Supporting Information

A Pd-Catalyzed Optional Approach for the Synthesis of Dibenzothiophenes

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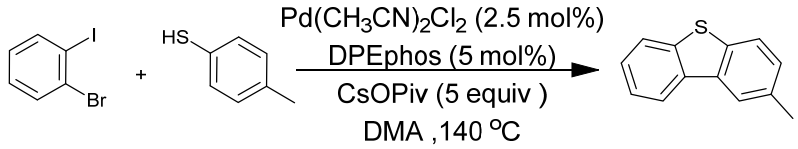
General Information

All reactions were carried out using Schlenk tube. All solvents were dried and distilled according to the standard methods before use. Unless otherwise noted, materials obtained from commercial suppliers were used without further purification. High Resolution mass spectrometry (HRMS) data report were performed on Waters Micromass GCT Premier, ionization mode: EI+ and IonSpec 4.7 Tesla FTMS. 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 ºC). ^{1}H and ^{13}C NMR data were recorded with Bruker Advance 400 MHz spectrometers with tetramethylsilane as an internal standard. All chemical shifts (δ) are reported in ppm and coupling constants (*J*) in Hz. The chemical shifts (δ) were given in part per million relatives to internal tetramethylsilane (0 ppm for ^{1}H) and $CDCl_3$ (77.0 ppm for ^{13}C).

General Experimental Procedures

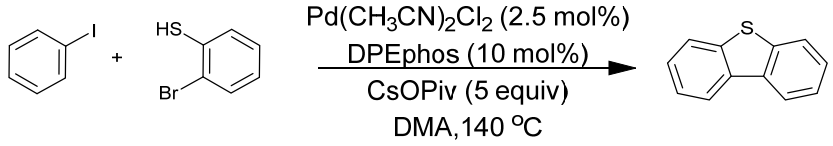
A. Synthesis of CsOPiv : To an oven tidy round bottomed flask, PivOH (20 mmol), Cs_2CO_3 (10 mmol), 20mL water were added under air atmosphere in the reaction. The reaction was then heated up to 70 ºC and kept stirring for 2 hours, the resulting mixture was dried by rotary evaporators, after this, we get the white solid 4.63g, 99% yield.

B. Typical Procedure for the Synthesis of 2-methyldibenzo[b,d]thiophene (3a) by *o*-Bromo-iodobenzenes Coupled with Benzenethiols.



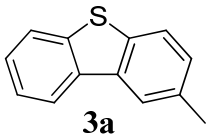
General procedure: To an oven dried schlenk tube containing 4-methylbenzenethiol (24.8 mg, 0.2 mmol), $Pd(CH_3CN)_2Cl_2$ (0.005 mmol, 1.30 mg) , DPEphos (0.010 mmol, 5.39 mg) andCsOPiv (235 mg, 1.0 mmol), DMA(N,N-Dimethylacetamide) (2 mL) was added in glove box under argon atmosphere. Sealed with a septa, *o*-bromoiodobenzene were injected into the reaction tube via syringe. The mixture was then heated to 140 ℃ and stirred for 24 hours. After quenched by saturated ammonium chloride solution, the reaction mixture was extracted with ethyl acetate (3 * 15 mL). The organic layers were combined, dried (Na_2SO_4) and filtered, and the solvent was removed under reduced pressure. Column chromatography on silica gel (petroleum ether) afforded the desired product **3a** in 91% yield (34.2 mg).

C. Typical Procedure for the Synthesis of dibenzothiophene (3u) by Iodobenzene Coupled with o-Bromo-benzenethiol.



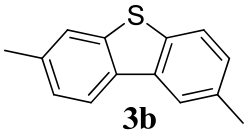
General procedure: To an oven dried schlenk tube, $Pd(CH_3CN)_2Cl_2$ (0.005 mmol, 1.30 mg) , DPEphos (0.020 mmol, 10.78 mg) and CsOPiv (1.0 mmol, 235 mg) were added, followed by DMA (2 mL) in glove box under argon atmosphere. Sealed with a septa, iodobenzene (0.25 mmol, 51.0 mg) and 2-bromobenzenethiol (0.2 mmol, 38.0 mg) were injected into the reaction tube via syringe. The mixture was then heated to 140 °C and stirred for 24 hours. After quenched by saturated ammonium chloride solution, the reaction mixture was extracted with ethyl acetate (3 * 15 mL). The organic layers were combined, dried (Na_2SO_4) and filtered, and the solvent was removed under reduced pressure. Column chromatography on silica gel (petroleum ether) afforded the desired product **3u** in 85% yield (31.3 mg).

Detailed descriptions for products:



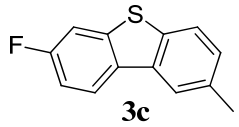
3a

2-methyldibenzo[b,d]thiophene (3a)[5] :white soild, yield: 34.2 mg, 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15-8.09 (m, 1H), 7.96 (s, 1H), 7.87-7.80 (m, 1H), 7.73 (d, *J* = 8.2 Hz, 1H), 7.47-7.41 (m, 2H), 7.29 (d, *J* = 8.2 Hz, 1H), 2.53 (s, 3H)； ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.7, 136.3, 135.6, 135.3, 134.0, 128.1, 126.4, 124.1, 122.7, 122.3, 121.7, 121.4, 21.4.



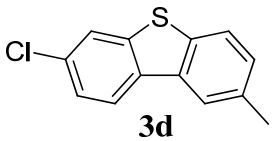
3b

2,7-dimethyldibenzo[b,d]thiophene (3b)[7]: white soild, yield: 34.4 mg, 81%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 8.1 Hz, 1H), 7.89 – 7.87 (m, 1H), 7.68 (d, *J* = 8.1 Hz, 1H), 7.60 (dd, *J* = 1.5, 0.7 Hz, 1H), 7.24 – 7.20 (m, 2H), 2.50 (s, 3H), 2.47 (s, 3H)； ^{13}C NMR (101 MHz, CDCl3) δ 140.0, 136.6, 136.0, 135.7, 133.9, 133.0, 127.6, 125.6, 122.7, 122.3, 121.4, 121.0, 21.4, 21.6.



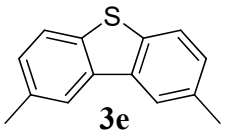
3c

7-fluoro-2-methyldibenzo[b,d]thiophene (3c): white soild, yield: 38.9 mg, 90%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 8.7, 5.2 Hz, 1H), 7.88 (s, 1H), 7.70 (d, *J* = 8.2 Hz, 1H), 7.51 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.28 (dd, *J* = 1.2, 1.6 Hz, 1H), 7.16 (td, *J* = 8.8, 2.4 Hz, 1H), 2.53 (s, 3H)； ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 160.5, 141.0, 136.2, 134.9, 134.5, 131.8, 127.8, 122.4, 121.5, 112.7, 109.2, 21.5. ^{19}F NMR (377 MHz, $CDCl_3$) δ -114.71. HRMS: (EI) Calcd for $C_{13}H_9FS$ $[M]^+$: 216.0409, found:216.0422



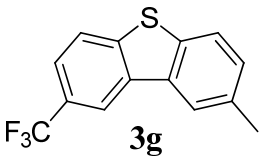
3d

7-chloro-2-methyldibenzo[b,d]thiophene (3d): white soild, yield: 41.4 mg, 89%; ^{1}H NMR (400 MHz, $CDCl_3$) 7.99 (d, J = 8.4 Hz, 1H), 7.89 (d, *J* = 1.7 Hz, 1H), 7.79 (d, *J* = 1.9 Hz, 1H), 7.70 (d, *J* = 8.3 Hz, 1H), 7.38 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.28 (dd, *J* = 8.2, 1.7 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) 140.9, 136.3, 134.8, 134.4, 133.9, 132.2, 128.4, 124.8, 122.4, 122.4 , 122.1, 121.7, 21.4. HRMS (EI) Calcd for $C_{13}H_9ClS$ $[M]^+$: 232.0113, found: 232.0105.



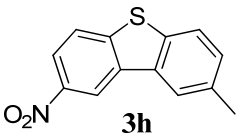
3e

2,8-dimethyldibenzo[b,d]thiophene (3e)[5]: white soild, yield: 28.0 mg, 66%; ^{1}H NMR (400 MHz, $CDCl_3$) 7.92 (s, 2H), 7.70 (d, *J* = 7.7 Hz, 2H), 7.25 (d, *J* = 7.6 Hz, 2H), 2.51 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.7, 135.5, 133.8, 128.0, 122.3, 121.6, 21.4.



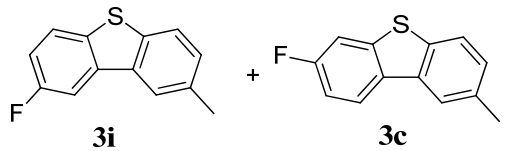
3g

2-methyl-8-(trifluoromethyl)dibenzo[b,d]thiophene(3g): white soild, yield: 45.3 mg, 85%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.95 (s, 1H), 7.87 (d, J = 8.4 Hz, 1H), 7.71 (d, *J* = 8.2 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.2, 136.8, 135.3, 134.8, 129.0, 126.7, 125.9, 123.1, 122.7, 122.4, 121.9, 118.4, 21.4; HRMS (EI) Calcd for $C_{14}H_9F_3S$ $[M]^+$: 266.0377, found: 266.0378.



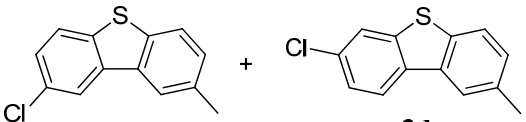
3h

2-methyl-8-nitrodibenzo[b,d]thiophene (3h): white soild, yield: 44.2 mg, 91%; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.96 (d, J = 2.3 Hz, 1H), 8.29 (dd, J = 8.8, 2.2 Hz, 1H), 8.05 (dd, J = 1.7, 0.8 Hz, 1H), 7.93 (d, J = 8.8 Hz, 1H), 7.77 (d, J = 8.2 Hz, 1H), 7.39 (dd, J = 8.3, 1.6 Hz, 1H), 2.57 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.4, 145.2, 137.2, 135.7, 135.4, 134.7, 129.7, 123.1, 122.6, 122.3, 120.9, 116.8, 21.5; HRMS (EI) Calcd for $C_{14}H_9NO_2S$ $[M]^+$: 243.0354, found: 243.0361.



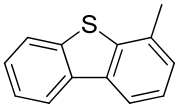
3i **3c**

2-fluoro-8-methyldibenzo[b,d]thiophene(3i) with 7-fluoro-2-methyldibenzo [b,d] thiophene (3c) (1:1) : white soild, yield: 31.1 mg, 72%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (ddd, *J* = 8.7, 5.2, 0.9 Hz, 1H), 7.86 (dt, *J* = 1.7, 0.9 Hz, 2H), 7.78 – 7.67 (m, 4H), 7.50 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.31 – 7.24 (m, 2H), 7.20 – 7.12 (m, 2H), 2.51 (s, 6H); ^{13}C NMR (101 MHz,$CDCl_3$) δ 162.5, 160.0, 141.0, 137.7 , 136.7, 136.1, 135.1, 134.9, 134.8, 134.4, 134.2, 131.8, 128.7, 128.8, 127.8, 123.7, 122.5, 122.3, 121.9, 121.4, 114.7, 112.6, 109.1, 107.6, 21.4, 21.4; HRMS: (EI) Calcd for $C_{13}H_9FS$ $[M]^+$: 216.0409, found: 216.0422.



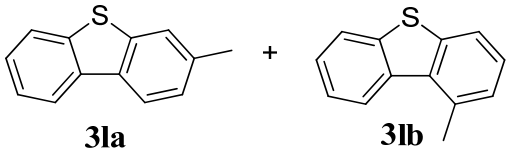
3j **3d**

2-chloro-8-methyldibenzo[b,d]thiophene (3j) with 7-chloro-2-methyl dibenzo [b,d] thiophene (3d) (1:1) : white soild, yield: 34.5 mg, 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 2.0 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.85 (s, 2H), 7.76 (d, *J* = 1.8 Hz, 1H), 7.71 – 7.65 (m, 3H), 7.37 – 7.34 (m, 2H), 7.29 – 7.24 (m, 2H), 2.50 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.9, 137.8, 137.1, 136.7, 136.2, 134.7, 134.6, 134.4, 134.3, 133.8, 132.2, 130.4, 128.8, 128.3, 126.6, 124.8, 123.6, 122.4, 122.4, 122.3, 122.1, 121.8, 121.6, 121.3, 21.4, 21.4; HRMS (EI) Calcd for $C_{13}H_9ClS$ $[M]^+$: 232.0113, found: 232.0105.



