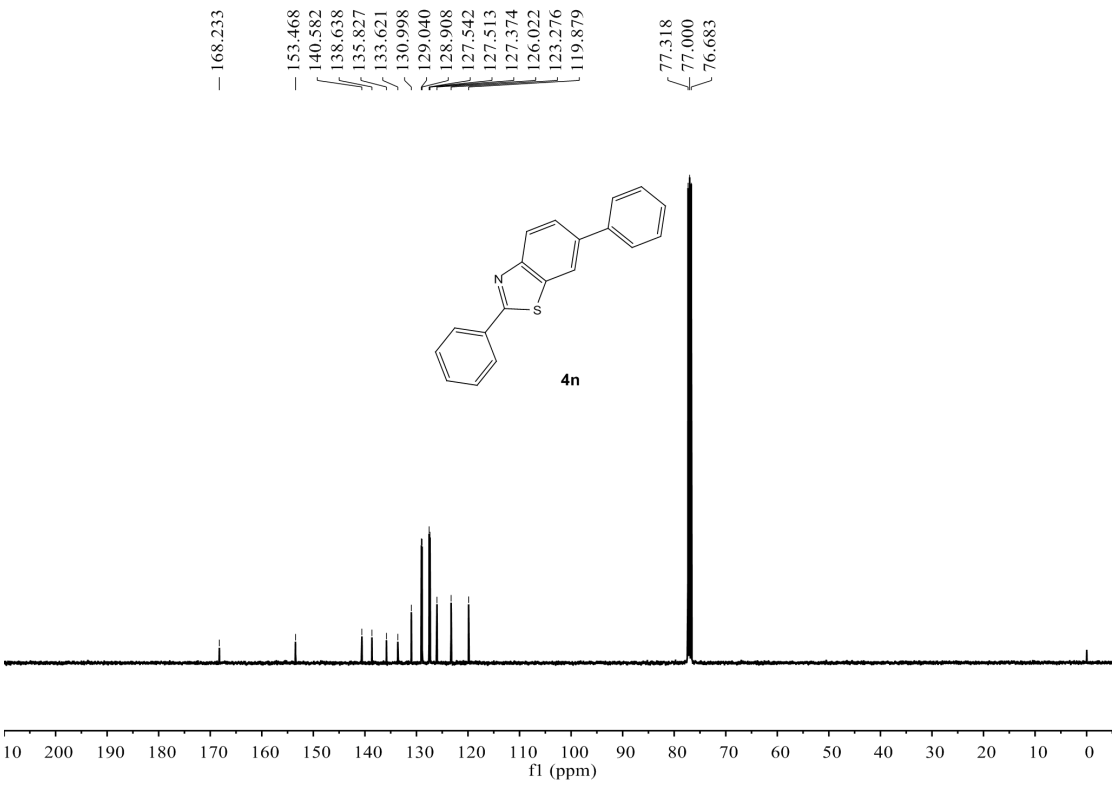
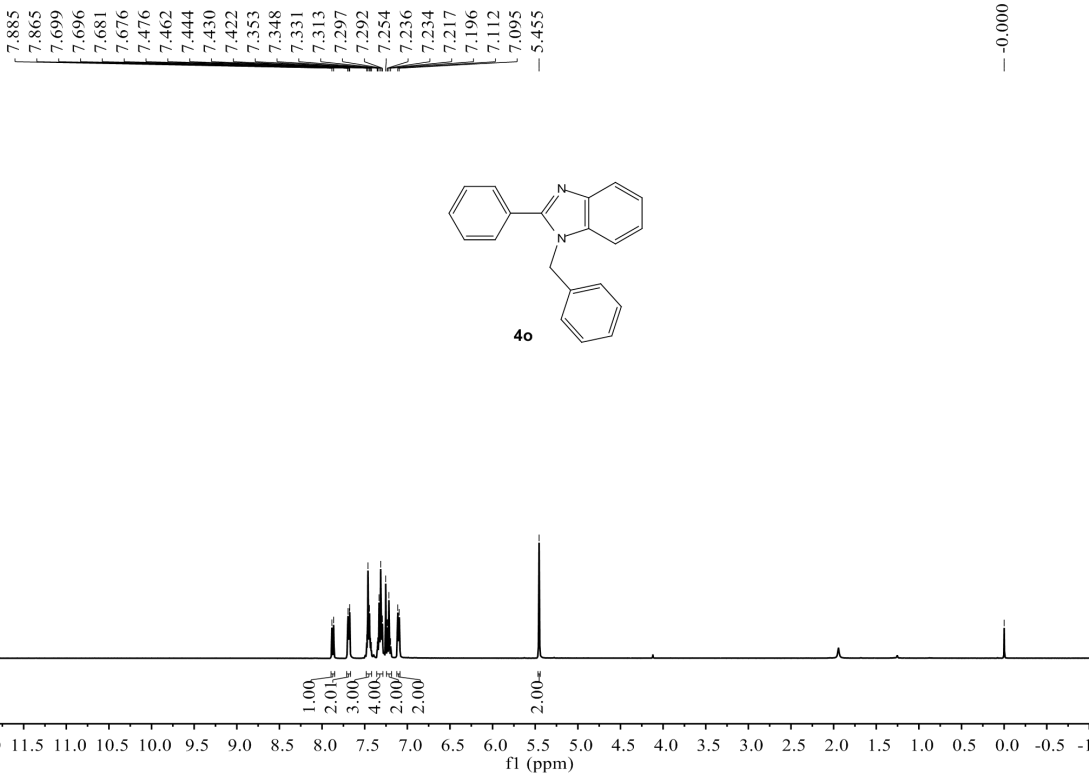
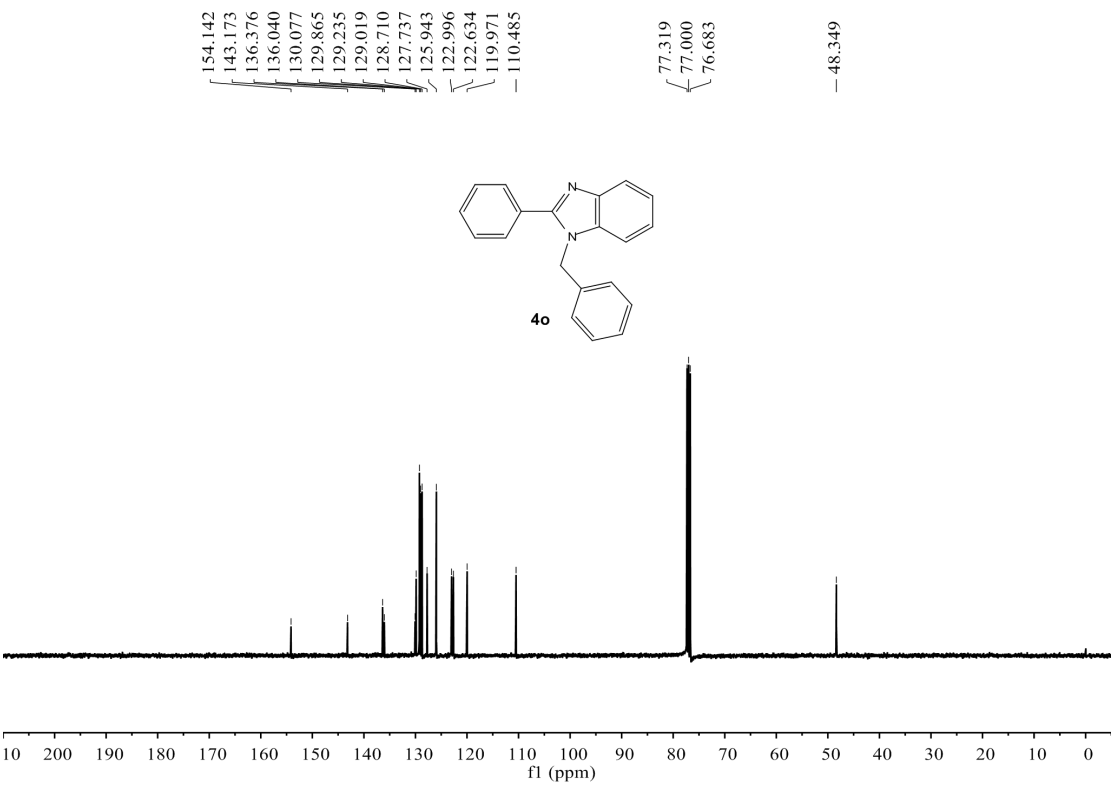
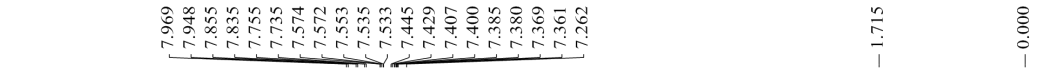
148.677
135.075
133.777
130.711
128.943
127.446
124.496
122.498
117.662
77.321
77.000
76.686
35.048
31.527
4m
f1 (ppm)


8.134
8.125
8.113
8.107
8.105
8.101
7.745
7.741
7.724
7.719
7.681
7.678
7.673
7.660
7.525
7.517
7.508
7.501
7.482
7.463
7.406
7.404
7.401
7.390
7.385
7.370
7.367
7.364
7.257
1.597
0.000
N
S
4n
4.00
1.00
2.00
5.00
1.00
f1 (ppm)


168.233
153.468
140.582
138.638
135.827
133.621
130.998
129.040
128.908
127.542
127.513
127.374
126.022
123.276
119.879
77.318
77.000
76.683
N
S
4n
f1 (ppm)


7.885
7.865
7.699
7.696
7.681
7.676
7.476
7.462
7.444
7.430
7.422
7.353
7.348
7.331
7.313
7.297
7.292
7.254
7.236
7.234
7.217
7.196
7.112
7.095
5.455
-0.000
4o
1.00
2.01
3.00
4.00
2.00
2.00
2.00
f1 (ppm)


154.142
143.173
136.376
136.040
130.077
129.865
129.235
129.019
128.710
127.737
125.943
122.996
122.634
119.971
110.485
77.319
77.000
76.683
48.349
4o
f1 (ppm)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7.948
7.855
7.835
7.755
7.735
7.574
7.572
7.553
7.535
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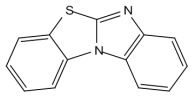
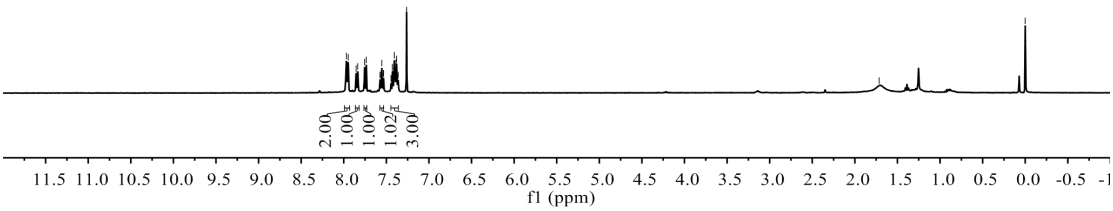
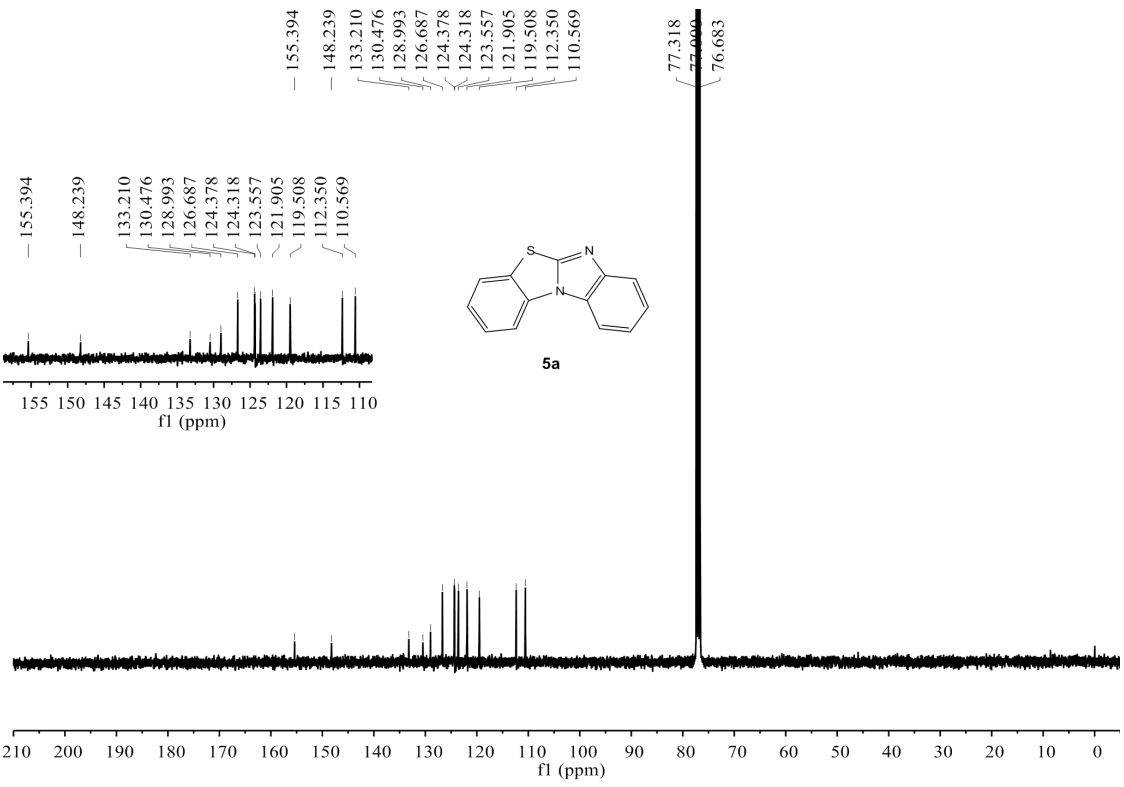
7.445
7.429
7.407
7.400
7.385
7.380
7.369
7.361
7.262
1.715
0.000