3k

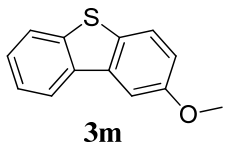
4-methyldibenzo[b,d]thiophene (3k):[5] white soild, yield: 34.8 mg, 88%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 – 8.10 (m, 1H), 8.00 (d, *J* = 7.9 Hz, 1H), 7.90 – 7.83 (m, 1H), 7.48 – 7.42 (m, 2H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.27 (d, *J* = 7.2 Hz, 1H), 2.58 (s, 3H)； ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.5, 139.1, 136.1, 135.3, 132.2, 126.9, 126.5, 124.6, 124.3, 122.8, 121.7, 119.0, 20.5.



3la **3lb**

1-methyldibenzo[b,d]thiophene(3la)[5] **compound with 3-methyldibenzo[b,d]thiop hene (3lb)**[4] **(5:1) in Path A and B ,** white soild, yield: 35.7 mg, 90% (in path A), 85% (in Path B) **; 1-methyldibenzo[b,d]thiophene(3la)**[5]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 8.05 (m, 1H), 8.00 (d, *J* = 8.1 Hz, 1H), 7.83 – 7.78 (m, 1H), 7.62 (dt, *J* = 1.5, 0.8 Hz, 1H), 7.42 – 7.38 (m, 2H), 7.24 (ddd, *J* = 8.1, 1.6, 0.7 Hz, 1H), 2.48(s,3H);

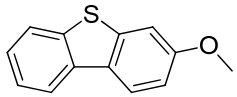
3-methyldibenzo[b,d]thiophene (3lb)[4]**:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 – 8.33 (m, 1H), 7.89 – 7.85 (m, 1H), 7.72 (ddd, *J* = 8.0, 1.2, 0.6 Hz, 1H), 7.47 – 7.43 (m, 3H), 7.36 – 7.31 (m, 1H), 2.90 (s, 3H).



3m

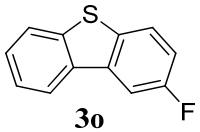
2-methoxydibenzo[b,d]thiophene (3m)[5]: white soild, yield: 30.8 mg, 72% (in path A) or 60% (in path B); ^{1}H NMR (400 MHz,$CDCl_3$) δ 8.11 – 8.04 (m, 1H), 7.84 – 7.77 (m, 1H), 7.69 (d, *J* = 8.7 Hz, 1H), 7.59 (d, *J* = 2.5 Hz, 1H), 7.45 – 7.38 (m, 2H), 7.07 (ddd, *J* = 8.7, 2.6, 1.0 Hz, 1H),

3.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.5, 140.4, 136.4, 135.3, 131.1, 126.6, 124.0, 123.3, 122.8, 121.4, 115.7, 104.8, 55.5.



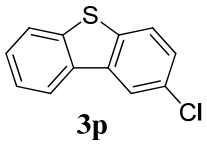
3n

3-methoxydibenzo[b,d]thiophene (3n)[4]: white soild, yield: 28.2 mg, 66%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (m, 2H), 7.81 (d, *J* = 7.3 Hz, 1H), 7.41 (m, 2H), 7.33 (d, *J* = 2.2 Hz, 1H), 7.05 (dd, *J* = 8.7, 2.3 Hz, 1H), 3.91 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.0, 140.9, 138.5, 135.4, 129.0, 125.4, 124.3, 122.6, 122.2, 120.7, 113.4, 105.7, 55.6.



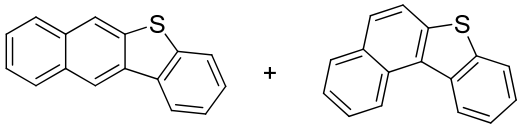
3o

2-fluorodibenzo[b,d]thiophene (3o)[5]: white soild, yield: 20.2 mg, 50% (in path A) or 81% (in path B) ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.02 (m, 1H), 7.85 – 7.72 (m, 3H), 7.47 – 7.43 (m, 2H), 7.19 (td, *J* = 8.7, 2.5 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.1, 159.7, 140.6, 136.8, 134.6, 126.9, 124.3, 123.7, 122.8, 121.6, 114.9, 107.7.



3p

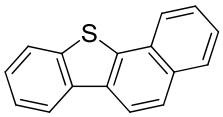
2-chlorodibenzo[b,d]thiophene (3p)[5]: white soild, yield: 28.8 mg, 66% (in path A) or 90% (in Path B); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (dd, *J* = 7.7, 2.0 Hz, 2H), 7.84 (dd, J = 5.9, 2.7 Hz, 1H), 7.74 (d, *J* = 8.5 Hz, 1H), 7.47 (dd, *J* = 6.5, 3.2 Hz, 2H), 7.40 (dd, J = 8.5, 1.9 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.1, 137.5, 136.9, 134.5, 130.6, 127.3, 126.9, 124.6, 123.7, 122.9, 121.8, 121.5.



3sa **3sb**

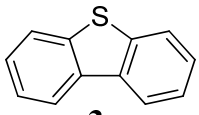
benzo[b]naphtho[1,2-d]thiophene(3sa)[3] **compound with benzo[b]naphtha[2,3-d] thiophene(3sb)**[2] **(1:1)**: white soild, yield: 44.5 mg, 95%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.00 (d, *J* = 8.5 Hz, 1H), 8.85 (d, *J* = 8.3 Hz, 1H), 8.59 (s, 1H), 8.28 – 8.23 (m, 2H), 8.04 – 7.97 (m, 2H),

7.92 – 7.86 (m, 2H), 7.73 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.58 (dtd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 7.52 – 7.45 (m, 5H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.0, 139.6, 138.5, 137.6, 136.6, 135.0, 132.5, 133.1, 131.8, 130.7, 130.6, 129.4, 128.9, 128.3, 127.8, 127.6, 127.1, 127.0, 125.9, 125.2, 125.1, 124.8, 124.7, 124.6, 124.5, 123.1, 123.1, 122.8, 121.9, 121.0, 120.5, 119.9.



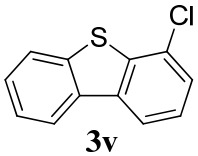
3t

benzo[b]naphtho[2,1-d]thiophene (3t)[5]: white soild, yield: 43.1 mg, 92%(in path A) or 30% (in Path B);[1]H NMR (400 MHz, $CDCl_3$) δ 8.25 – 8.09 (m, 3H), 7.97 (m, 2H), 7.87 (d, *J* = 8.6 Hz, 1H), 7.59 (m, 2H), 7.54 – 7.42 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.0, 137.2, 136.5, 132.6, 132.3, 128.9, 128.8, 126.7, 126.2, 126.1, 125.4, 124.5, 124.4, 122.9, 121.5, 119.6.



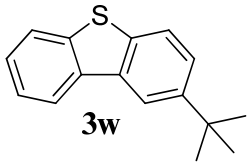
3u

dibenzo[b,d]thiophene (3u)[5]: white soild, yield: 30.5 mg,85%; ^{1}H NMR (400 MHz, CDCl3) δ 8.22 (dd, *J* = 5.9, 3.2 Hz, 2H), 7.92 (dd, *J* = 5.9, 3.3 Hz, 2H), 7.52 (ddd, *J* = 6.0, 3.2, 0.9 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.4,135.5, 126.6, 124.3, 122.7, 121.5.



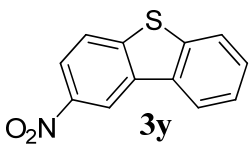
3v

4-chlorodibenzo[b,d]thiophene (3v)[1]: white soild, yield: 30.5 mg,70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (ddd, *J* = 7.2, 2.5, 1.5 Hz, 1H), 8.04 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.90 – 7.85 (m, 1H), 7.51 – 7.43 (m, 3H), 7.41 (td, *J* = 7.7, 1.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.3, 138.8, 137.1, 135.7, 128.2, 127.2, 126.2, 125.5, 124.7, 122.9, 122.0, 119.7.



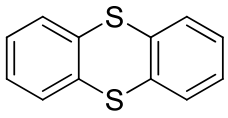
3w

2-(tert-butyl)dibenzo[b,d]thiophene (3w)[5]: colorless liquid, yield: 40.3 mg, 84%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 – 8.11 (m, 2H), 7.89 – 7.79 (m, 1H), 7.80 – 7.72 (m, 1H), 7.52 (dd, *J* = 8.4, 1.9 Hz, 1H), 7.48 – 7.39 (m, 2H), 1.44 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.6, 139.8, 136.4, 135.7, 135.3, 126.4, 124.8, 124.1, 122.8, 122.2, 121.3, 117.8, 34.8, 31.6.



3y

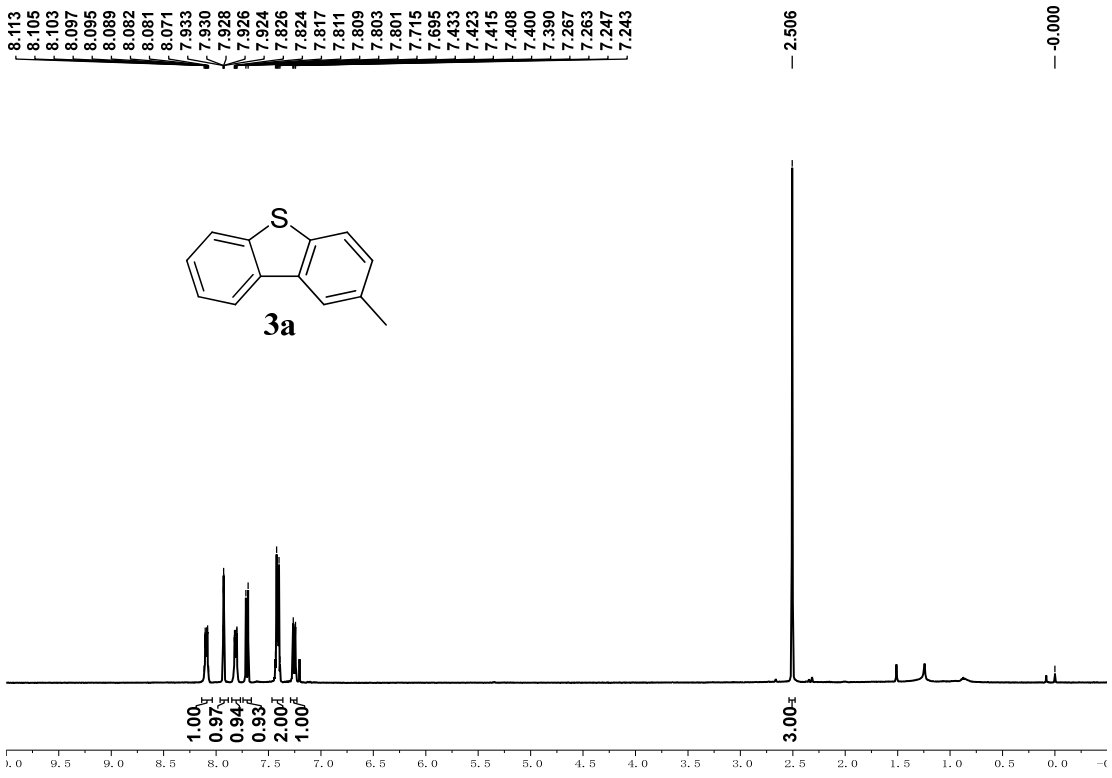
2-nitrodibenzo[b,d]thiophene (3y)[3]: white soild, yield: 18.3 mg, 40% or 75% (1-Bromo-4-nitrobenenzene as substrate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (s, 1H), 8.35 – 8.19 (m, 2H), 8.05 – 7.84 (m, 2H), 7.67 – 7.47 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.0, 145.3, 140.2, 135.9, 134.5, 128.2, 125.3, 123.1, 123.0, 122.2, 121.0, 117.0.