S
N
N

5a


2.00
1.00
1.00
1.02
3.00
11.5 11.0 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 -0.5 -1
f1 (ppm)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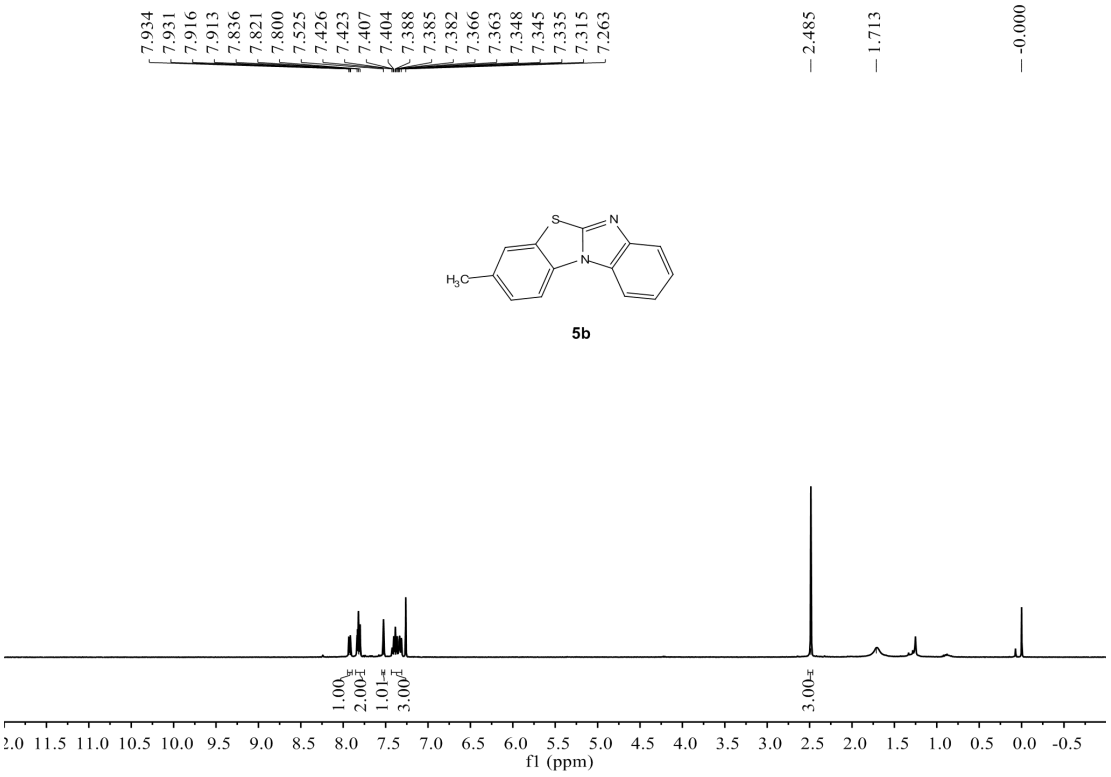
130.476
128.993
126.687
124.378
124.318
123.557
121.905
119.508
112.350
110.569
77.318
77.000
76.683
S
N
N
5a
155 150 145 140 135 130 125 120 115 110
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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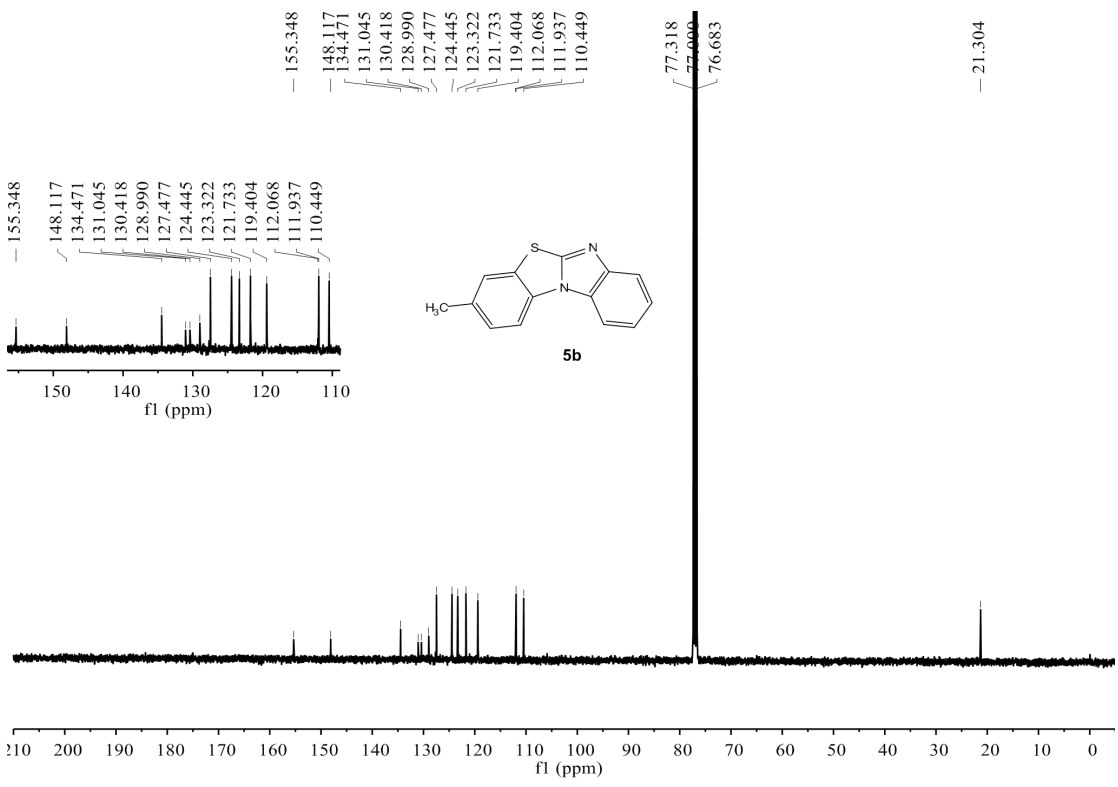
7.931
7.916
7.913
7.836
7.821
7.800
7.525
7.426
7.423
7.407
7.404
7.388
7.385
7.382
7.366
7.363
7.348
7.345
7.335
7.315
7.263
2.485
1.713
0.000
S
N
N
H3C
5b
1.00
2.00
1.01
3.00
3.00
f1 (ppm)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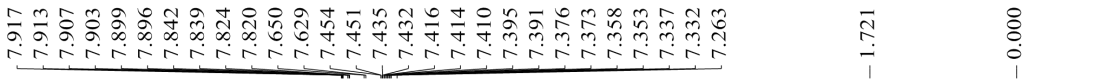
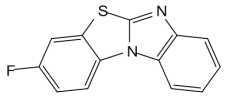
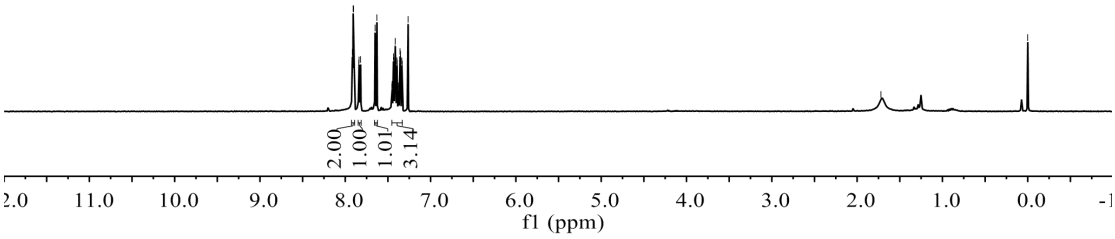
131.045
130.418
128.990
127.477
124.445
123.322
121.733
119.404
112.068
111.937
110.449
77.318
77.000
76.683
21.304
S
N
N
H3C
5b
f1 (ppm)
f1 (ppm)


7.917
7.913
7.907
7.903
7.899
7.896
7.842
7.839
7.824
7.820
7.650
7.629
7.454
7.451
7.435
7.432
7.416
7.414
7.410
7.395
7.391
7.376
7.373
7.358
7.353
7.337
7.332
7.263
1.721
0.000


S
N
N
F

5c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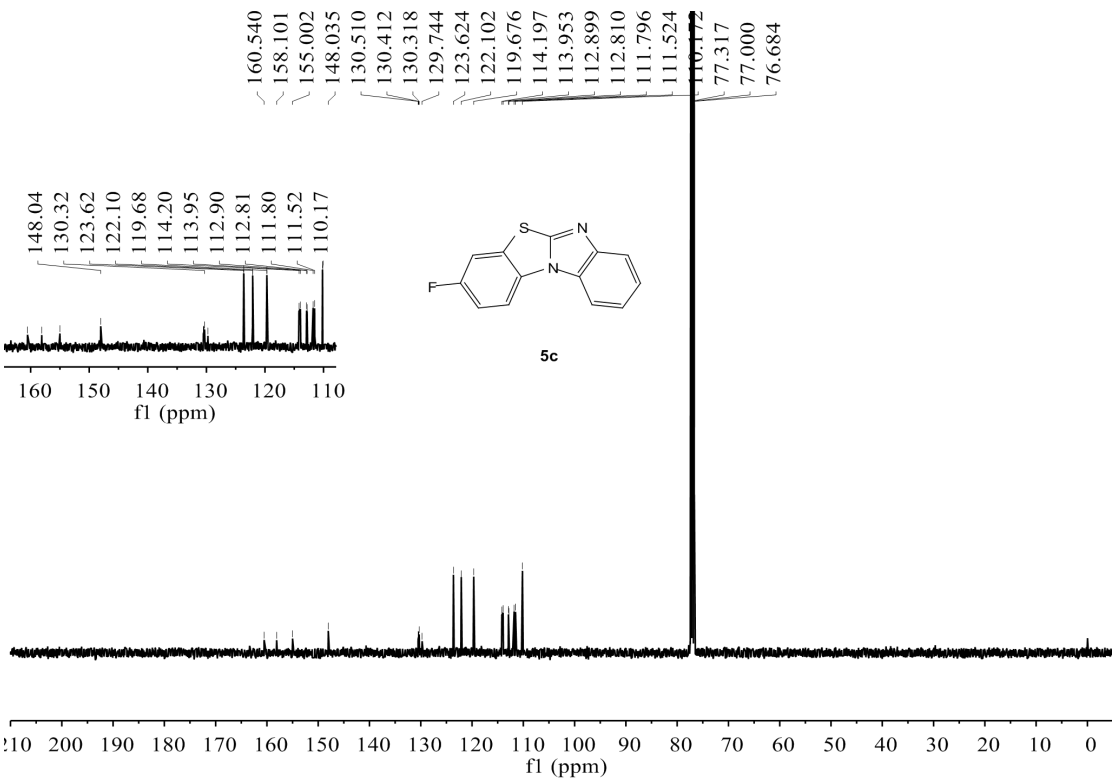
1.00
1.01
3.14
f1 (ppm)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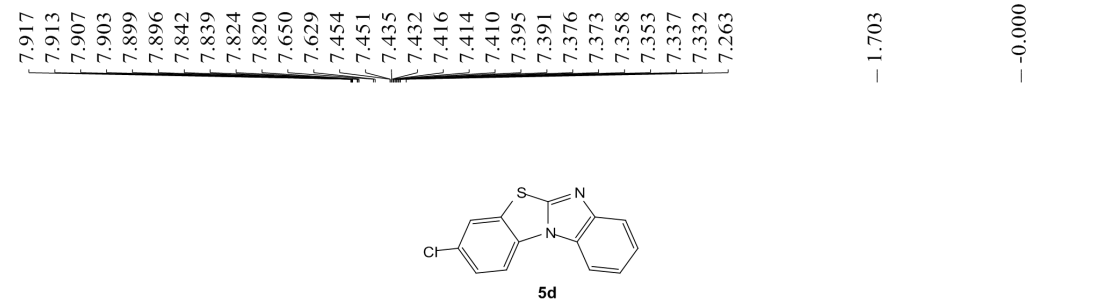
148.035
130.510
130.412
130.318
129.744
123.624
122.102
119.676
114.197
113.953
112.899
112.810
111.796
111.524
77.317
77.000
76.684
148.04
130.32
123.62
122.10
119.68
114.20
113.95
112.90
112.81
111.80
111.52
110.17
S
N
N
F
f1 (ppm)
f1 (ppm)