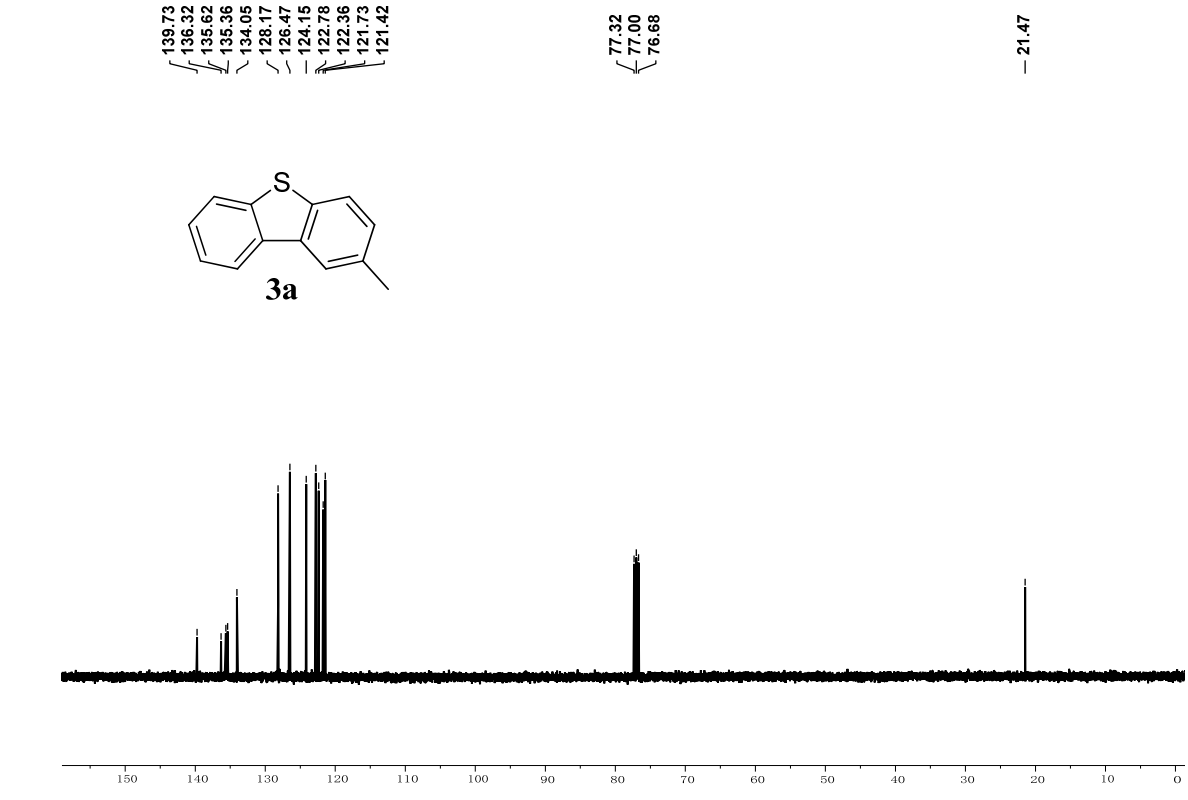


6

Thianthrene (6)[6]: yield: 76%； ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 5.8, 3.4 Hz, 4H), 7.23 (dd, *J* = 5.8, 3.3 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.5, 128.7, 127.6.

Copies of Product ^{1}H NMR and ^{13}C NMR



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7.958
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7.881
7.690
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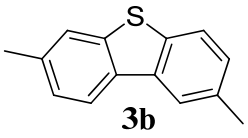
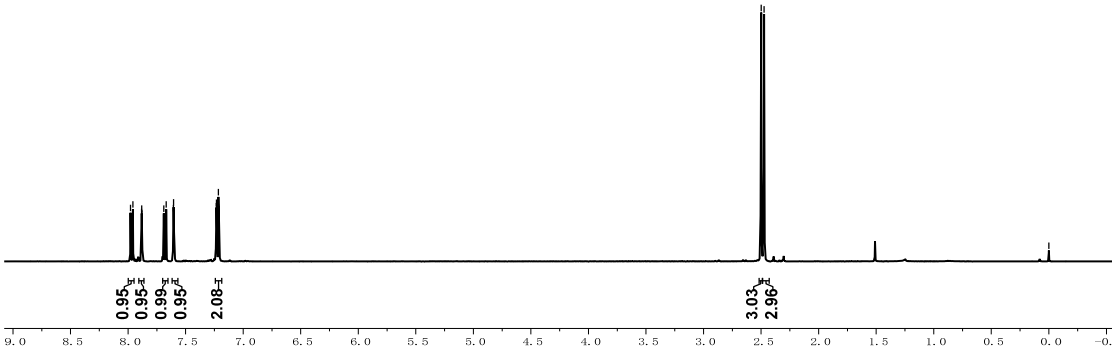
7.606
7.604
7.232
7.230
7.215
7.212
7.210
2.499
2.475
-0.000



3b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3.03
2.96
9.0
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8.0
7.5
7.0
6.5
6.0
5.5
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4.0
3.5
3.0
2.5
2.0
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1.0
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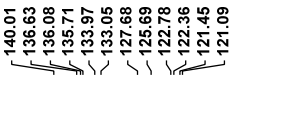
0.0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136.08
135.71
133.97
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125.69
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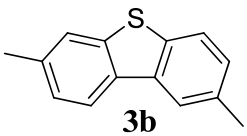
121.09
77.32
77.00
76.68
21.64
21.46



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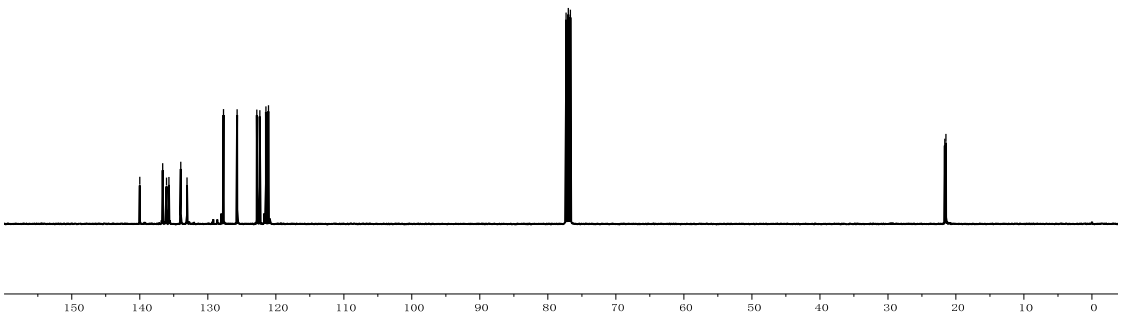
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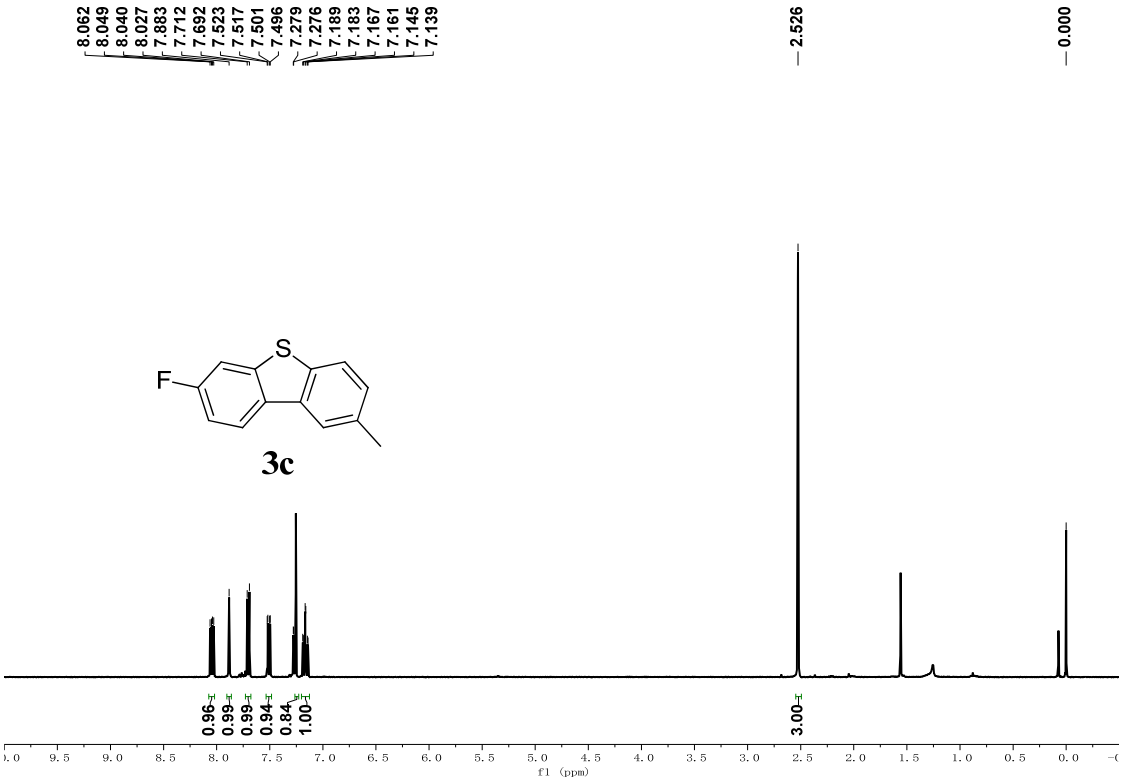
120
110
100
90
80
70
60
50
40
30
20
10
0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7.692
7.523
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7.501
7.496
7.279
7.276
7.189
7.183
7.167
7.161
7.145
7.139
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S
F
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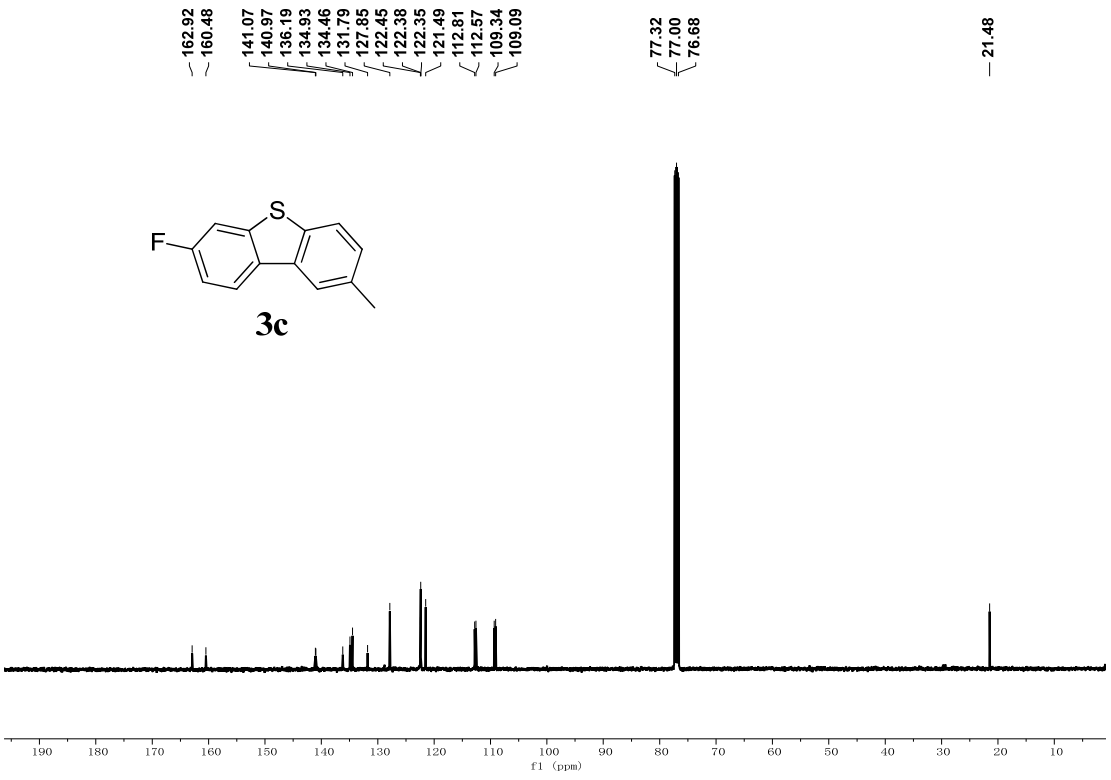
0.99
0.99
0.94
0.84
1.00
3.00
f1 (ppm)