5c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7.913
7.907
7.903
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7.896
7.842
7.839
7.824
7.820
7.650
7.629
7.454
7.451
7.435
7.432
7.416
7.414
7.410
7.395
7.391
7.376
7.373
7.358
7.353
7.337
7.332
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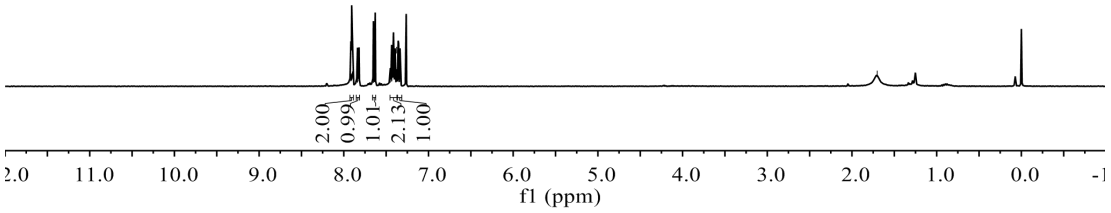
1.703
-0.000
S
N
N
Cl
5d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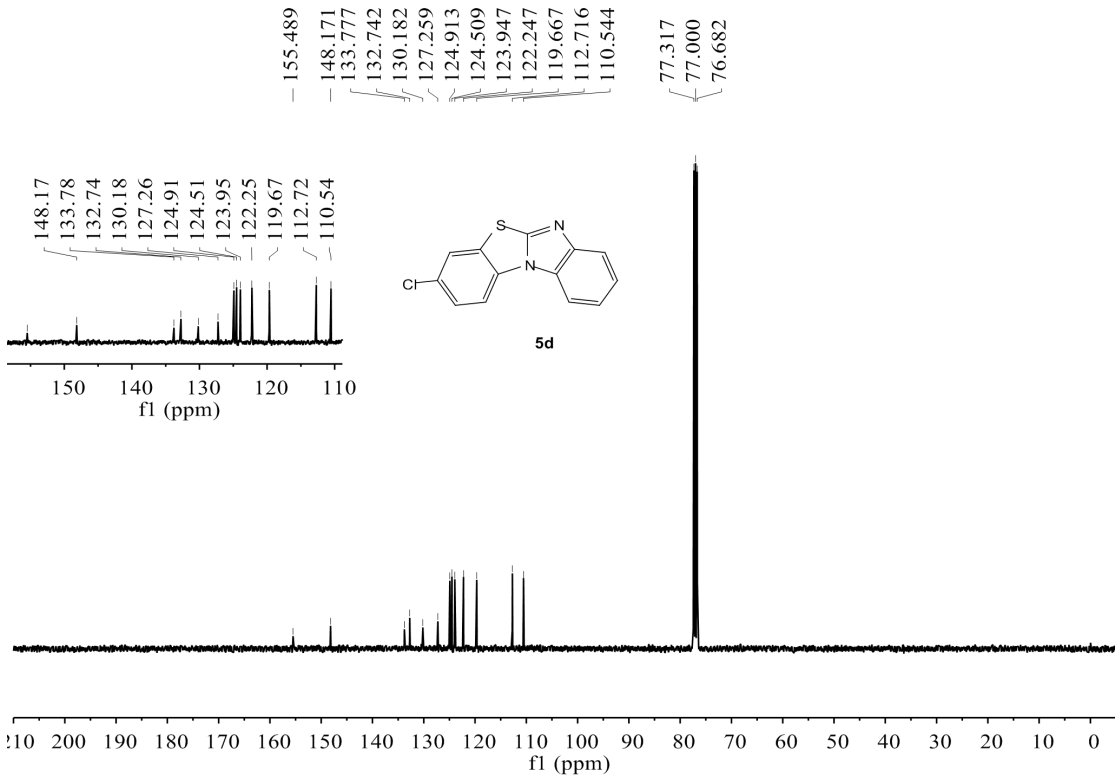
0.99
1.01
2.13
1.00
f1 (ppm)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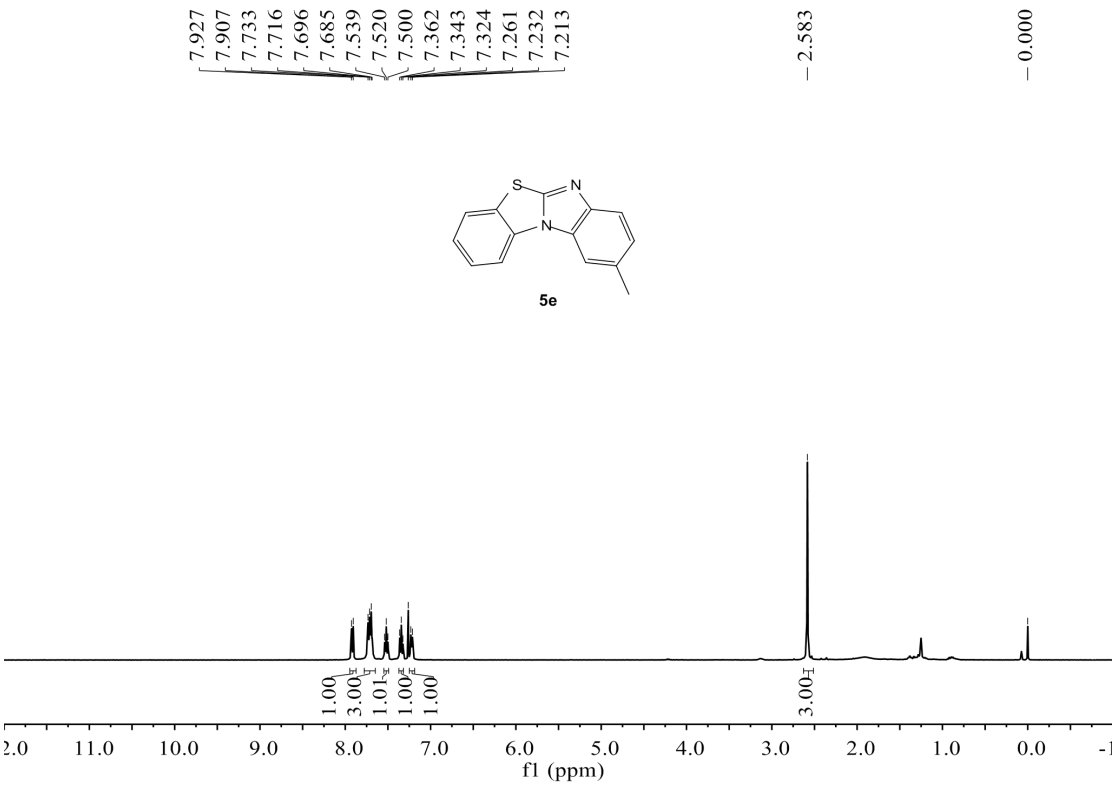
124.913
124.509
123.947
122.247
119.667
112.716
110.544
77.317
77.000
76.682
148.17
133.78
132.74
130.18
127.26
124.91
124.51
123.95
122.25
119.67
112.72
110.54
S
N
N
Cl
5d
f1 (ppm)
f1 (ppm)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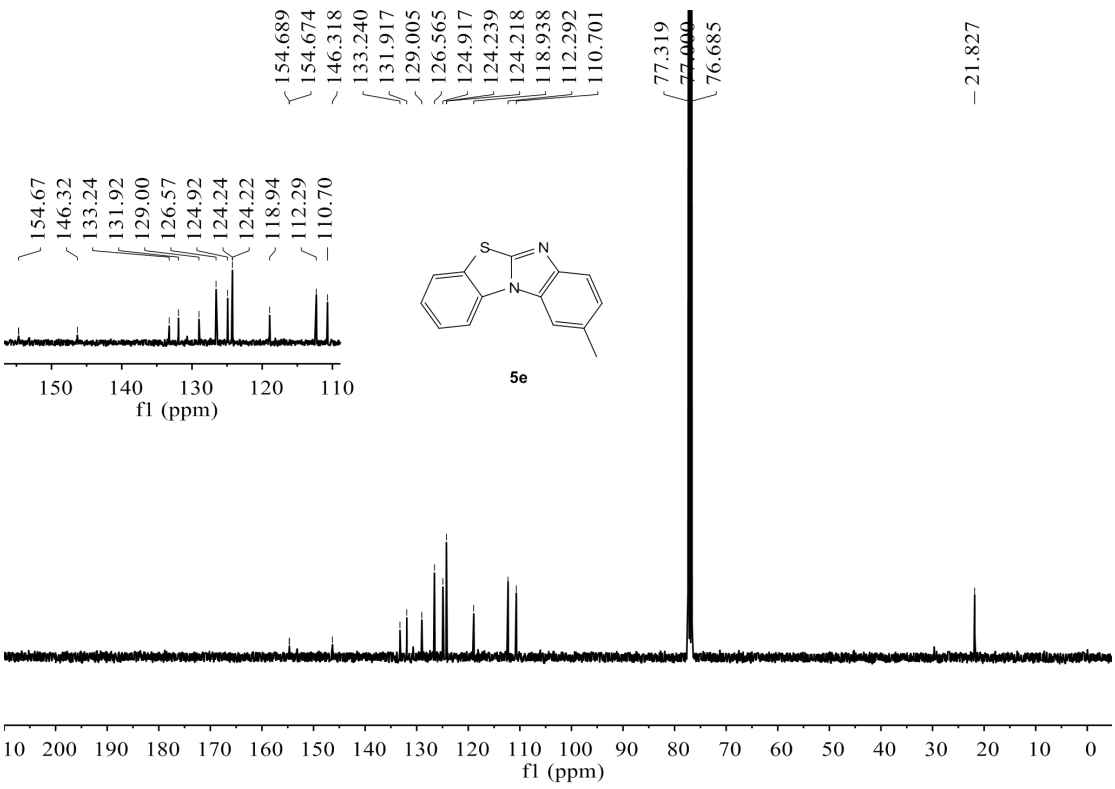
7.685
7.539
7.520
7.500
7.362
7.343
7.324
7.261
7.232
7.213
2.583
0.000
S
N
N
5e
1.00
3.00
1.01
1.00
1.00
3.00
f1 (ppm)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129.005
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124.917
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124.218
118.938
112.292
110.701
77.319
77.000
76.685
21.827
154.67
146.32
133.24
131.92
129.00
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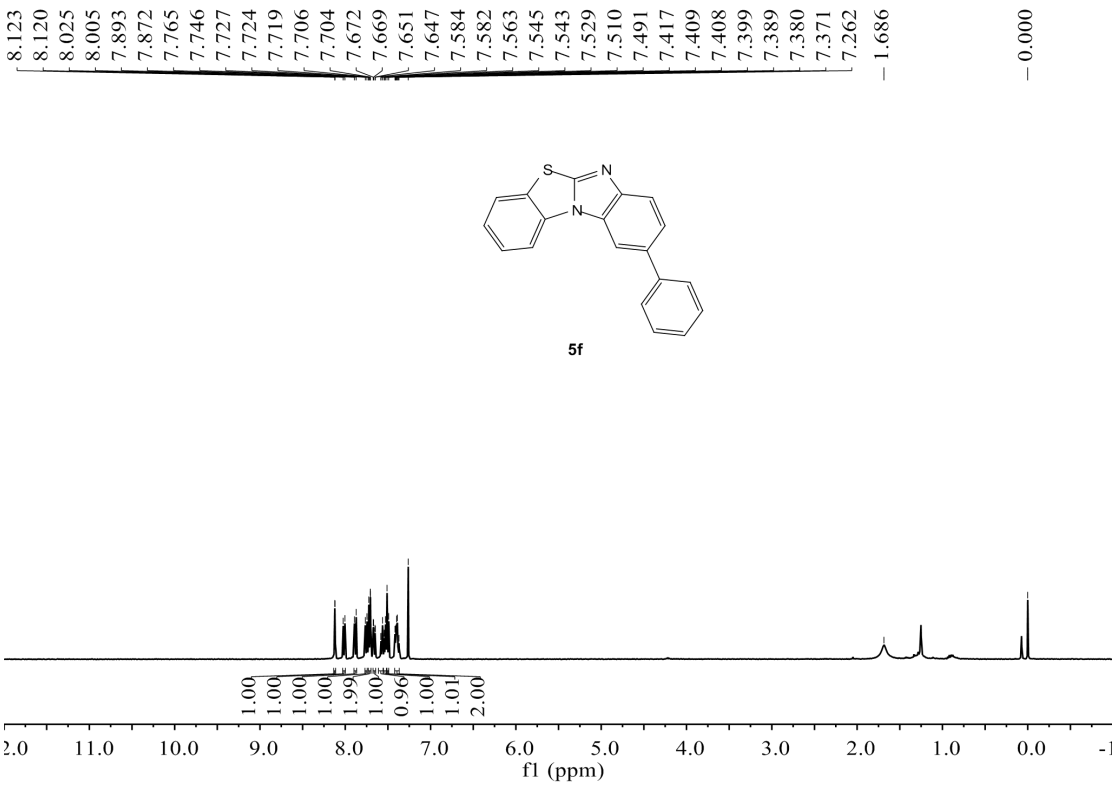
124.22
118.94
112.29
110.70
S
N
N
5e
f1 (ppm)
f1 (ppm)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8.120
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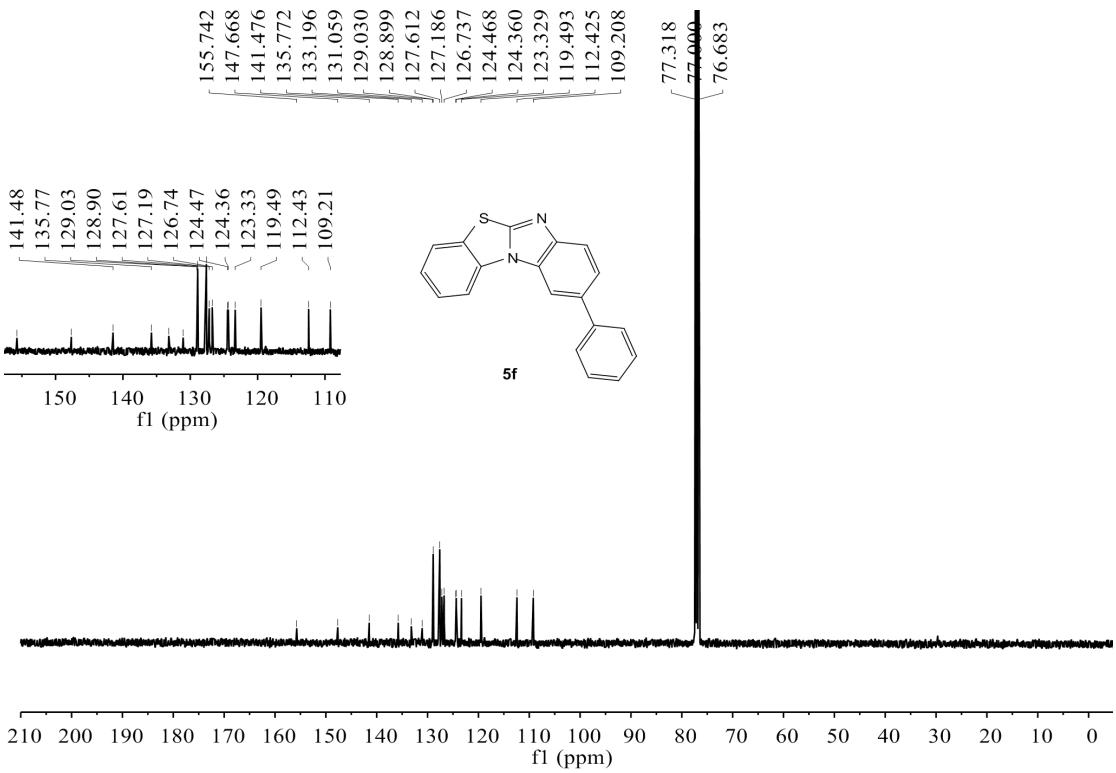
7.872
7.765
7.746
7.727
7.724
7.719
7.706
7.704
7.672
7.669
7.651
7.647
7.584
7.582
7.563
7.545
7.543
7.529
7.510
7.491
7.417
7.409
7.408
7.399
7.389
7.380
7.371
7.262
1.686
0.000
S
N
N
5f
1.00
1.00
1.00
1.00
1.99
1.00
0.96
1.00
1.01
2.00
2.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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141.476
135.772
133.196
131.059
129.030
128.899
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127.186
126.737
124.468
124.360
123.329
119.493
112.425
109.208
77.318
77.000
76.683
141.48
135.77
129.03
128.90
127.61
127.19
126.74
124.47
124.36
123.33
119.49
112.43
109.21
S
N
N
5f
150
140
130
120
110
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
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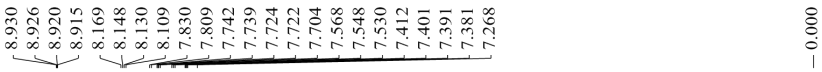
70
60
50
40
30
20
10
0
f1 (ppm)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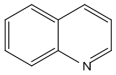
8.926
8.920
8.915
8.169
8.148
8.130
8.109
7.830
7.809
7.742
7.739
7.724
7.722
7.704
7.568
7.548
7.530
7.412
7.401
7.391
7.381
7.268
0.000



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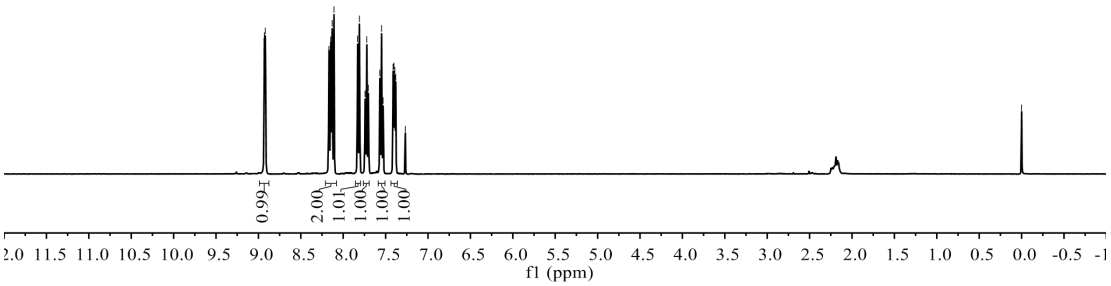
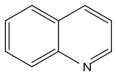

0.99
2.00
1.01
1.00
1.00
1.00
f1 (ppm)


150.373
148.245
136.013
129.482
128.313
127.811
126.565
121.100
77.318
77.000
76.682



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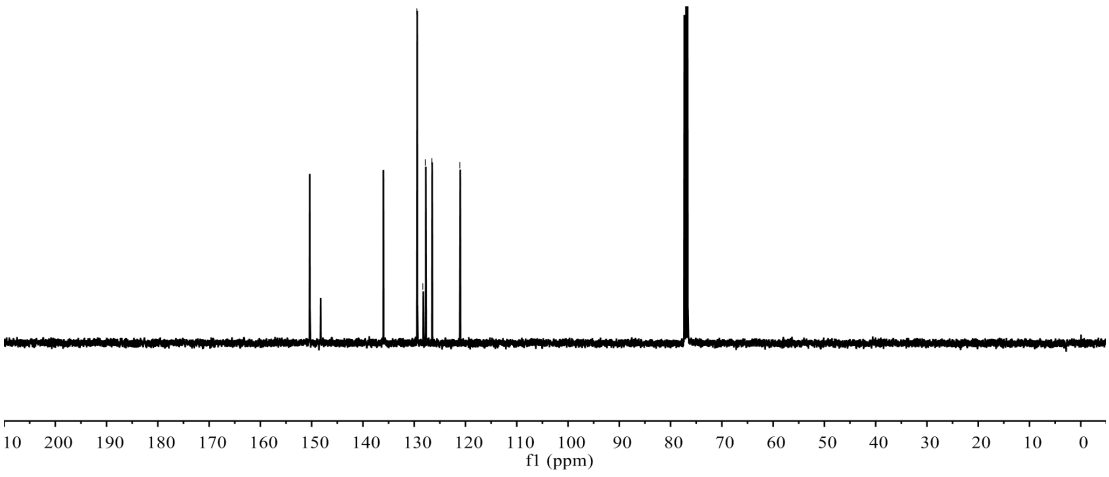
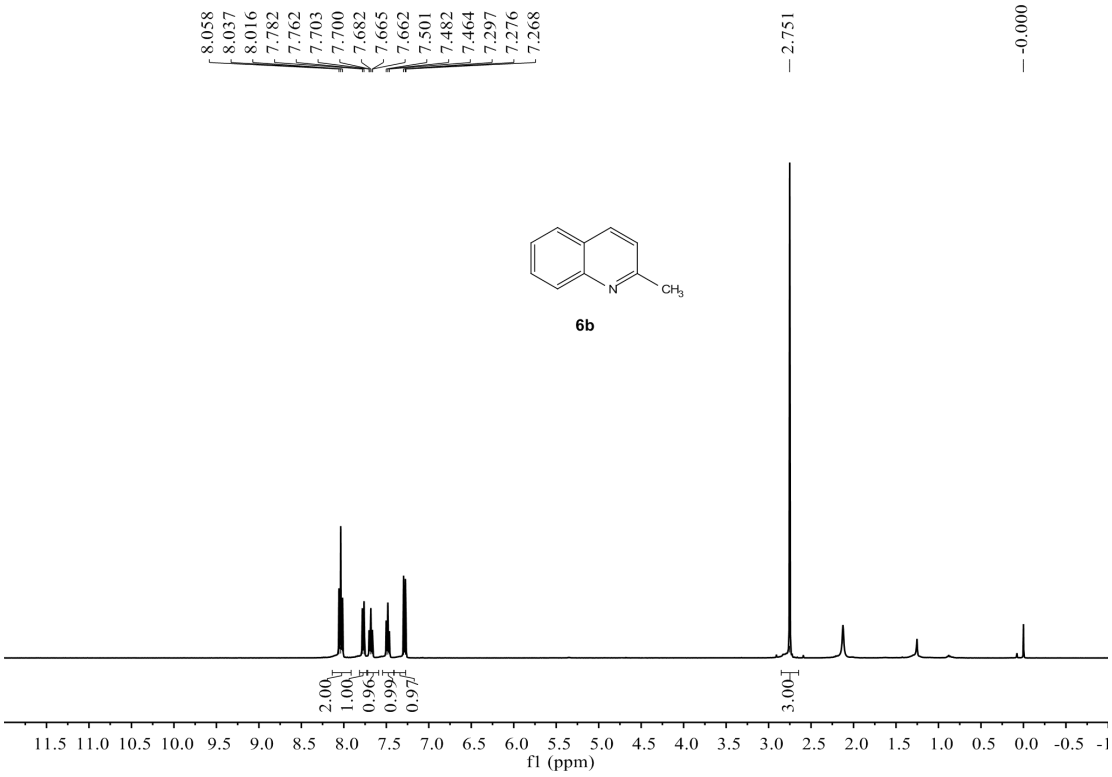