3c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134.93
134.46
131.79
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122.45
122.38
122.35
121.49
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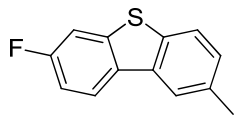
112.57
109.34
109.09
77.32
77.00
76.68
21.48
S
F
f1 (ppm)

3c


S
F

3c

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-111.0
-111.5
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-116.5
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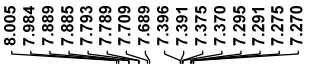
-117.5
f1 (ppm)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7.275
7.270


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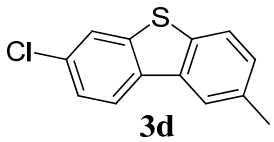
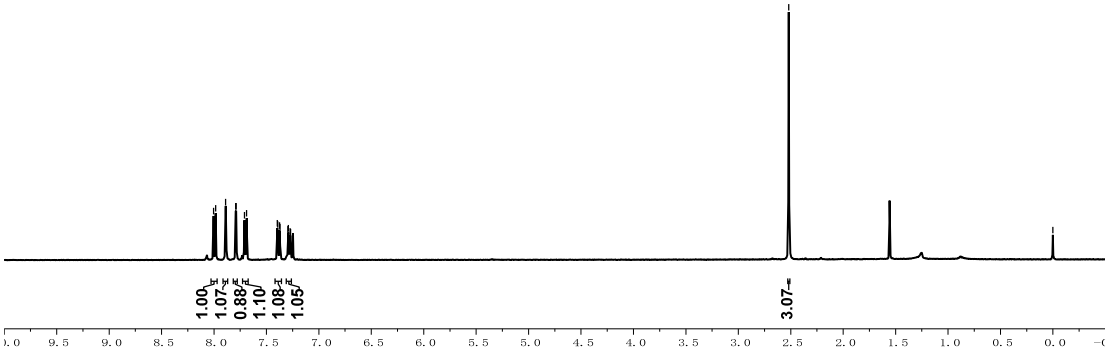
0.001


S
Cl

3d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1.05
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6.0
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4.0
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3.0
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2.0
1.5
1.0
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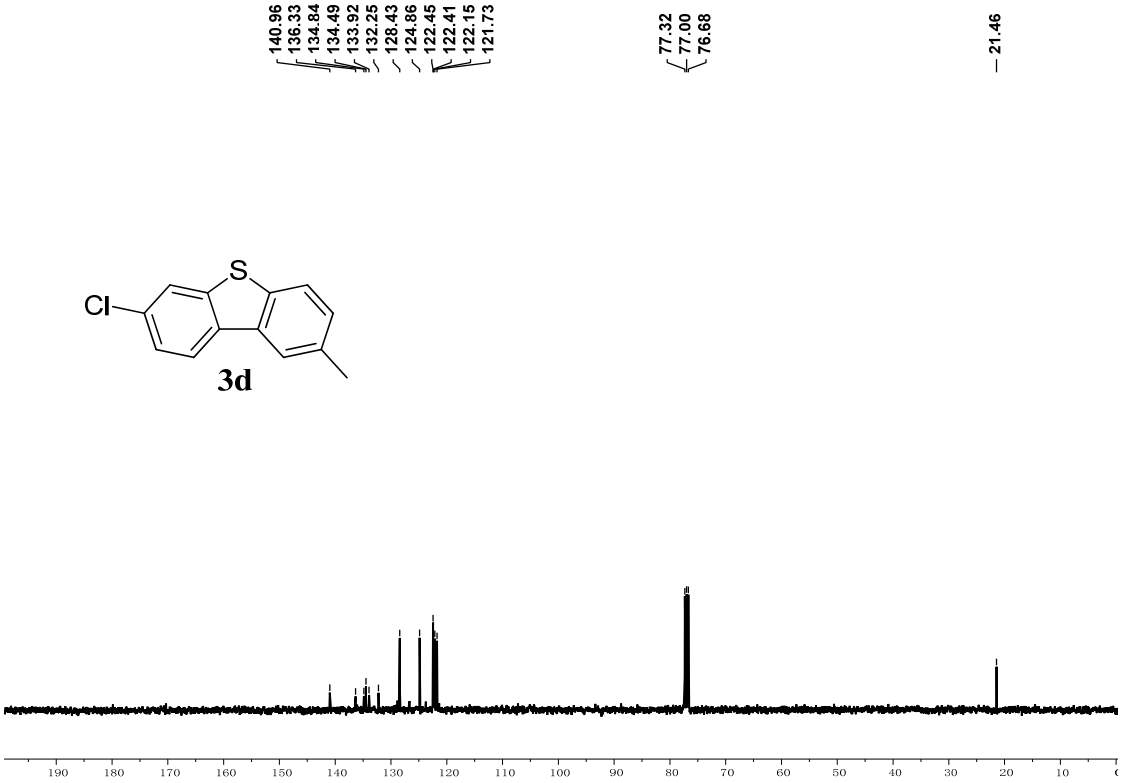
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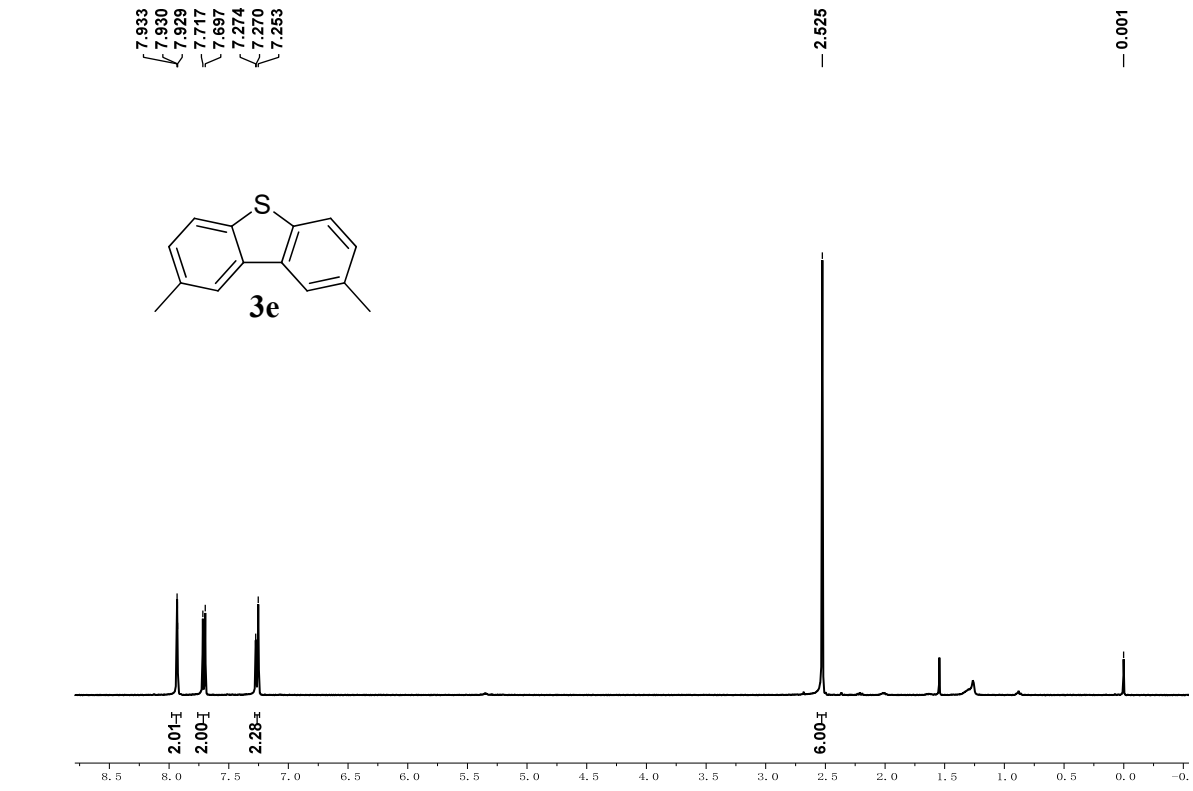
134.84
134.49
133.92
132.25
128.43
124.86
122.45
122.41
122.15
121.73
77.32
77.00
76.68
21.46
Cl
S
3d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10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7.697
7.274
7.270
7.253
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0.001
S
3e
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2.00
2.28
6.00
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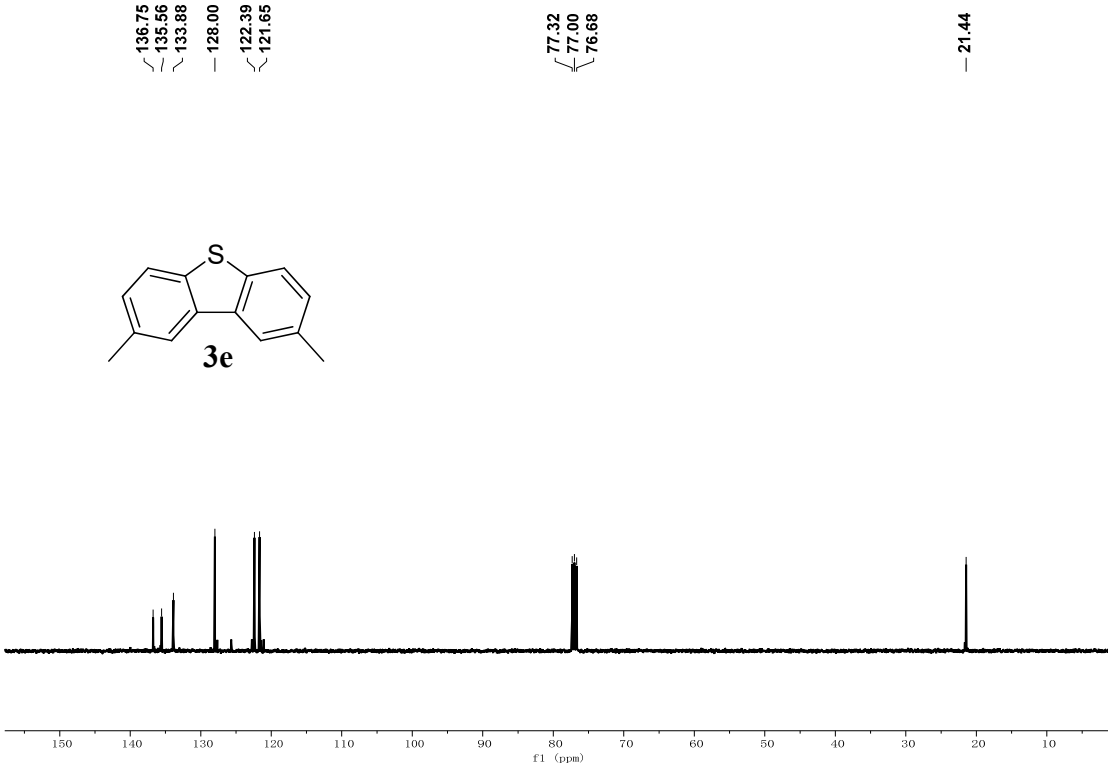
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121.65
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77.00
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S
3e
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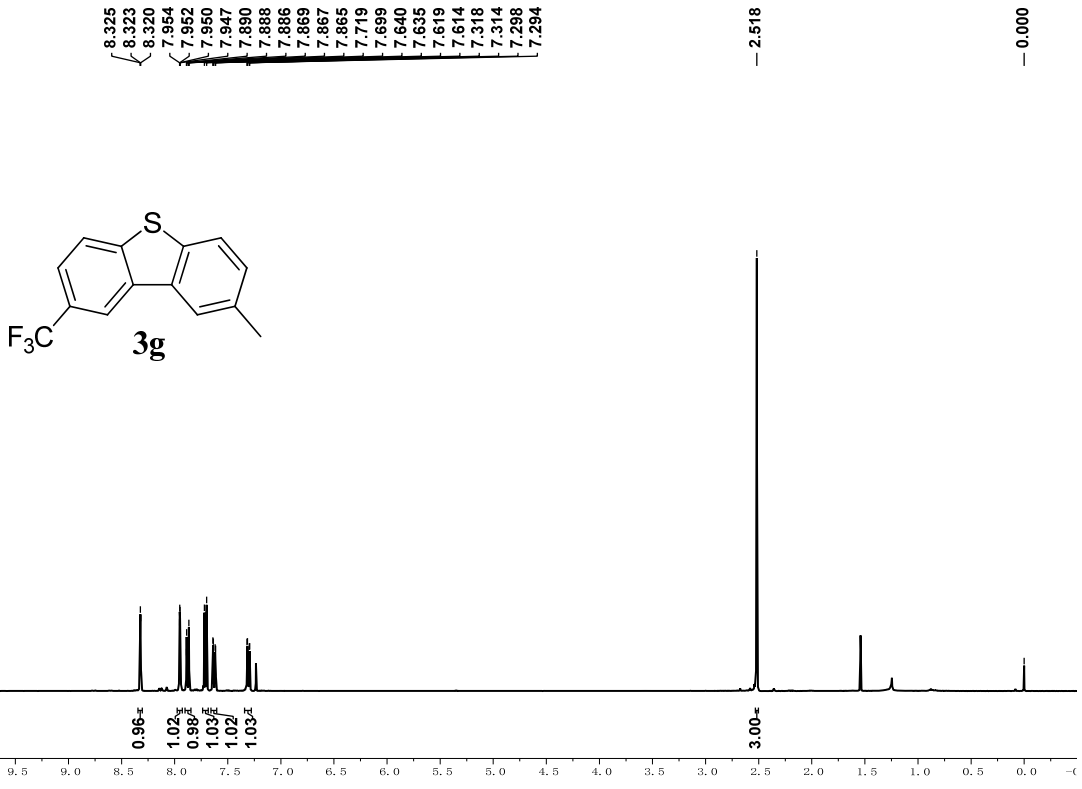
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.867
7.865
7.719
7.699
7.640
7.635
7.619
7.614
7.318
7.314
7.298
7.294
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S
F3C
3g
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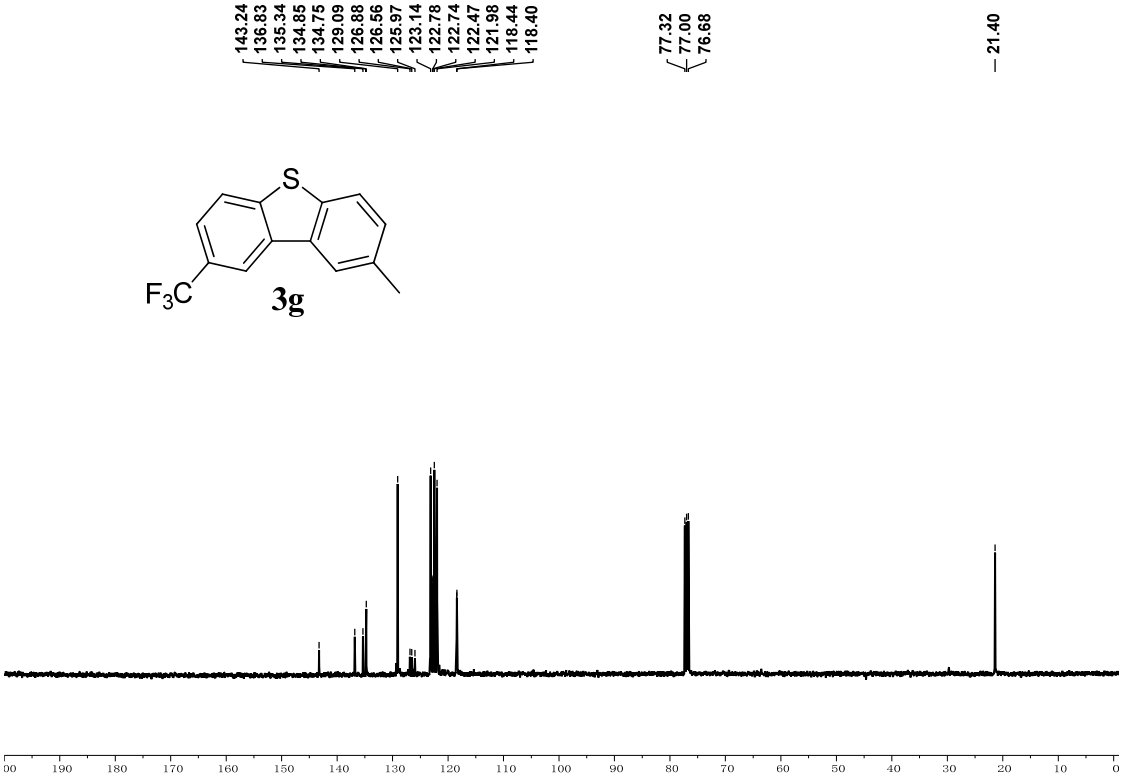
0.98
1.03
1.02
1.03
3.00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76.68
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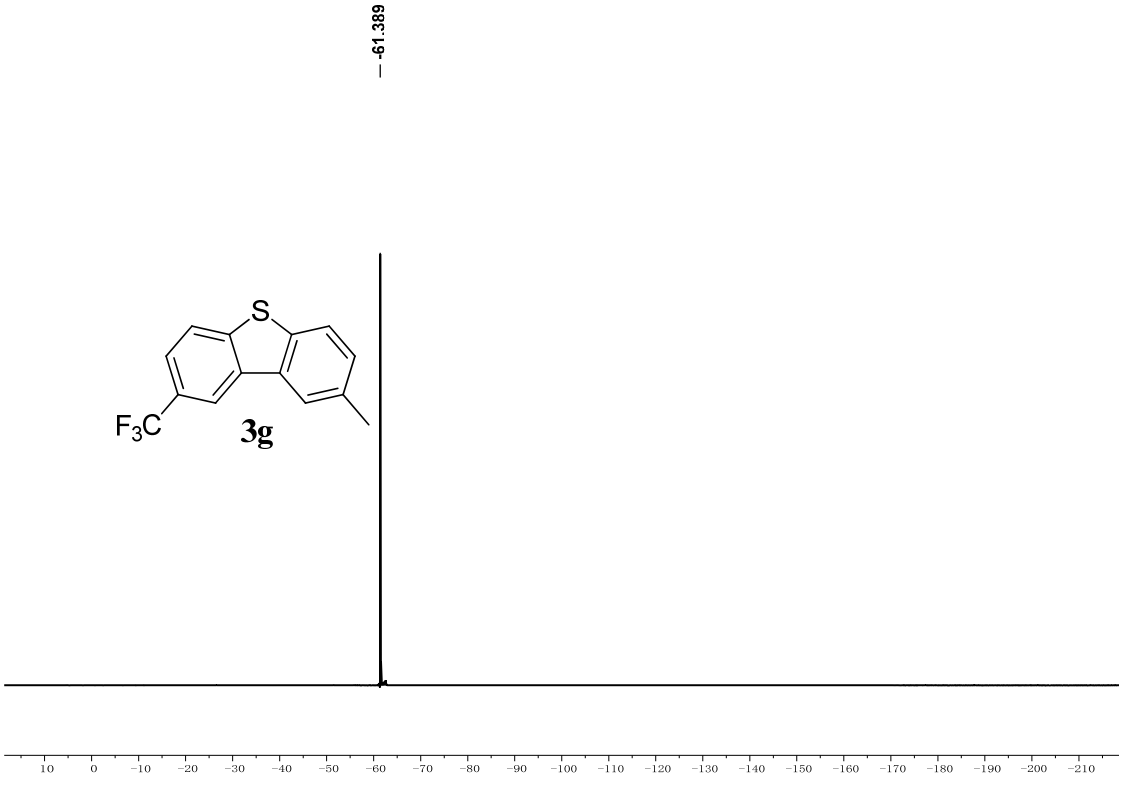
S
F3C
3g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F3C
3g