f1 (ppm)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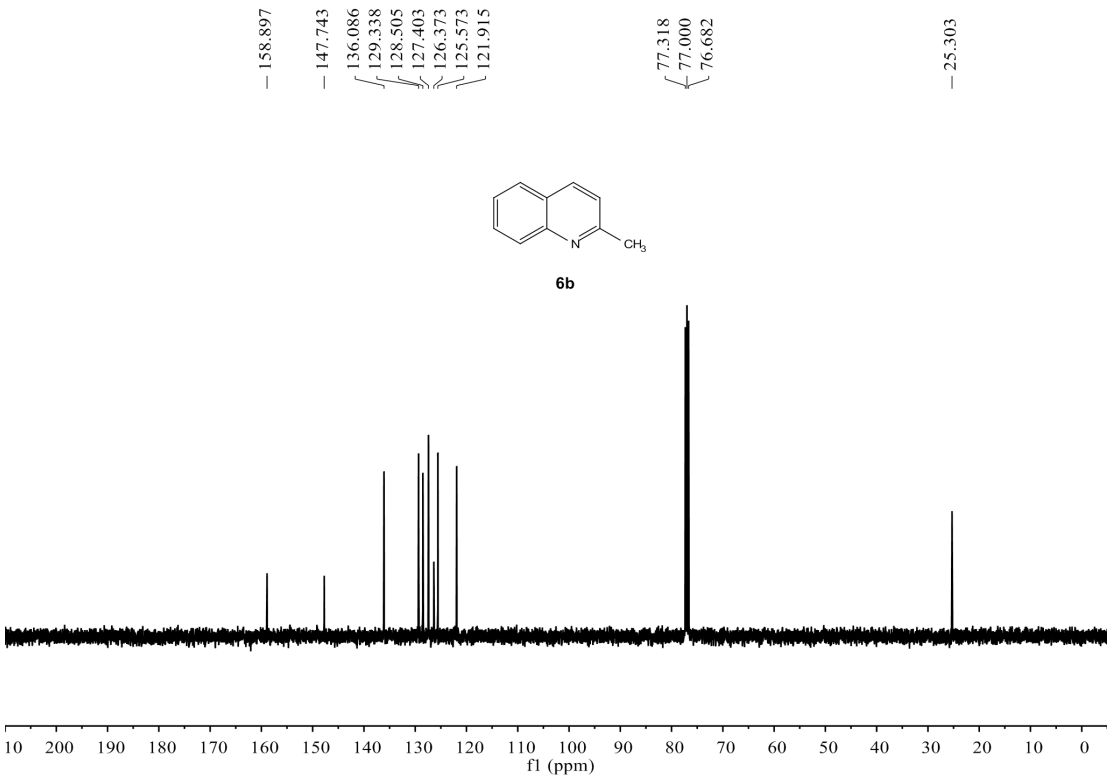
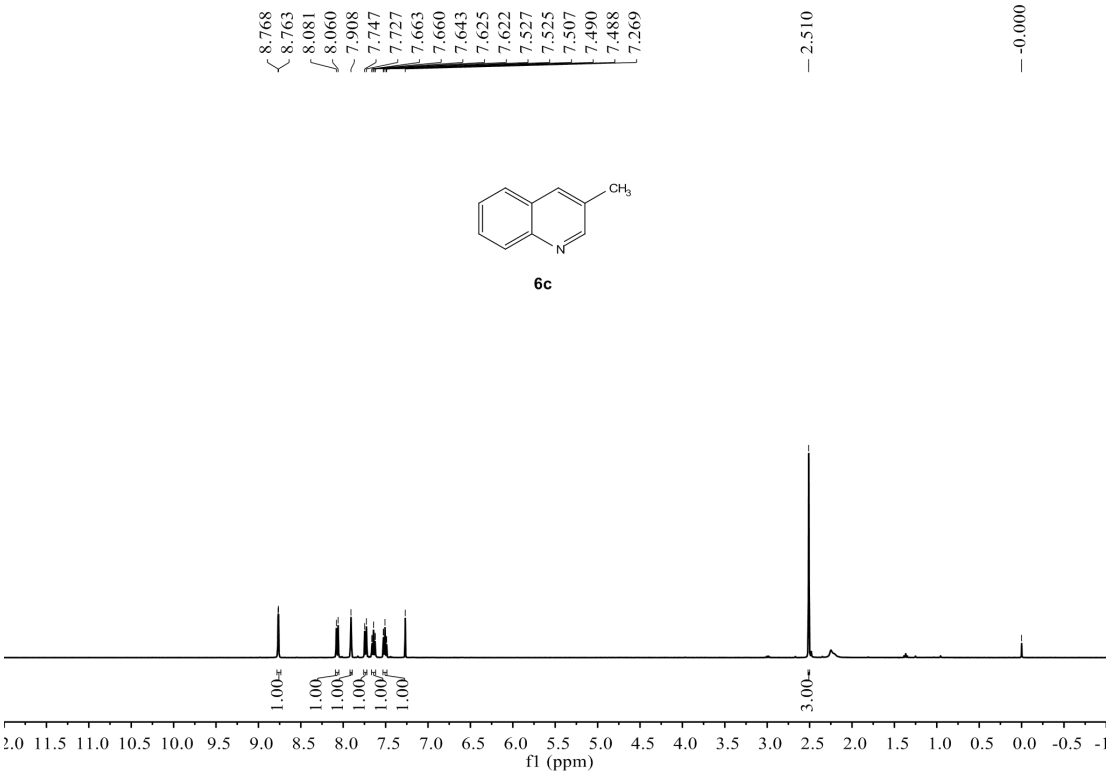
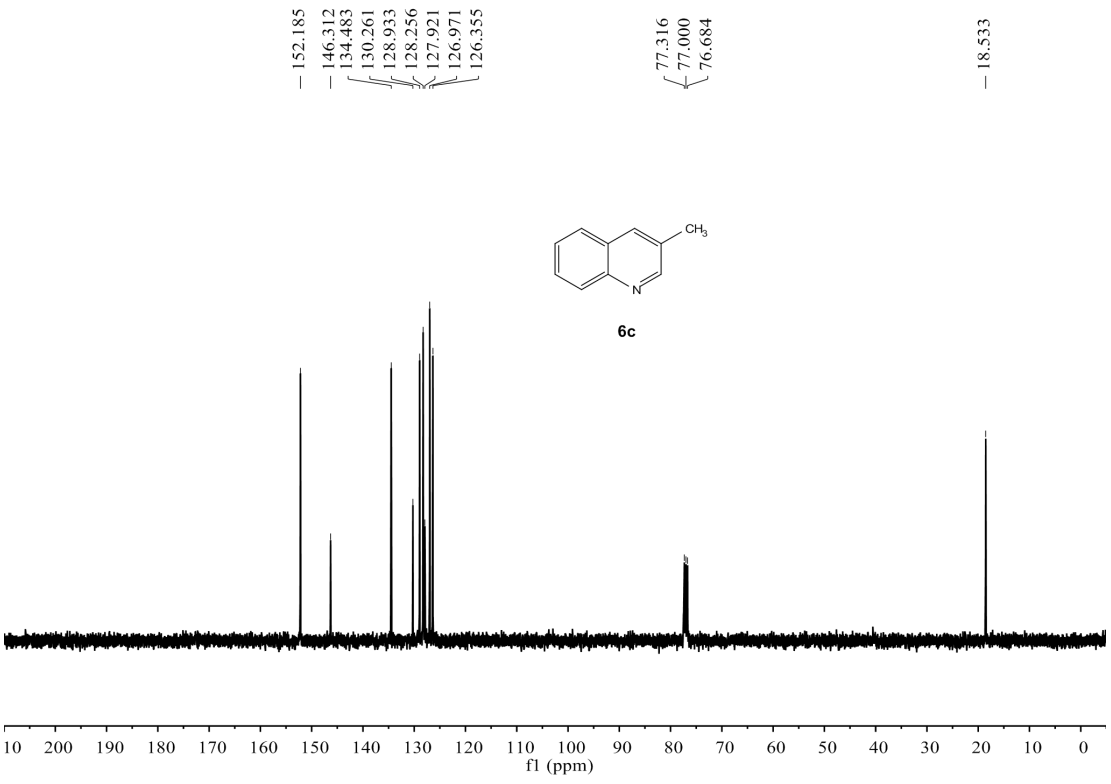
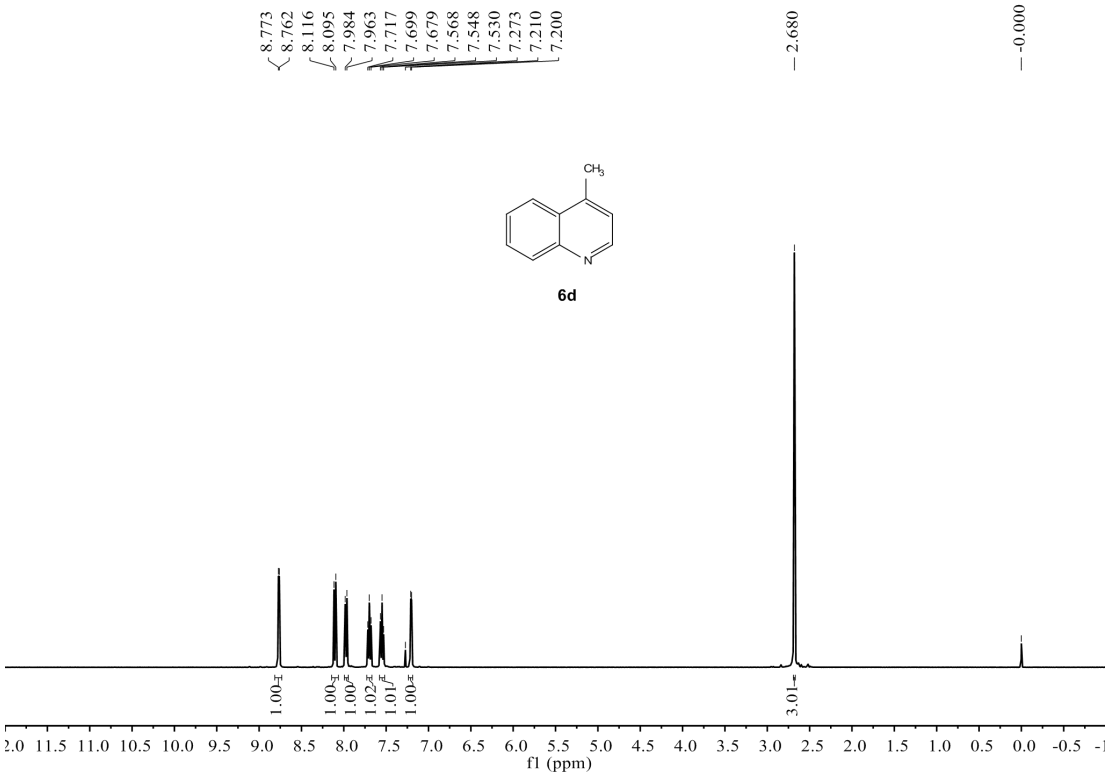
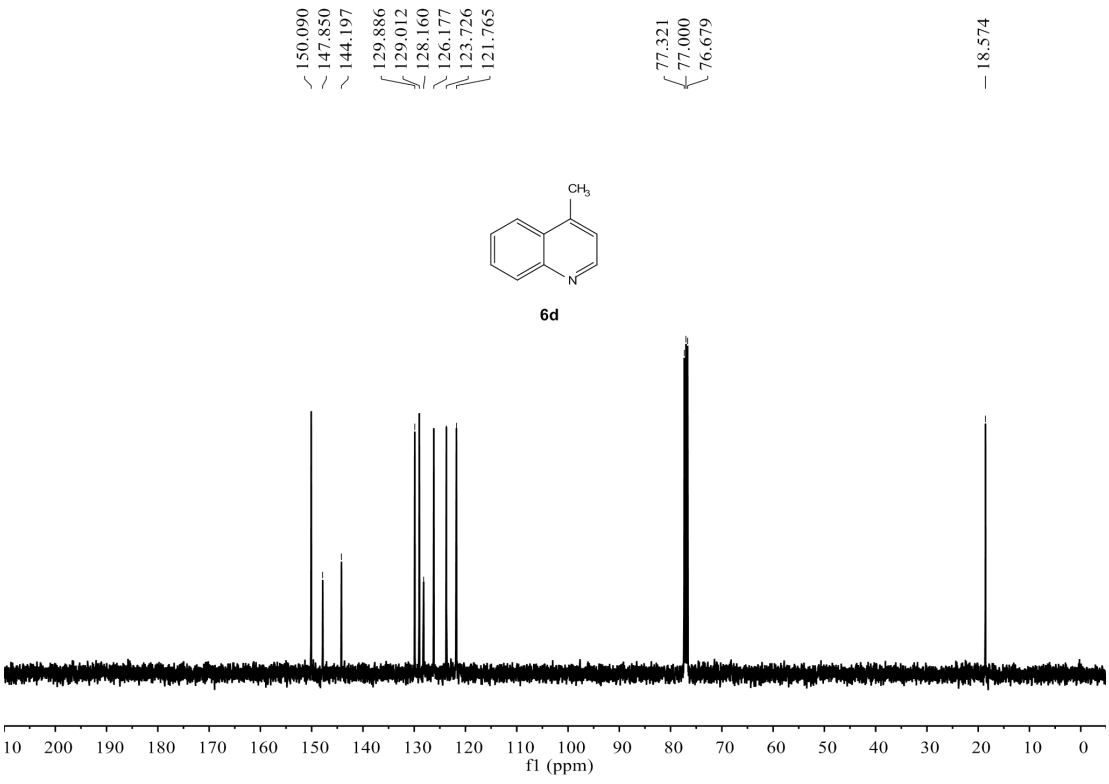
8.037
8.016
7.782
7.762
7.703
7.700
7.682
7.665
7.662
7.501
7.482
7.464
7.297
7.276
7.268
2.751
-0.000
N
CH3
6b
2.00
1.00
0.96
0.99
0.97
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

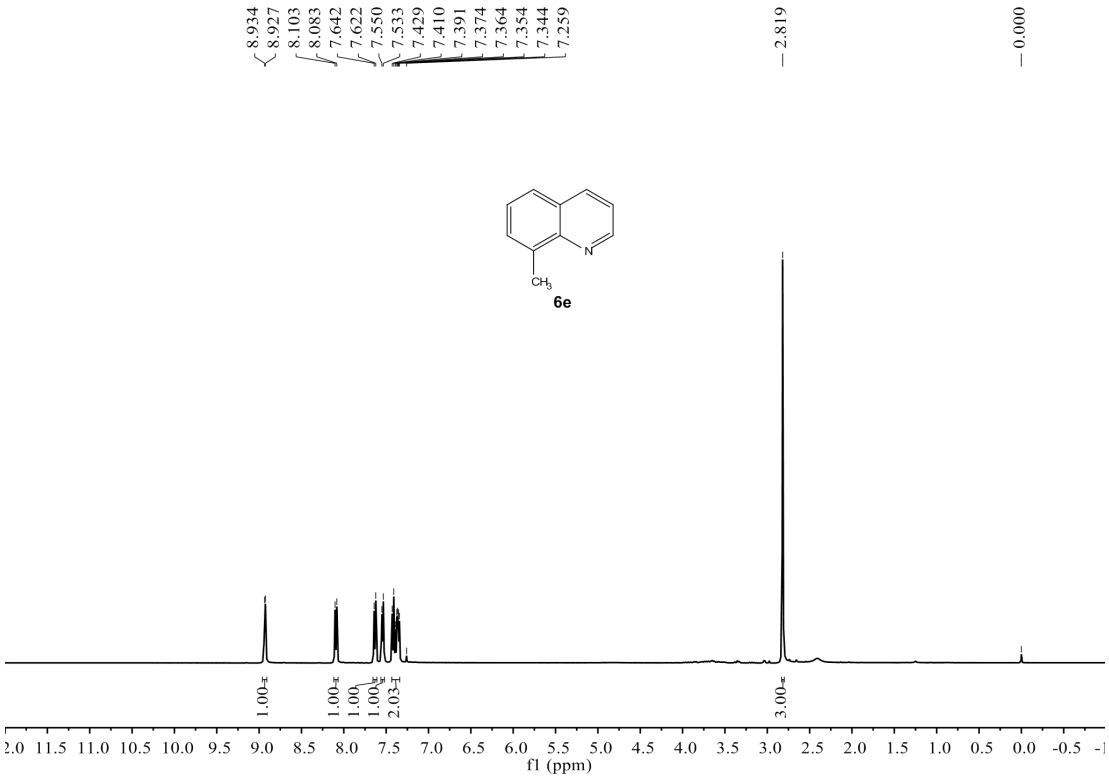

158.897
147.743
136.086
129.338
128.505
127.403
126.373
125.573
121.915
77.318
77.000
76.682
25.303
N
CH3
6b
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