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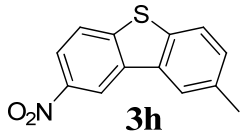
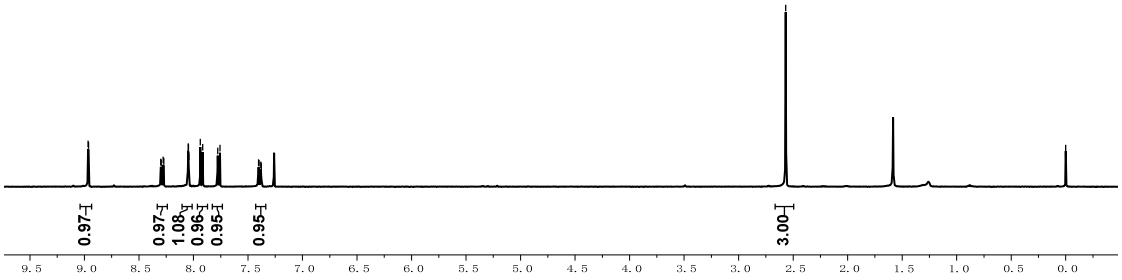

S
O2N

3h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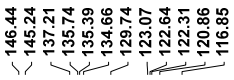
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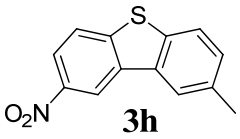
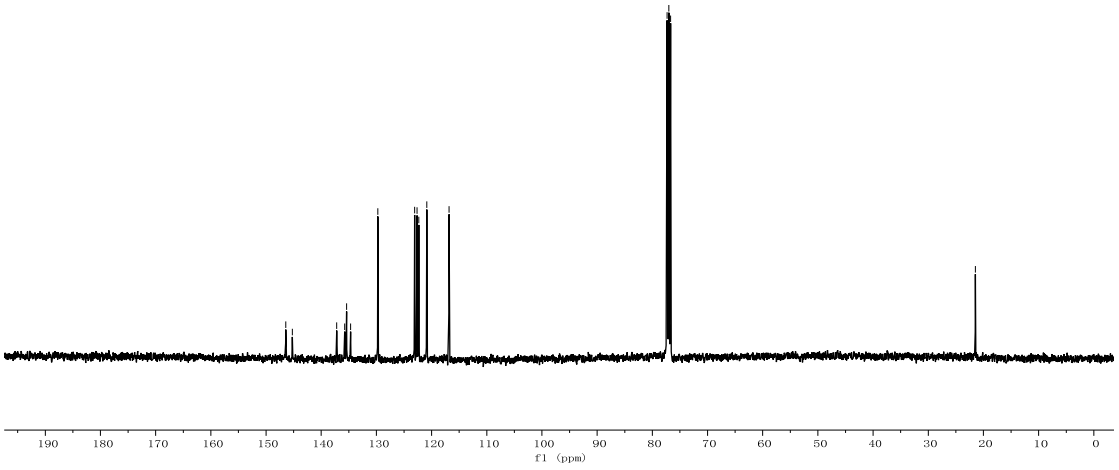

S
O2N

3h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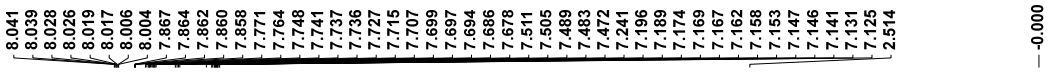
f1 (ppm)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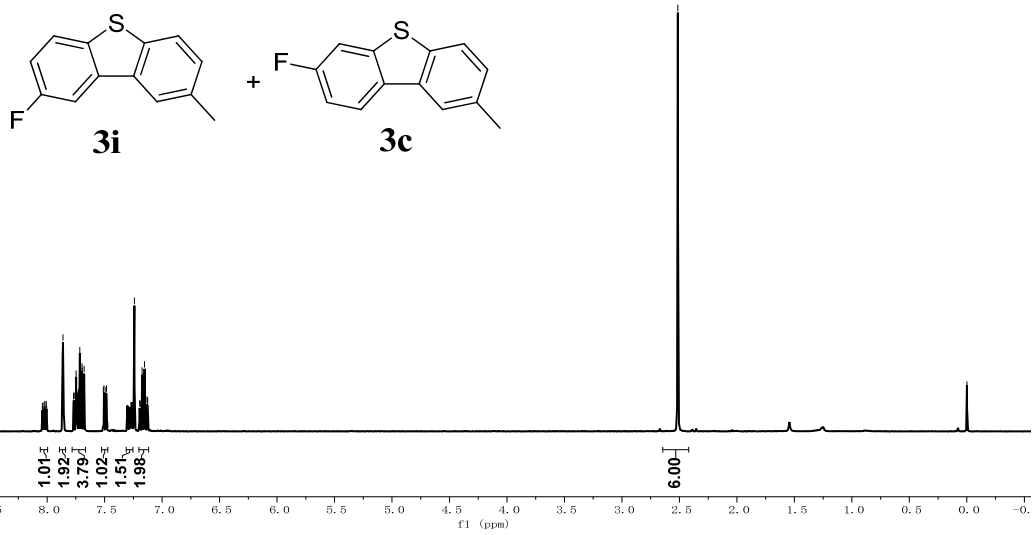
S
F
+
S
F
3i
3c
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1.98
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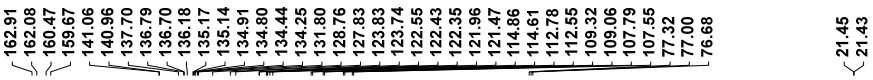
f1 (ppm)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122.55
122.43
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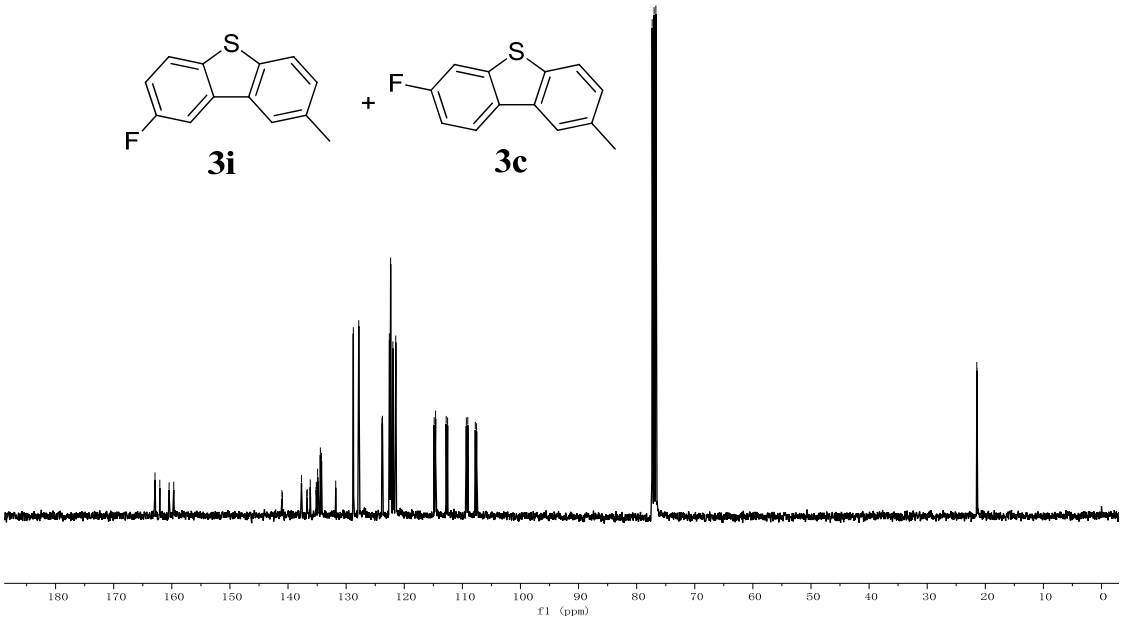
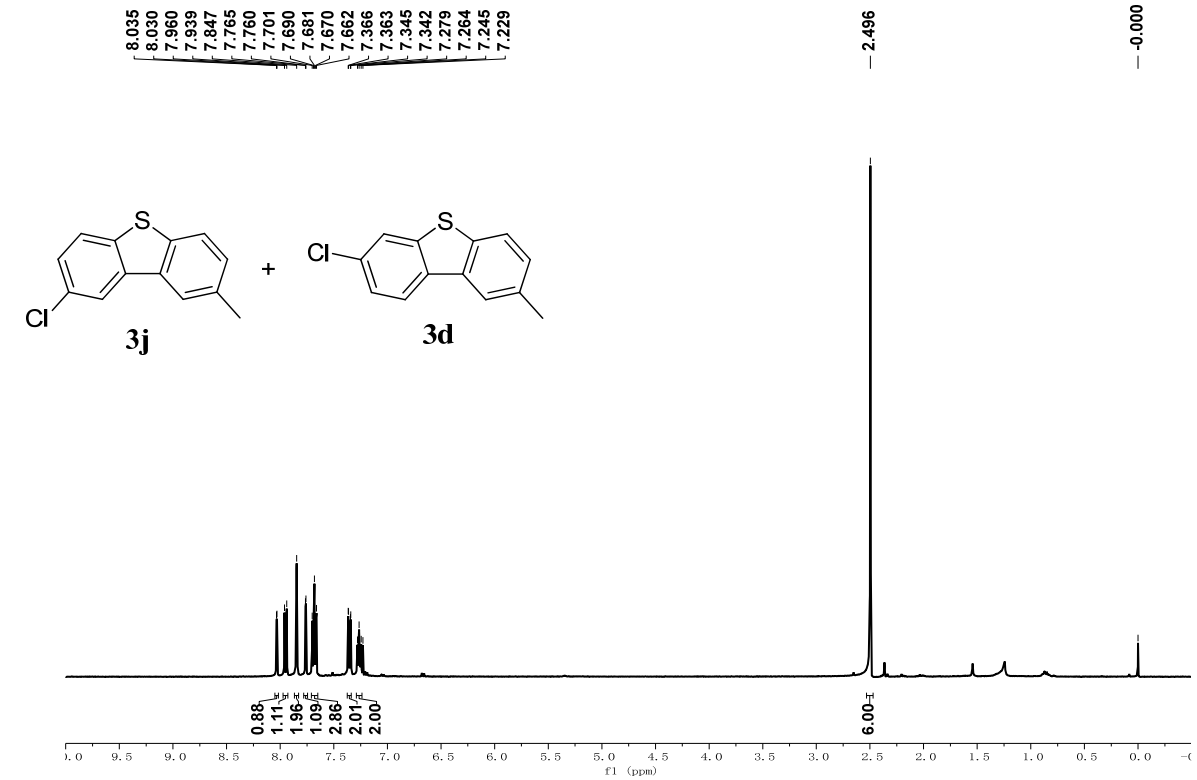