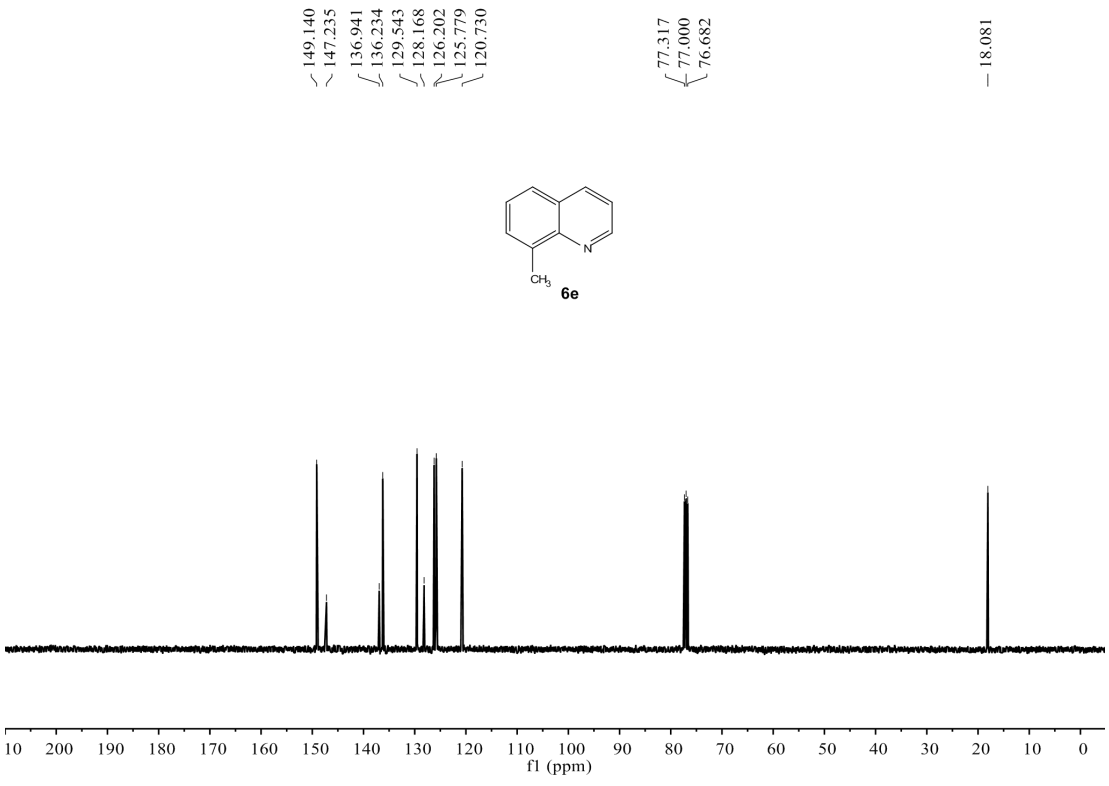

8.768
8.763
8.081
8.060
7.908
7.747
7.727
7.663
7.660
7.643
7.625
7.622
7.527
7.525
7.507
7.490
7.488
7.269
2.510
-0.000
CH3
N
6c
1.00
1.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)

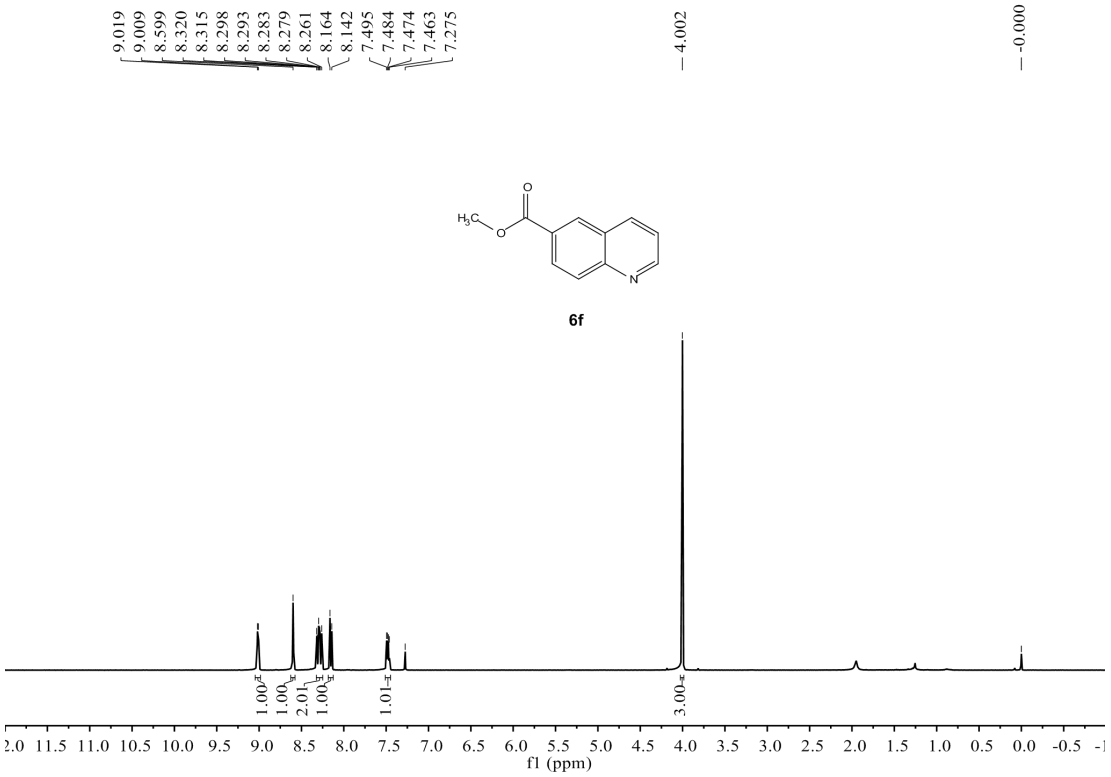

152.185
146.312
134.483
130.261
128.933
128.256
127.921
126.971
126.355
77.316
77.000
76.684
18.533
CH3
N
6c
f1 (ppm)

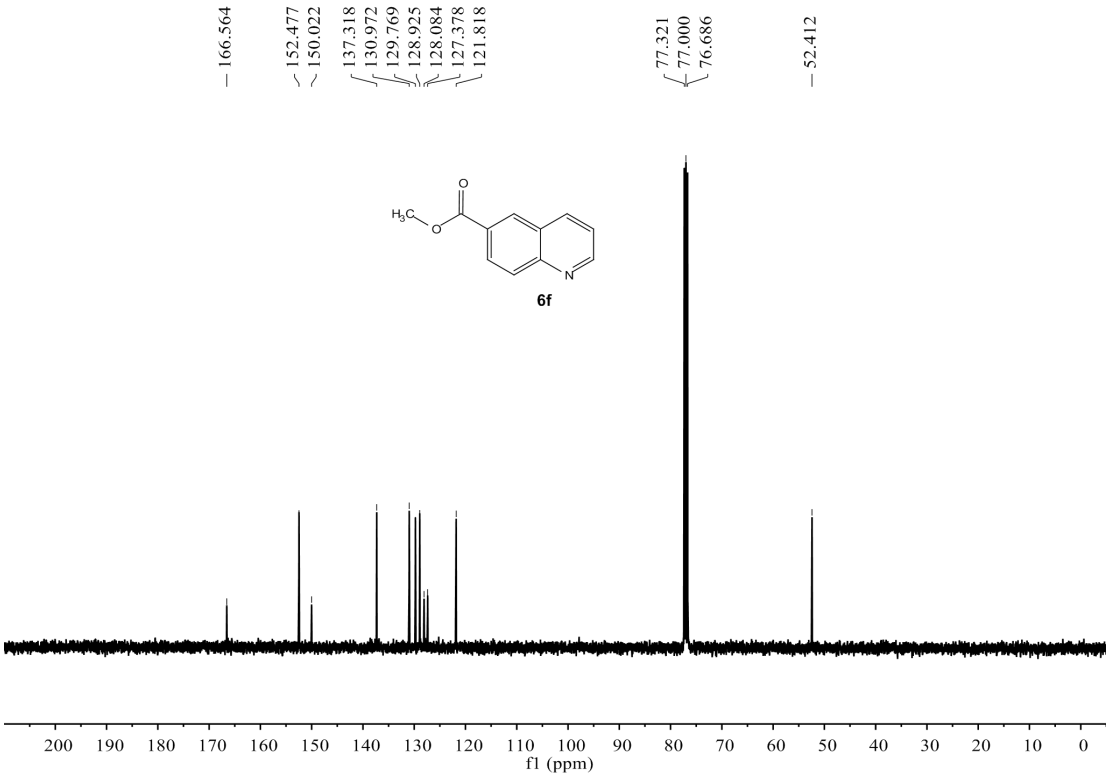

8.773
8.762
8.116
8.095
7.984
7.963
7.717
7.699
7.679
7.568
7.548
7.530
7.273
7.210
7.200
2.680
0.000
CH3
N
6d
1.00
1.00
1.00
1.02
1.01
1.00
3.01
f1 (ppm)

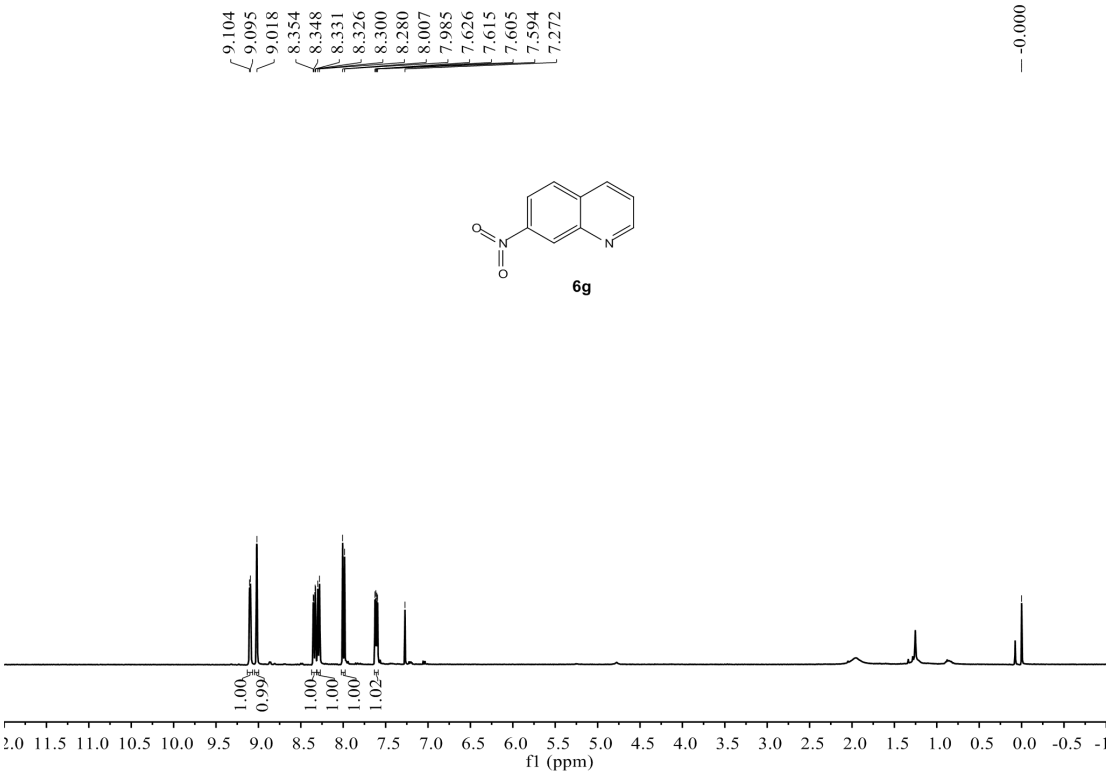

150.090
147.850
144.197
129.886
129.012
128.160
126.177
123.726
121.765
77.321
77.000
76.679
18.574
CH3
N
6d
f1 (ppm)

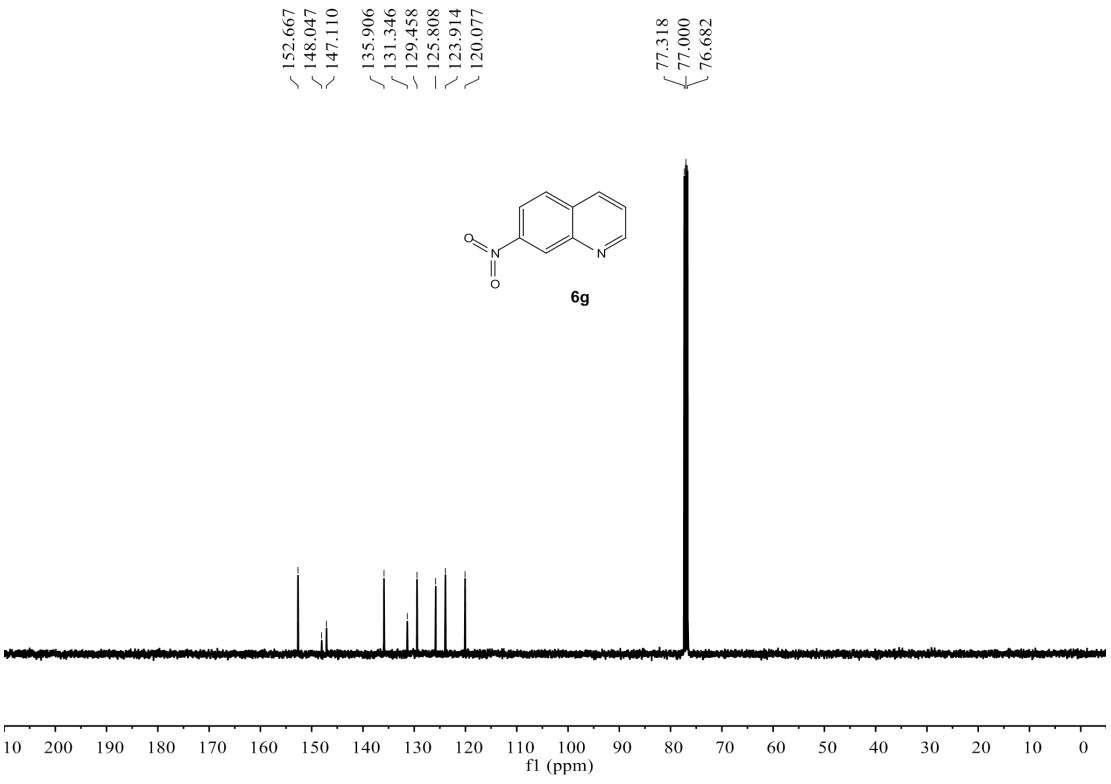

8.934
8.927
8.103
8.083
7.642
7.622
7.550
7.533
7.429
7.410
7.391
7.374
7.364
7.354
7.344
7.259
2.819
0.000
N
CH3
6e
1.00
1.00
1.00
2.03
3.00
f1 (ppm)