S
F
+
S
F
3i
3c
f1 (ppm)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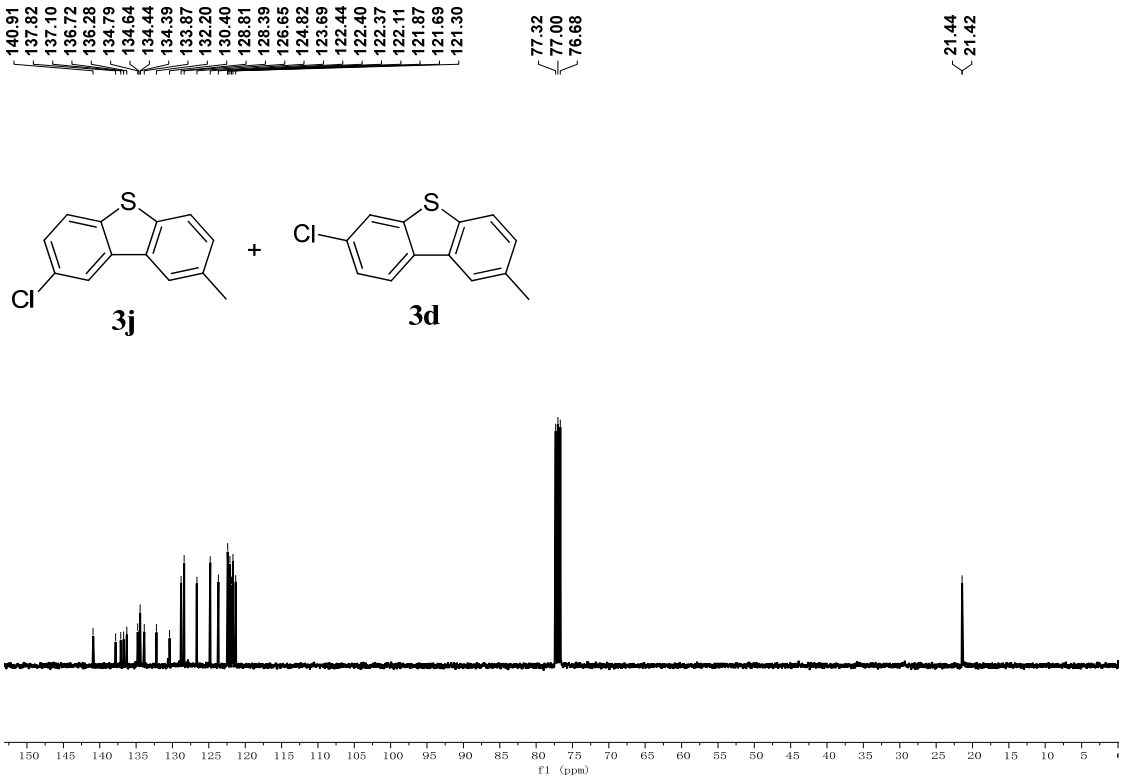
8.030
7.960
7.939
7.847
7.765
7.760
7.701
7.690
7.681
7.670
7.662
7.366
7.363
7.345
7.342
7.279
7.264
7.245
7.229
2.496
-0.000
S
Cl
+
S
Cl
3j
3d
0.88
1.11
1.96
1.09
2.86
2.01
2.00
6.00
f1 (ppm)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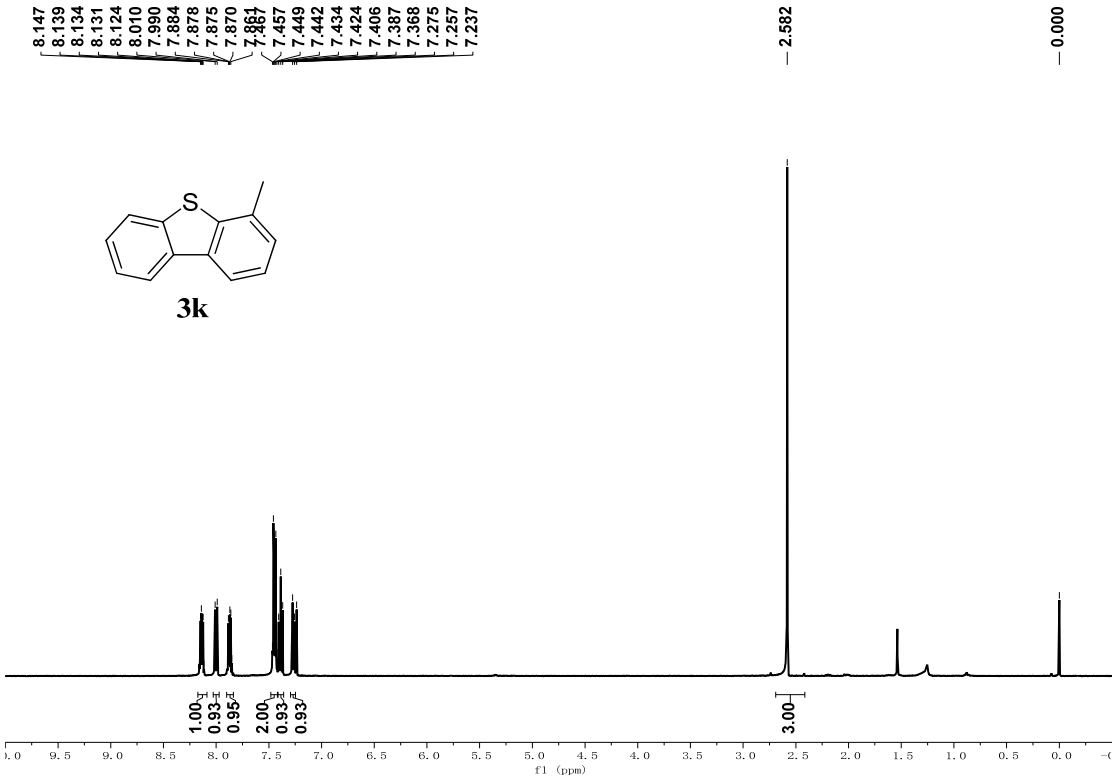
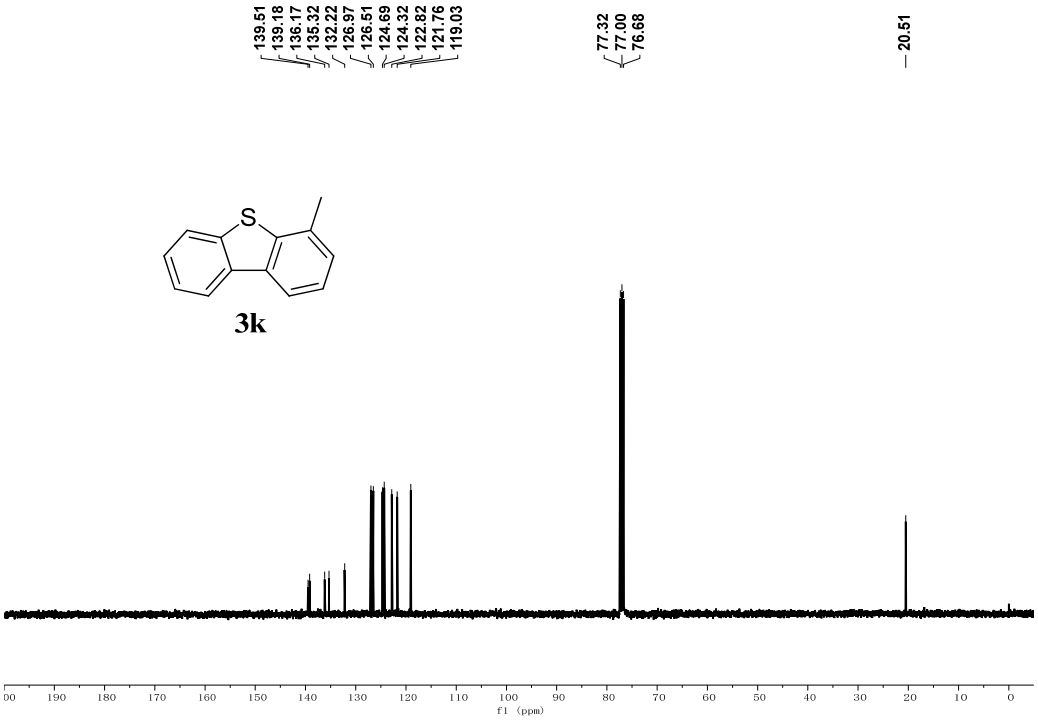
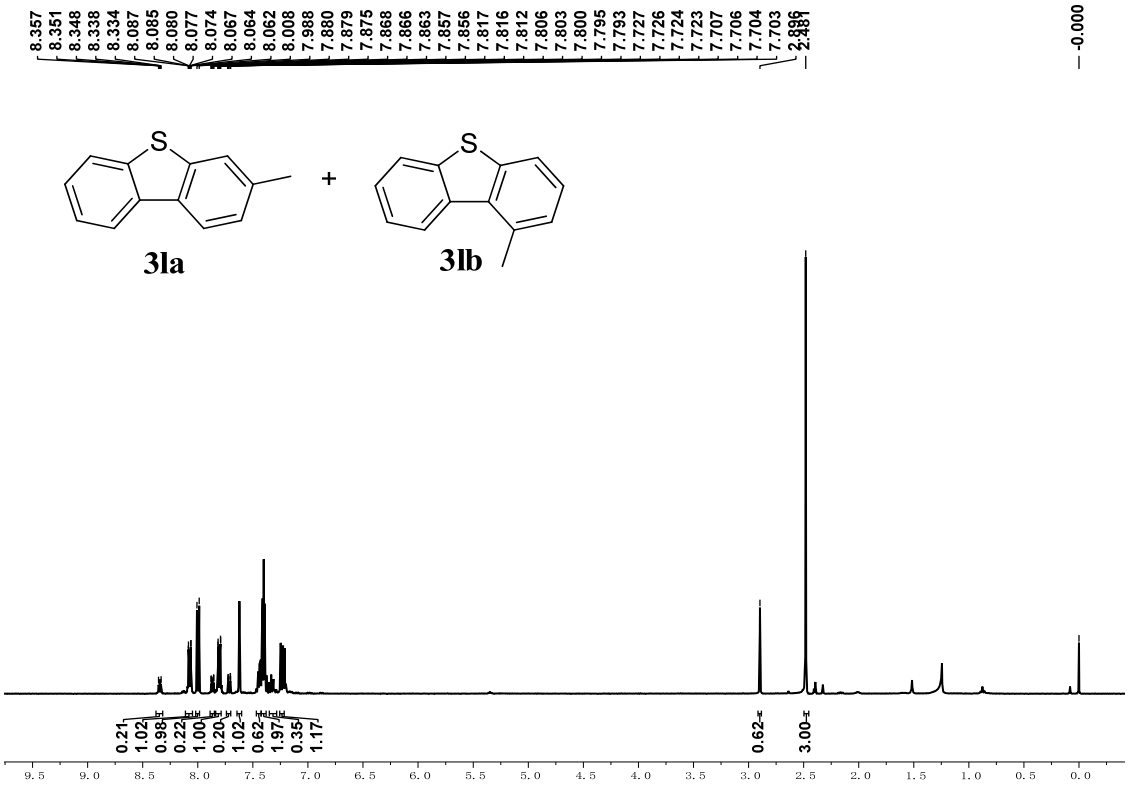
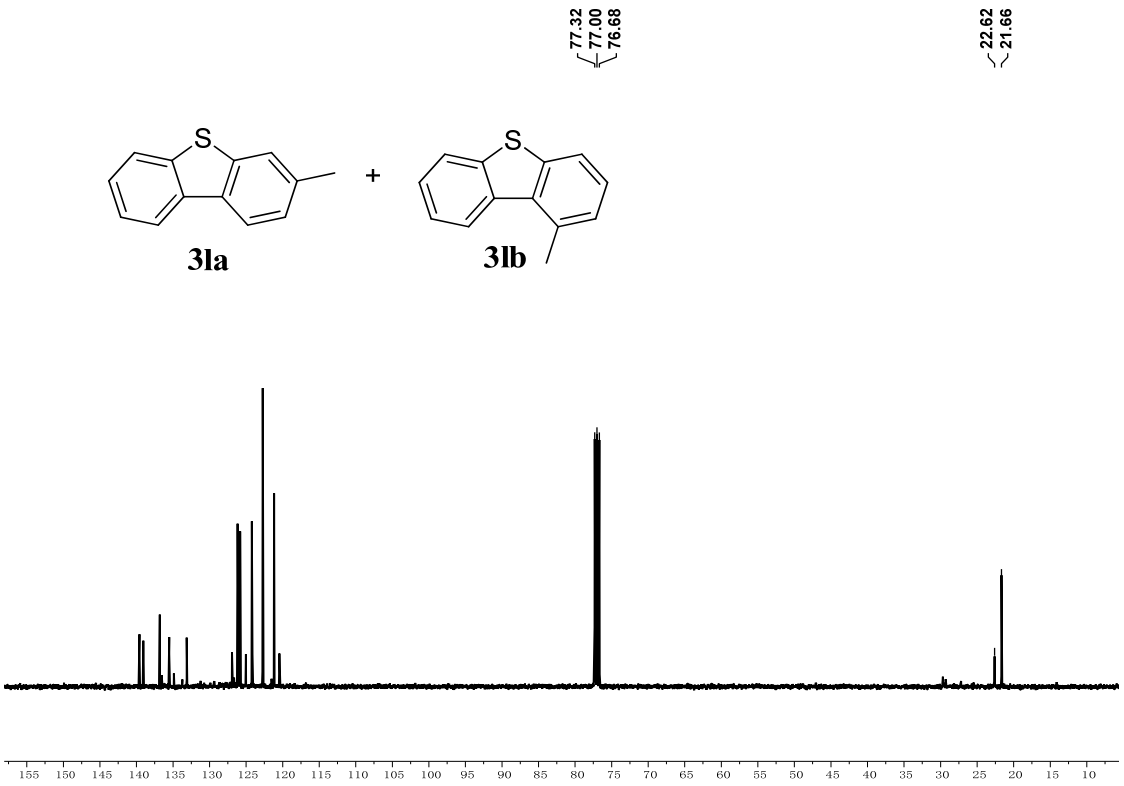
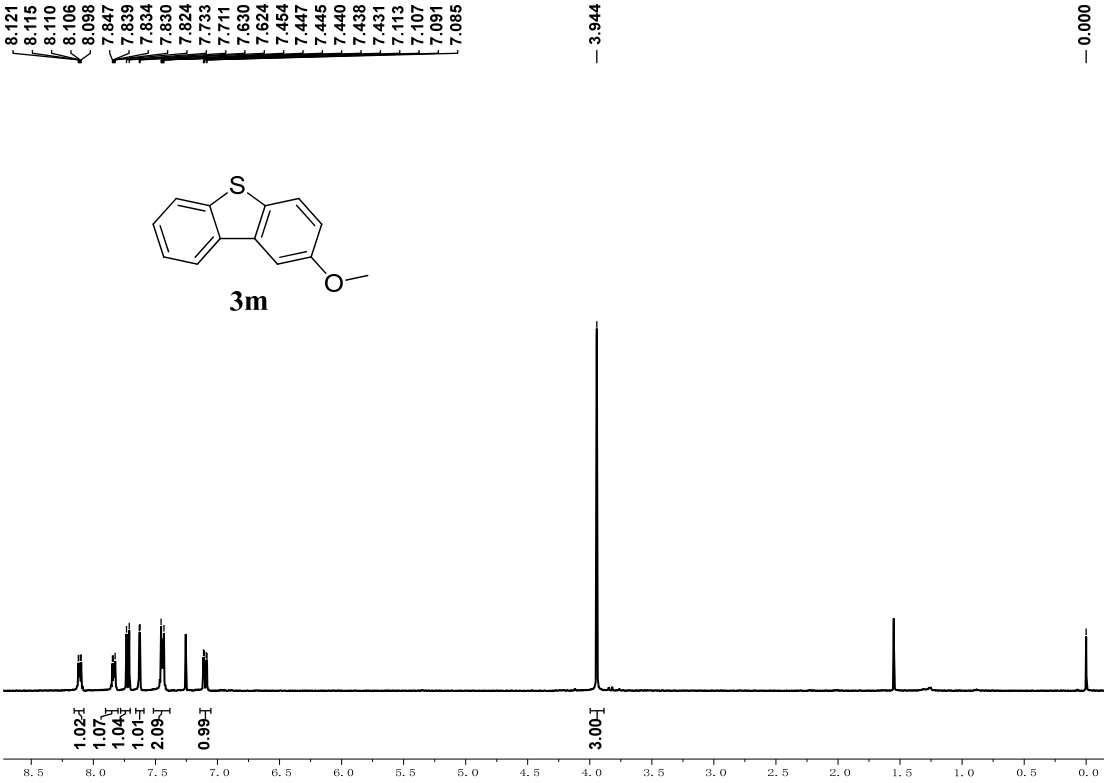
137.82
137.10
136.72
136.28
134.79
134.64
134.44
134.39
133.87
132.20
130.40
128.81
128.39
126.65
124.82
123.69
122.44
122.40
122.37
122.11
121.87
121.69
121.30
77.32
77.00
76.68
21.44
21.42
S
Cl
+
S
Cl
3j
3d
f1 (ppm)