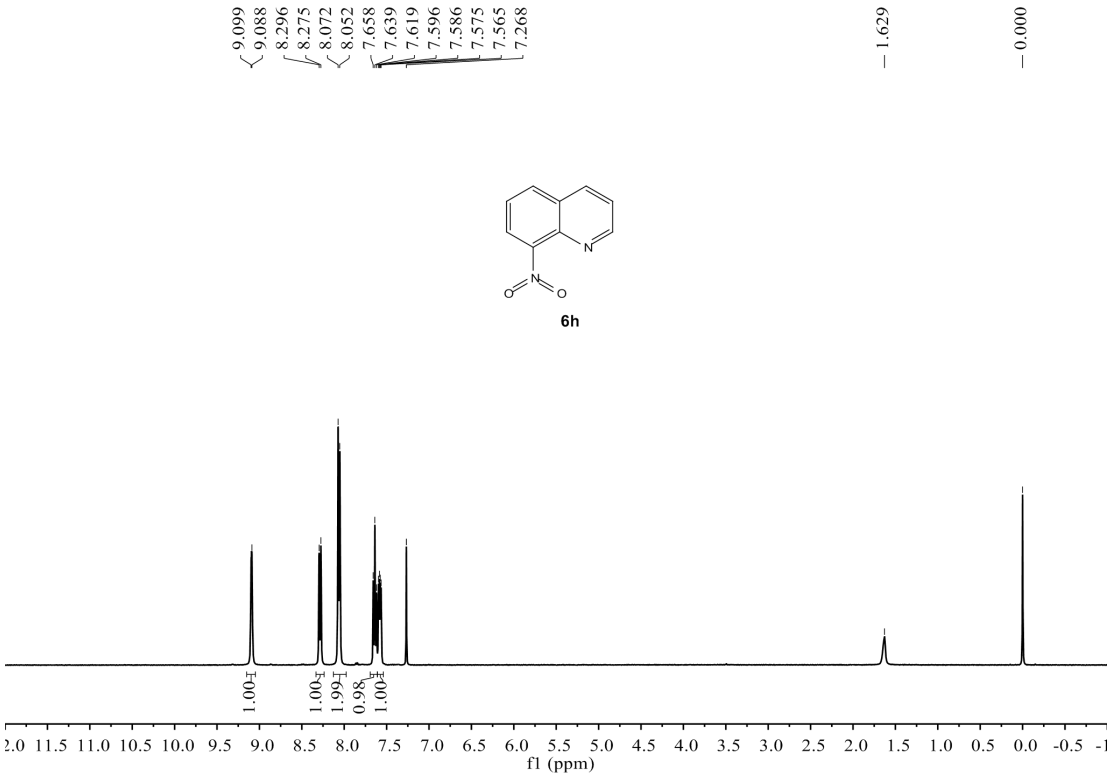

149.140
147.235
136.941
136.234
129.543
128.168
126.202
125.779
120.730
77.317
77.000
76.682
18.081
N
CH3
6e
f1 (ppm)

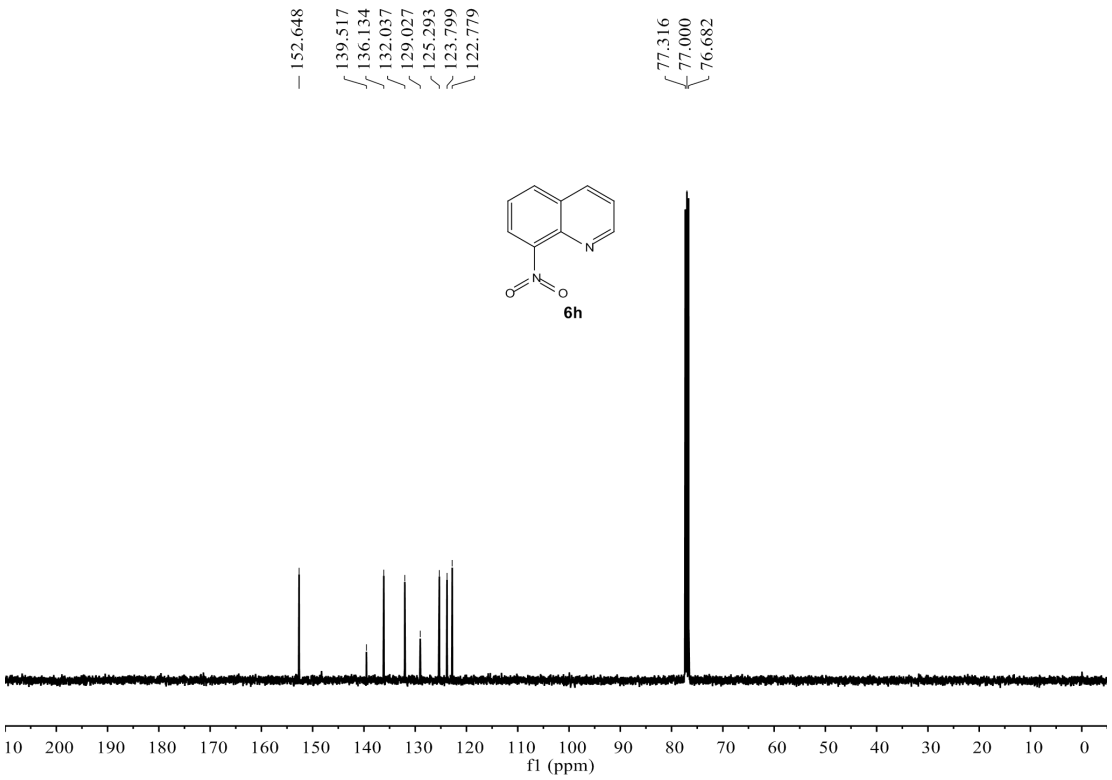

9.019
9.009
8.599
8.320
8.315
8.298
8.293
8.283
8.279
8.261
8.164
8.142
7.495
7.484
7.474
7.463
7.275
4.002
-0.000
O
H3C
O
N
6f
1.00
1.00
2.01
1.00
1.01
3.00
f1 (ppm)

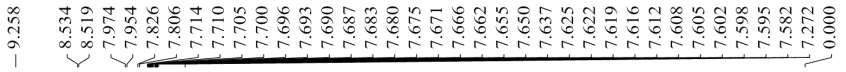

166.564
152.477
150.022
137.318
130.972
129.769
128.925
128.084
127.378
121.818
77.321
77.000
76.686
52.412
O
H3C
O
N
6f
f1 (ppm)

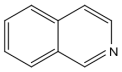

9.104
9.095
9.018
8.354
8.348
8.331
8.326
8.300
8.280
8.007
7.985
7.626
7.615
7.605
7.594
7.272
-0.000
6g
1.00
0.99
1.00
1.00
1.00
1.02
f1 (ppm)


152.667
148.047
147.110
135.906
131.346
129.458
125.808
123.914
120.077
77.318
77.000
76.682
6g
f1 (ppm)

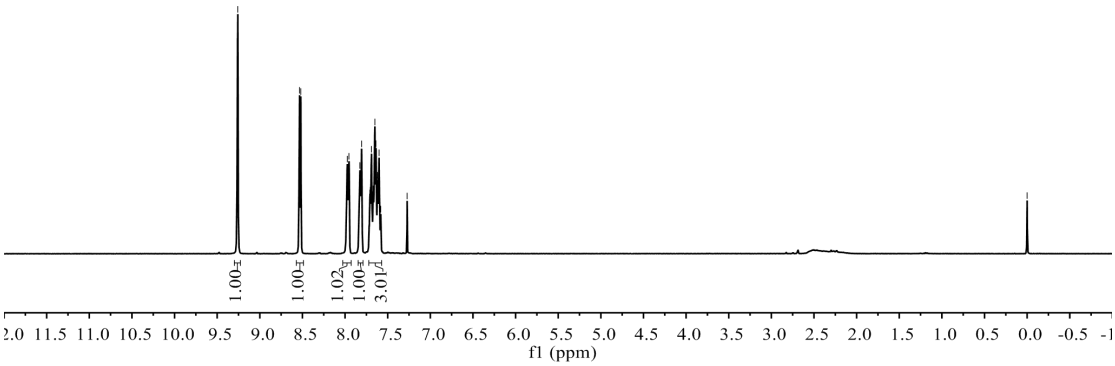

9.099
9.088
8.296
8.275
8.072
8.052
7.658
7.639
7.619
7.596
7.586
7.575
7.565
7.268
1.629
0.000
6h
1.00
1.00
1.99
0.98
1.00
f1 (ppm)

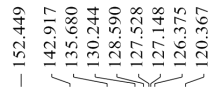

152.648
139.517
136.134
132.037
129.027
125.293
123.799
122.779
77.316
77.000
76.682
6h
f1 (ppm)

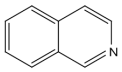

9.258
8.534
8.519
7.974
7.954
7.826
7.806
7.714
7.710
7.705
7.700
7.696
7.693
7.690
7.687
7.683
7.680
7.675
7.671
7.666
7.662
7.655
7.650
7.637
7.625
7.622
7.619
7.616
7.612
7.608
7.605
7.602
7.598
7.595
7.582
7.272
0.000



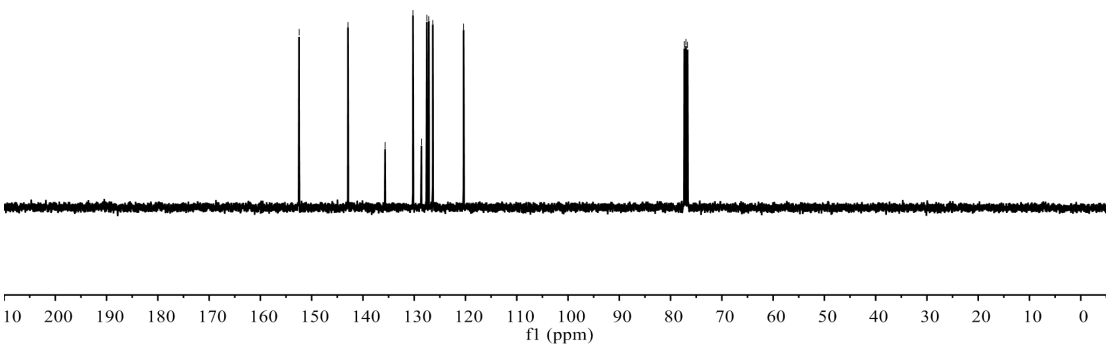
6i

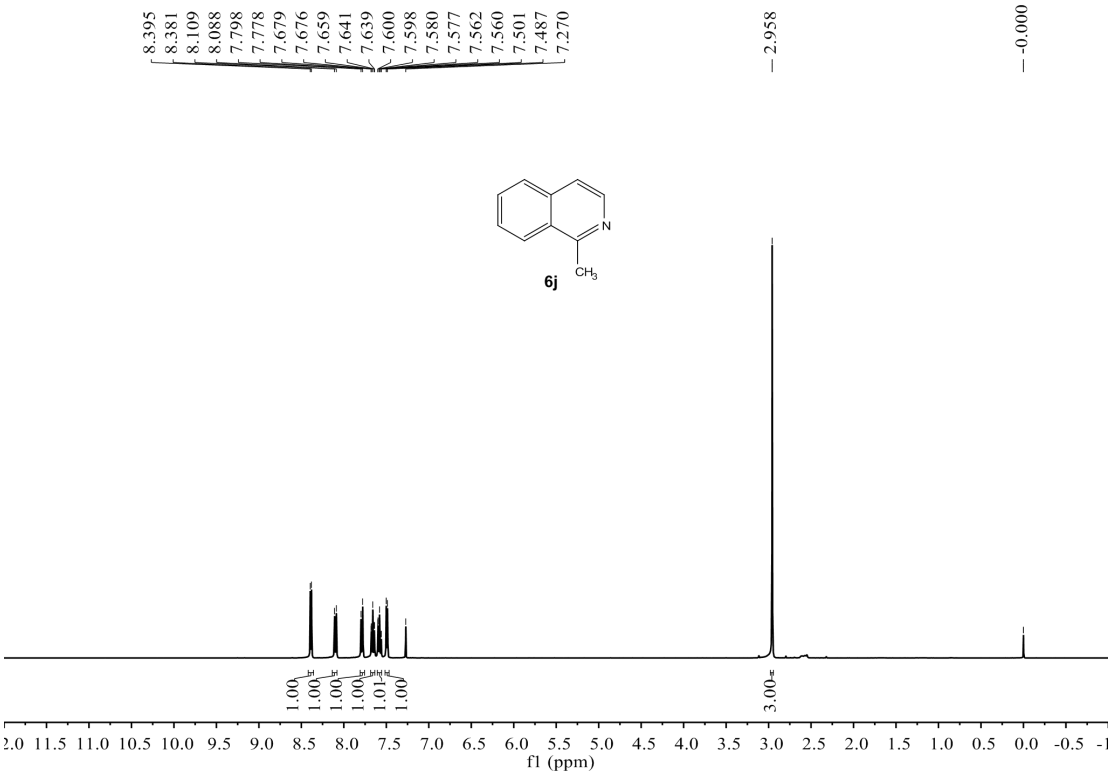

1.00
1.00
1.02
1.00
3.01
f1 (ppm)

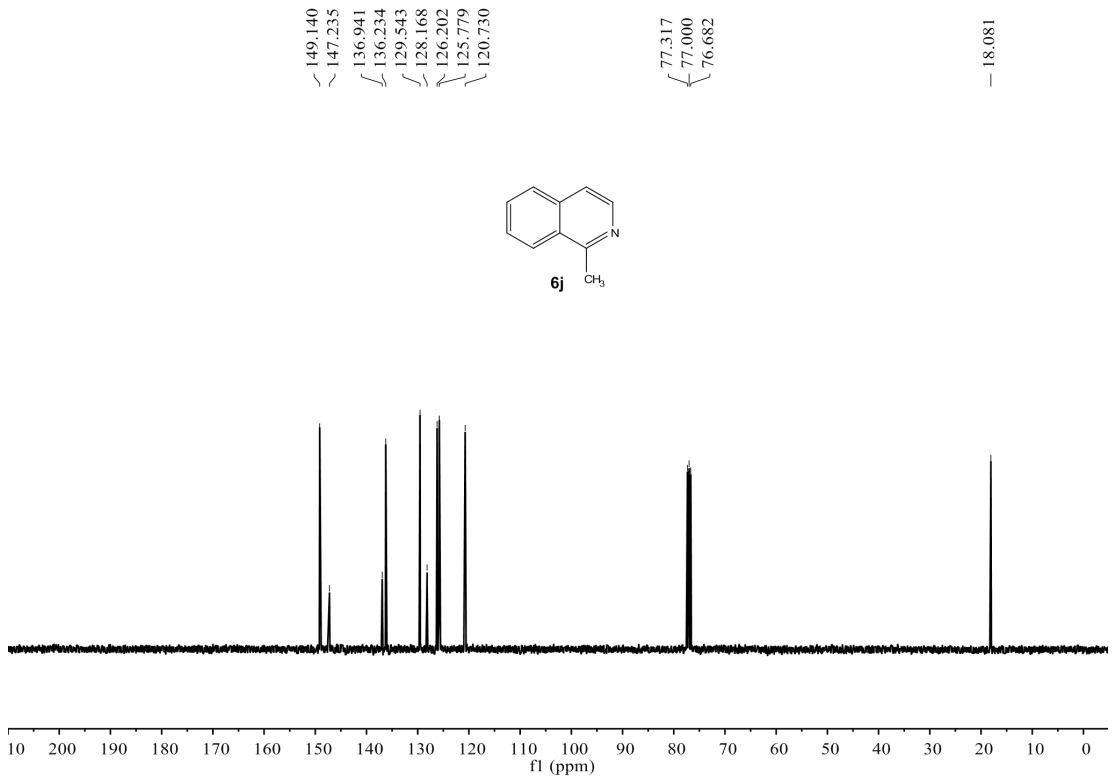

152.449
142.917
135.680
130.244
128.590
127.528
127.148
126.375
120.367
77.317
77.000
76.682

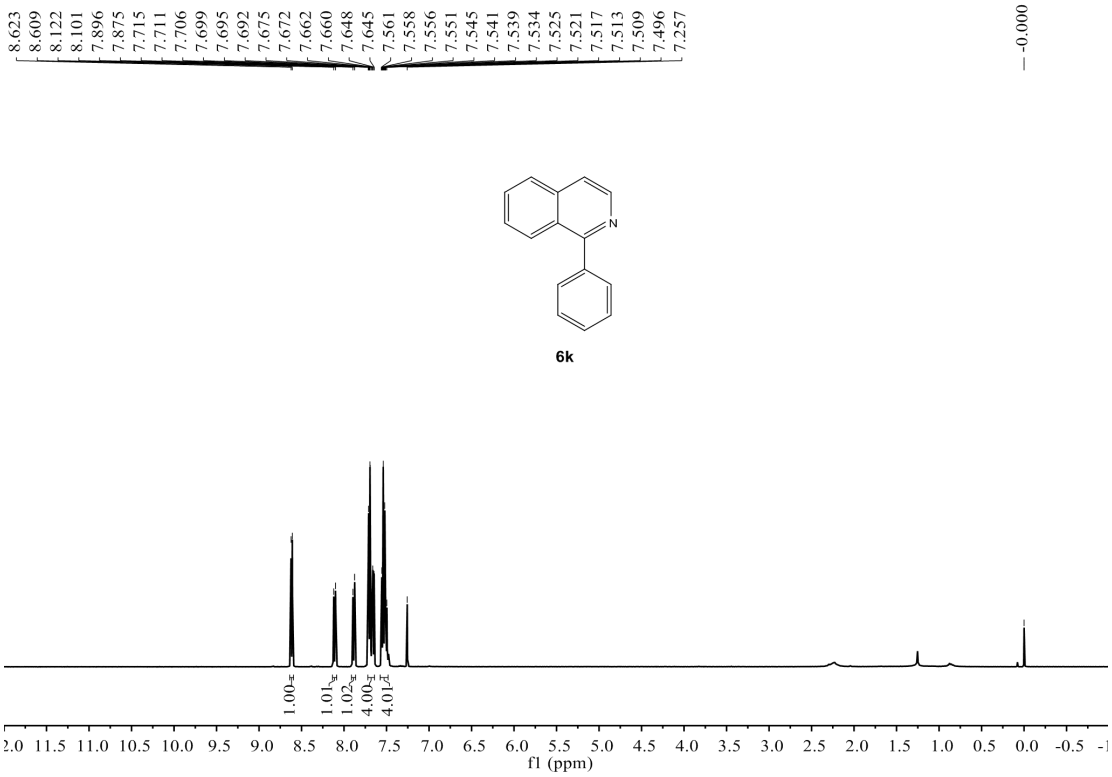


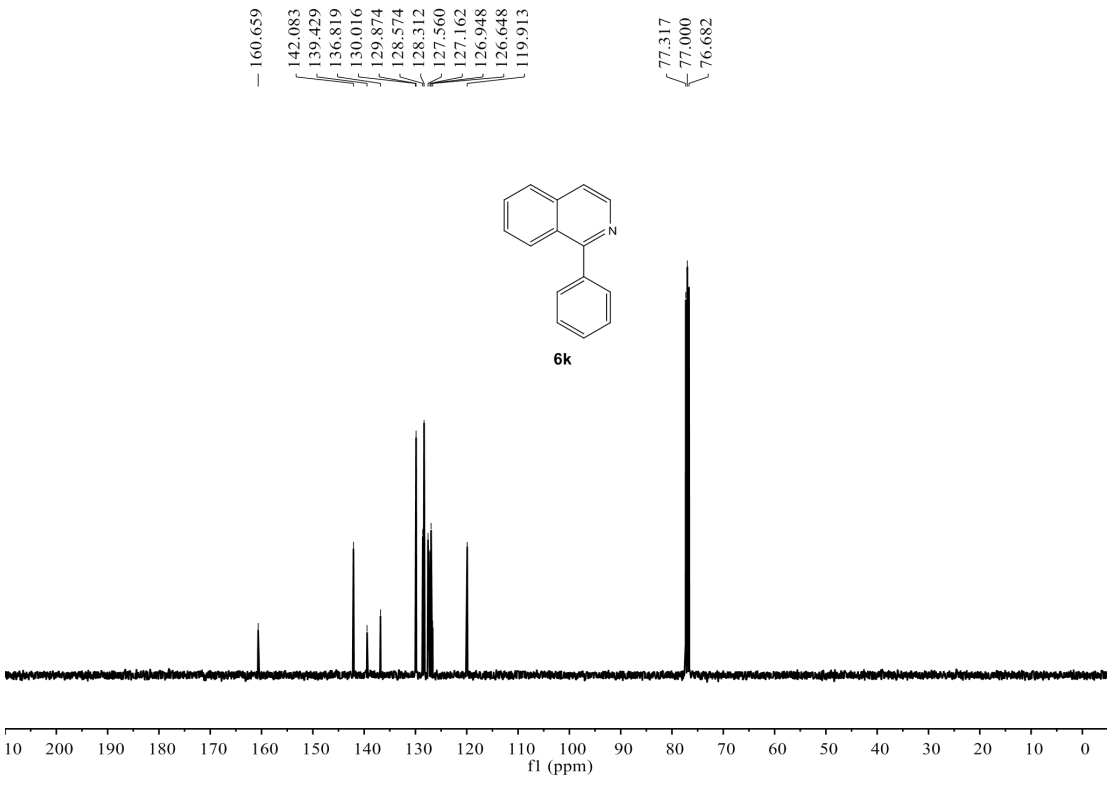
6i

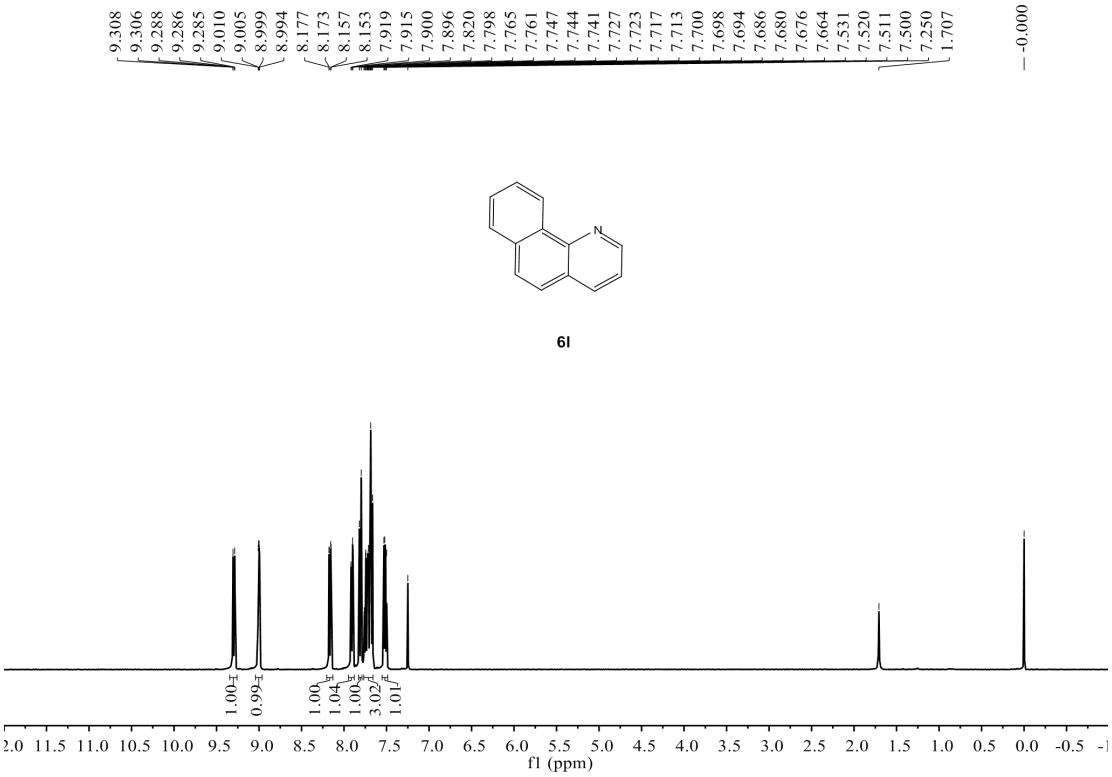

f1 (ppm)

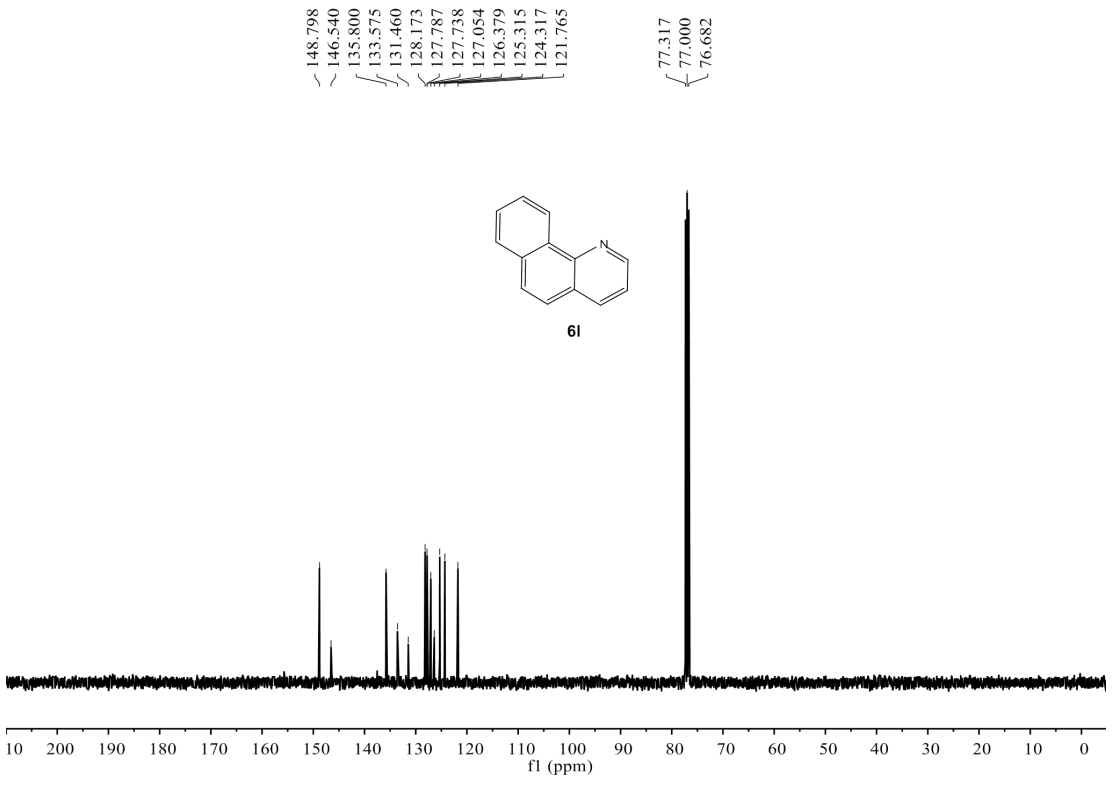

8.395
8.381
8.109
8.088
7.798
7.778
7.679
7.676
7.659
7.641
7.639
7.600
7.598
7.580
7.577
7.562
7.560
7.501
7.487
7.270
2.958
-0.000
N
CH3
6j
1.00
1.00
1.00
1.00
1.01
1.00
3.00
f1 (ppm)


149.140
147.235
136.941
136.234
129.543
128.168
126.202
125.779
120.730
77.317
77.000
76.682
18.081
N
CH3
6j
f1 (ppm)


8.623
8.609
8.122
8.101
7.896
7.875
7.715
7.711
7.706
7.699
7.695
7.692
7.675
7.672
7.662
7.660
7.648
7.645
7.561
7.558
7.556
7.551
7.545
7.541
7.539
7.534
7.525
7.521
7.517
7.513
7.509
7.496
7.257
-0.000
N
6k
1.00
1.01
1.02
4.00
4.01
f1 (ppm)


160.659
142.083
139.429
136.819
130.016
129.874
128.574
128.312
127.560
127.162
126.948
126.648
119.913
77.317
77.000
76.682
N
6k
f1 (ppm)


9.308
9.306
9.288
9.286
9.285
9.010
9.005
8.999
8.994
8.177
8.173
8.157
8.153
7.919
7.915
7.900
7.896
7.820
7.798
7.765
7.761
7.747
7.744
7.741
7.727
7.723
7.717
7.713
7.700
7.698
7.694
7.686
7.680
7.676
7.664
7.531
7.520
7.511
7.500
7.250
1.707
-0.000
N
6l
1.00
0.99
1.00
1.04
1.00
3.02
1.01
f1 (ppm)


148.798
146.540
135.800
133.575
131.460
128.173
127.787
127.738
127.054
126.379
125.315
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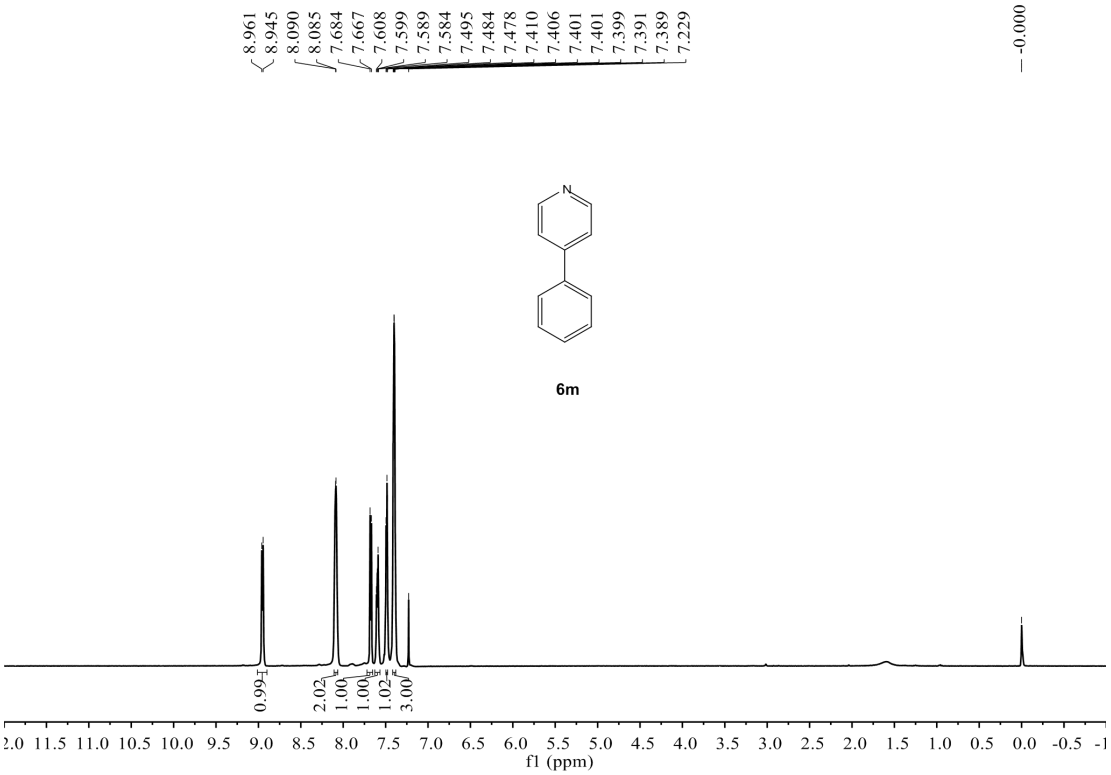
121.765
77.317
77.000
76.682
N
6l
f1 (ppm)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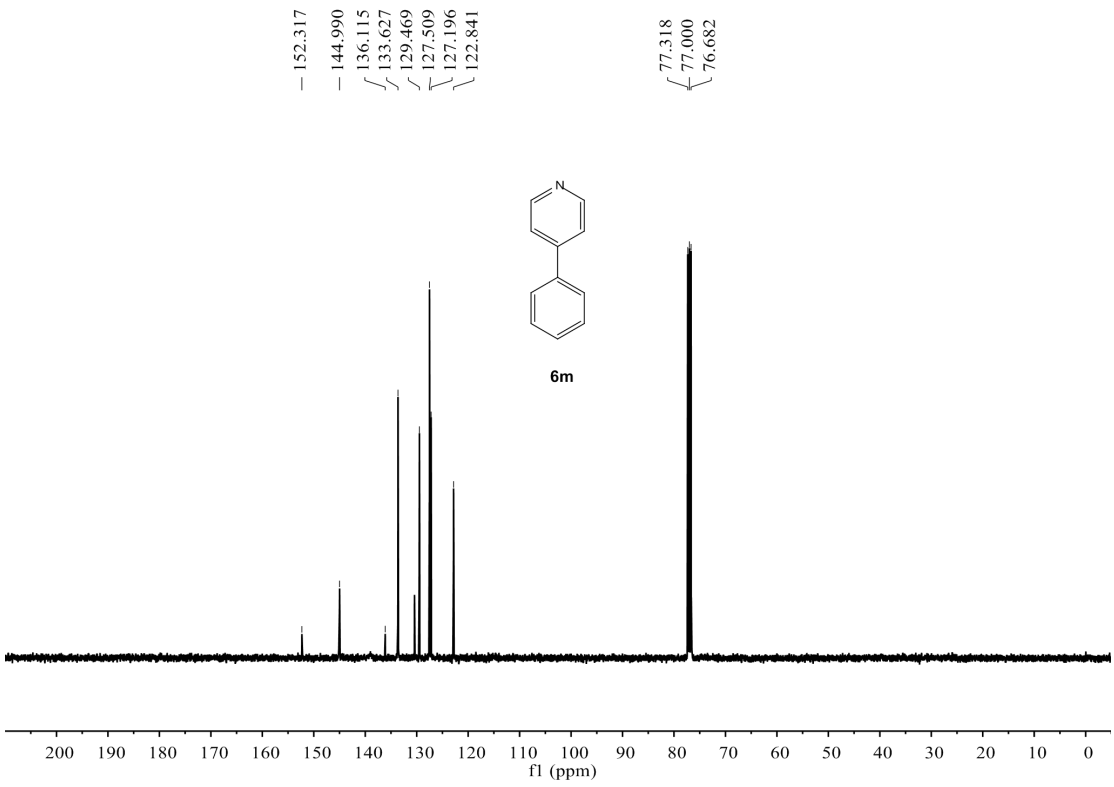
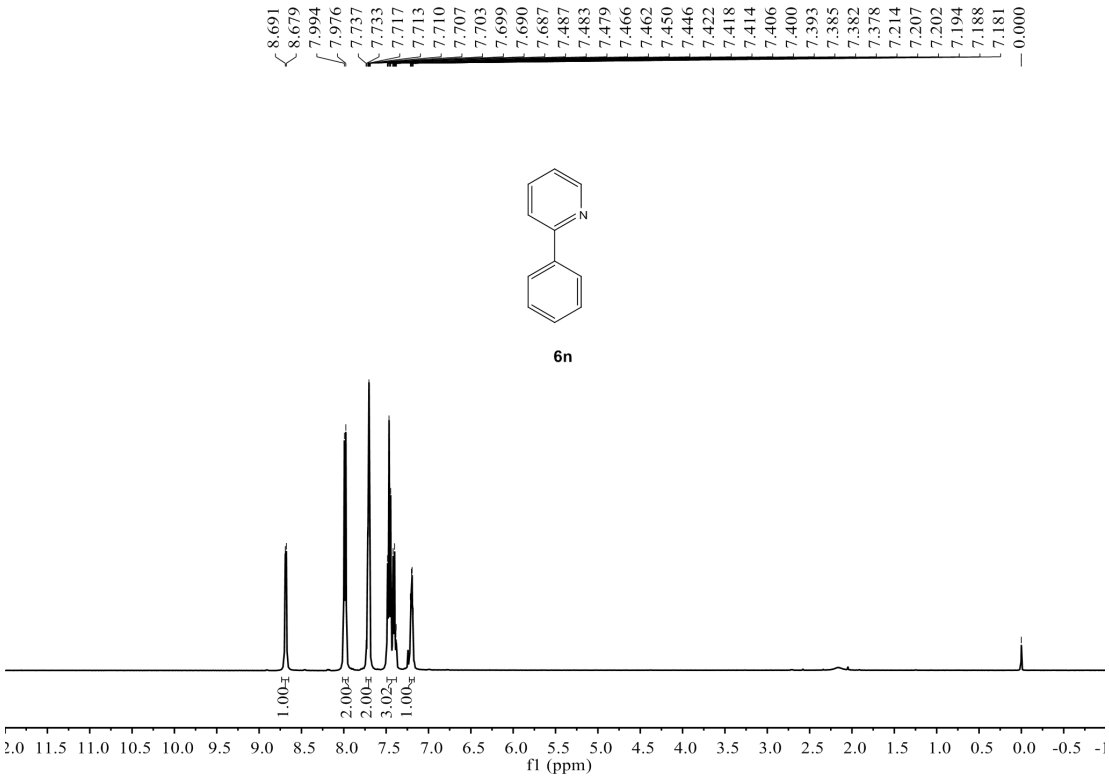
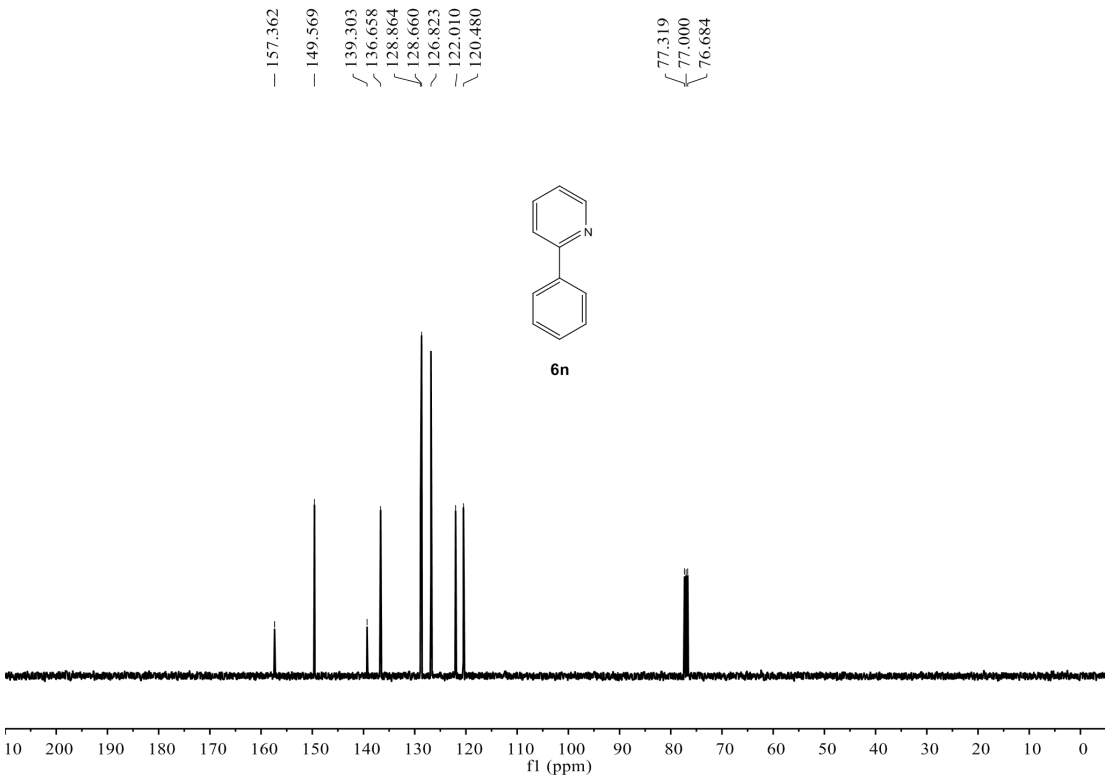
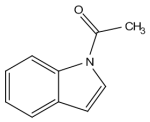
8.945
8.090
8.085
7.684
7.667
7.608
7.599
7.589
7.584
7.495
7.484
7.478
7.410
7.406
7.401
7.401
7.399
7.391
7.389
7.229
-0.000
6m
0.99
2.02
1.00
1.00
1.02
3.00
f1 (ppm)


152.317
144.990
136.115
133.627
129.469
127.509
127.196
122.841
77.318
77.000
76.682
6m
f1 (ppm)

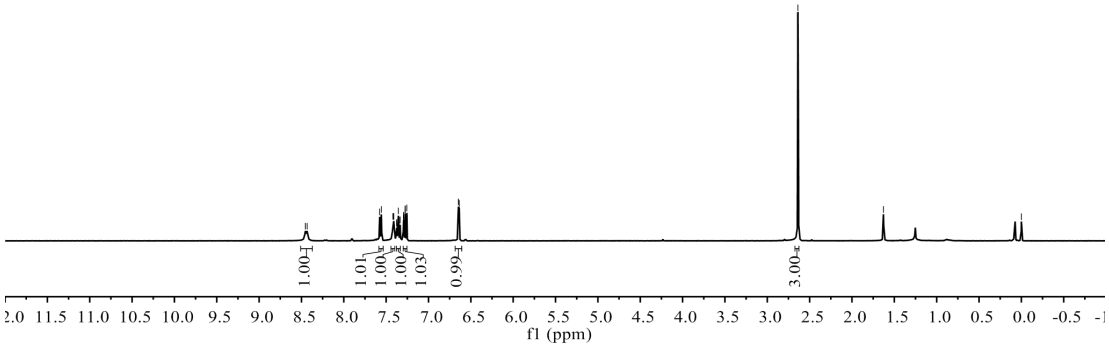

8.691
8.679
7.994
7.976
7.737
7.733
7.717
7.713
7.710
7.707
7.703
7.699
7.690
7.687
7.487
7.483
7.479
7.466
7.462
7.450
7.446
7.422
7.418
7.414
7.406
7.400
7.393
7.385
7.382
7.378
7.214
7.207
7.202
7.194
7.188
7.181
0.000
N
6n
1.00
2.00
2.00
3.02
1.00
f1 (ppm)

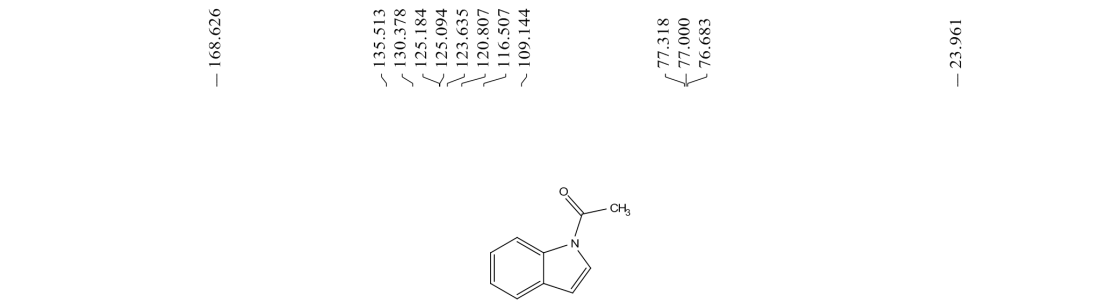

157.362
149.569
139.303
136.658
128.864
128.660
126.823
122.010
120.480
77.319
77.000
76.684
N
6n
f1 (ppm)


8.454
8.433
7.577
7.557
7.420
7.410
7.376
7.374
7.356
7.338
7.335
7.296
7.296
7.294
7.277
7.275
7.275
7.259
7.256
6.647
6.638
2.638
1.629
-0.000


O
CH3
N

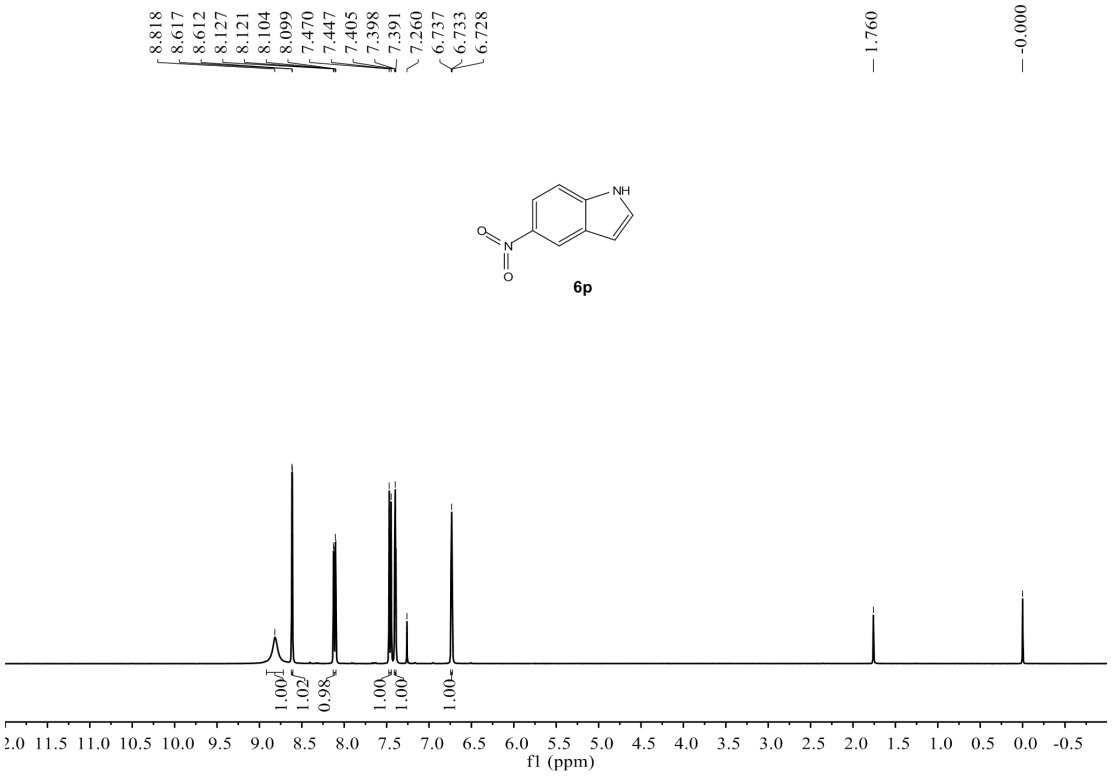
6o

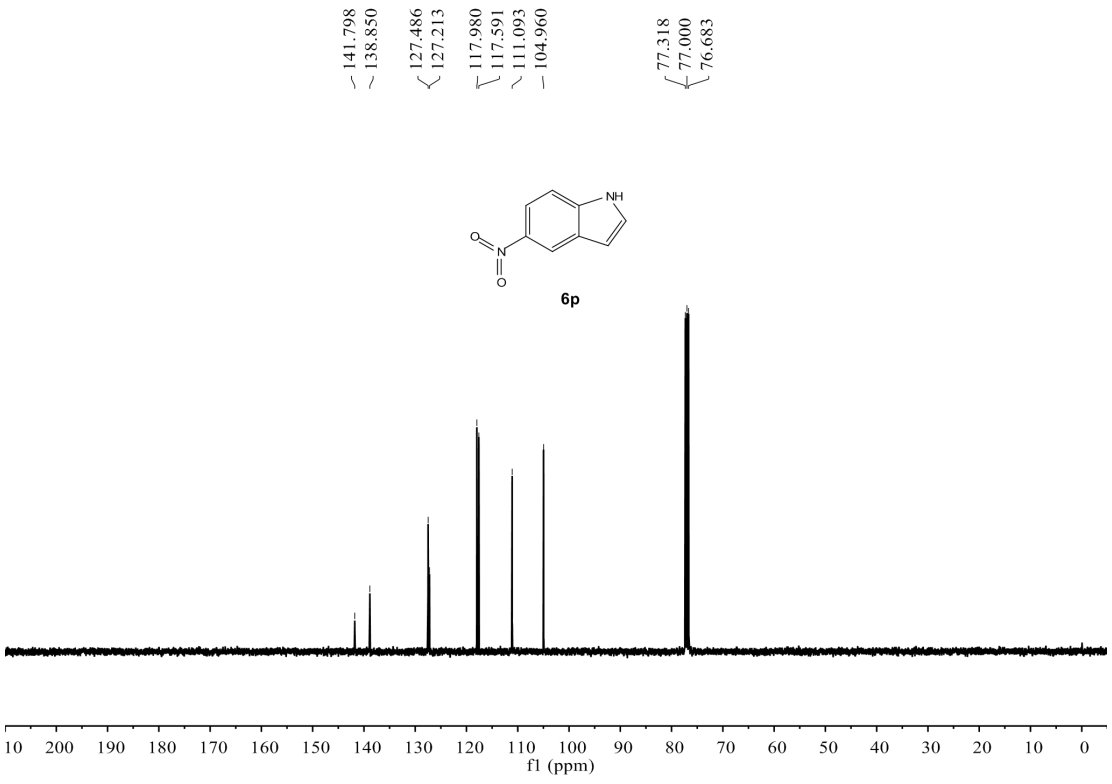

1.00
1.01
1.00
1.00
1.03
0.99
3.00
f1 (ppm)


168.626
135.513
130.378
125.184
125.094
123.635
120.807
116.507
109.144
77.318
77.000
76.683
23.961
f1 (ppm)

O
CH3
N

6o


8.818
8.617
8.612
8.127
8.121
8.104
8.099
7.470
7.447
7.405
7.398
7.391
7.260
6.737
6.733
6.728
1.760
-0.000
NH
O
N
O
6p
1.00
1.02
0.98
1.00
1.00
1.00
f1 (ppm)


141.798
138.850
127.486
127.213
117.980
117.591
111.093
104.960
77.318
77.000
76.683
NH
O
N
O
6p
f1 (ppm)