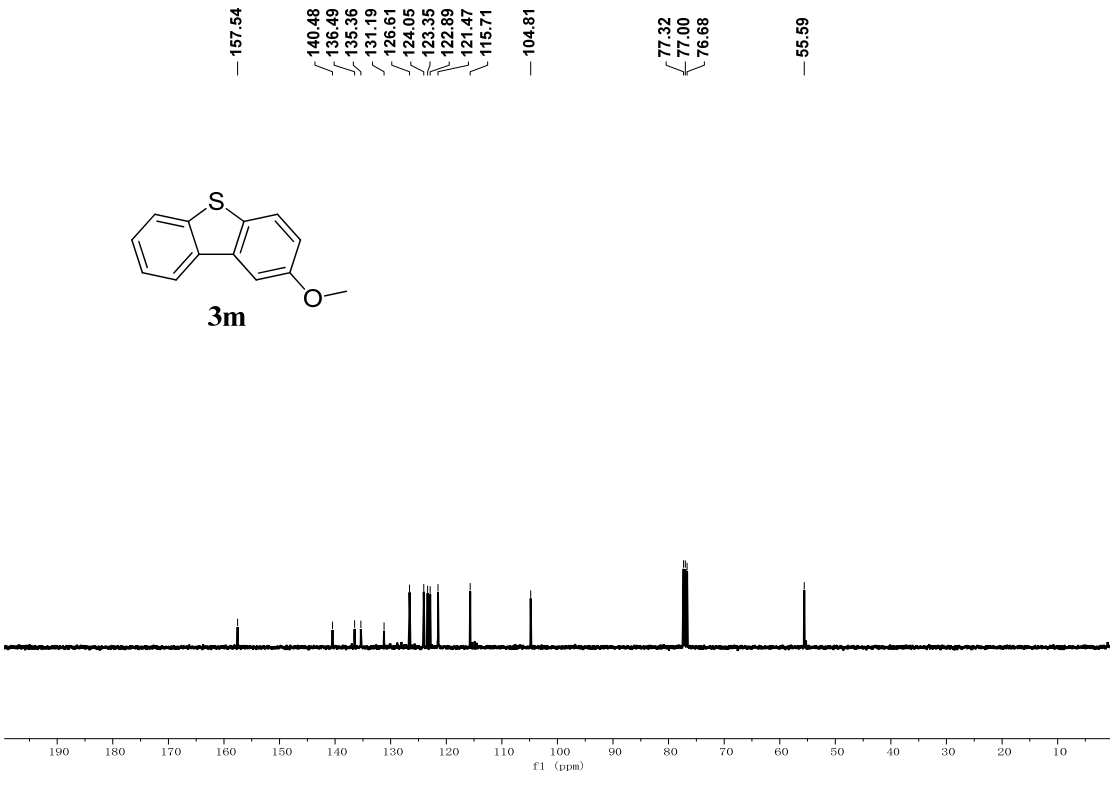

8.147
8.139
8.134
8.131
8.124
8.010
7.990
7.884
7.878
7.875
7.870
7.861
7.457
7.449
7.442
7.434
7.424
7.406
7.387
7.368
7.275
7.257
7.237
2.582
0.000
S
3k
1.00
0.93
0.95
2.00
0.93
0.93
3.00
f1 (ppm)

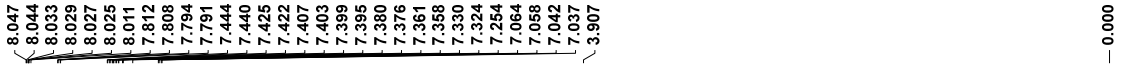

139.51
139.18
136.17
135.32
132.22
126.97
126.51
124.69
124.32
122.82
121.76
119.03
77.32
77.00
76.68
20.51
S
3k
f1 (ppm)

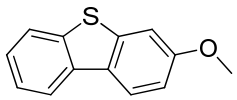

8.357
8.351
8.348
8.338
8.334
8.087
8.085
8.080
8.077
8.074
8.067
8.064
8.062
8.008
7.988
7.880
7.879
7.875
7.868
7.866
7.863
7.857
7.856
7.817
7.816
7.812
7.806
7.803
7.800
7.795
7.793
7.727
7.726
7.724
7.723
7.707
7.706
7.704
7.703
2.886
2.481
-0.000
3la
3lb
0.21
1.02
0.98
0.22
1.00
0.20
1.02
0.62
1.97
0.35
1.17
0.62
3.00


77.32
77.00
76.68
22.62
21.66
3la
3lb

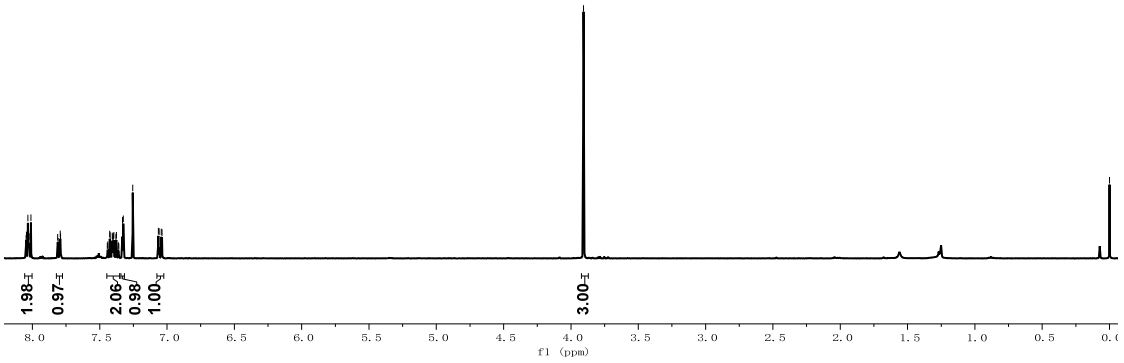

8.121
8.115
8.110
8.106
8.098
7.847
7.839
7.834
7.830
7.824
7.733
7.711
7.630
7.624
7.454
7.447
7.445
7.440
7.438
7.431
7.113
7.107
7.091
7.085
3.944
0.000
S
O
3m
1.02
1.07
1.04
1.01
2.09
0.99
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

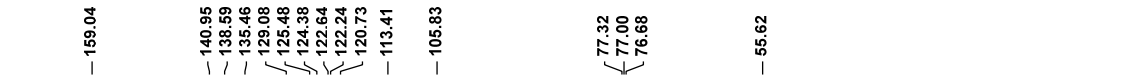

157.54
140.48
136.49
135.36
131.19
126.61
124.05
123.35
122.89
121.47
115.71
104.81
77.32
77.00
76.68
55.59
S
O
3m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

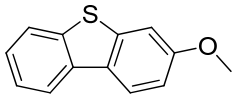

8.047
8.044
8.033
8.029
8.027
8.025
8.011
7.812
7.808
7.794
7.791
7.444
7.440
7.425
7.422
7.407
7.403
7.399
7.395
7.380
7.376
7.361
7.358
7.330
7.324
7.254
7.064
7.058
7.042
7.037
3.907
0.000



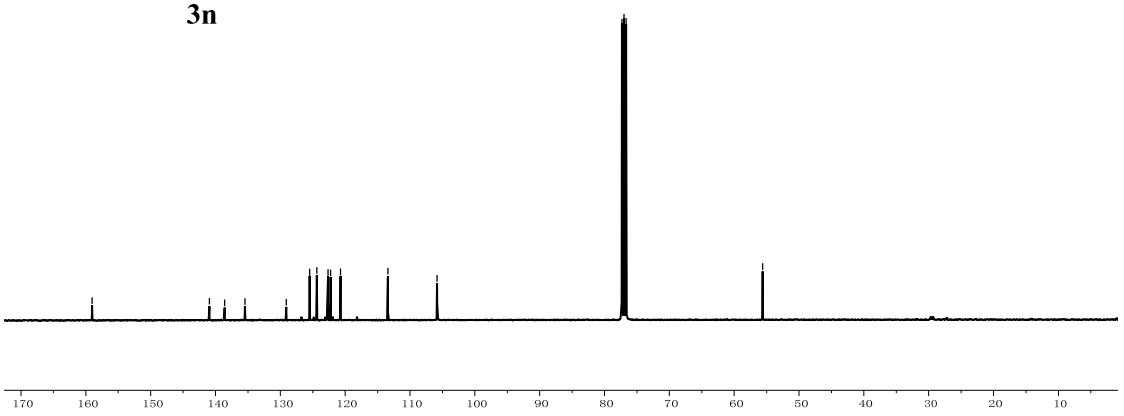
3n


1.98
0.97
2.06
0.98
1.00
3.00
f1 (ppm)


159.04
140.95
138.59
135.46
129.08
125.48
124.38
122.64
122.24
120.73
113.41
105.83
77.32
77.00
76.68
55.62



3n




8.068
8.065
8.061
8.051
8.045
7.854
7.847
7.839
7.834
7.824
7.820
7.817
7.797
7.791
7.774
7.768
7.765
7.752
7.743
7.731
7.484
7.480
7.466
7.462
7.456
7.450
7.443
7.438
7.433
7.420
7.416
7.233
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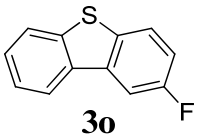
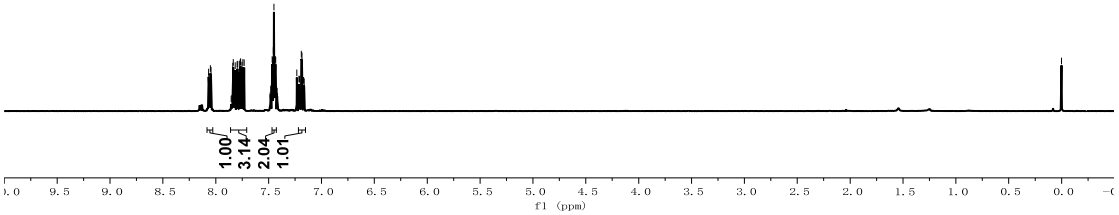
7.207
7.191
7.185
7.170
7.163
0.000


S
F

3o


1.00
3.14
2.04
1.01
f1 (ppm)


162.11
159.70
140.67
136.87
136.78
134.97
134.93
134.40
134.38
127.19
126.65
124.39
124.30
123.81
123.73
122.92
122.75
121.79
121.52
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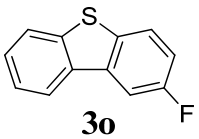
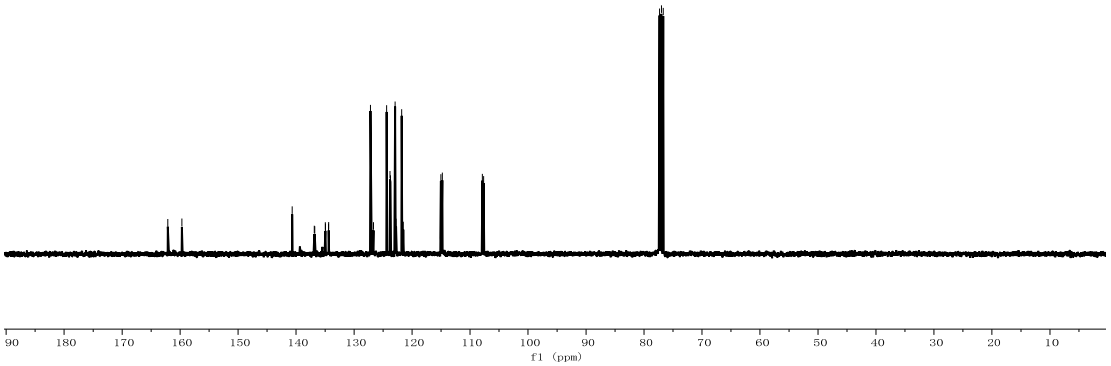
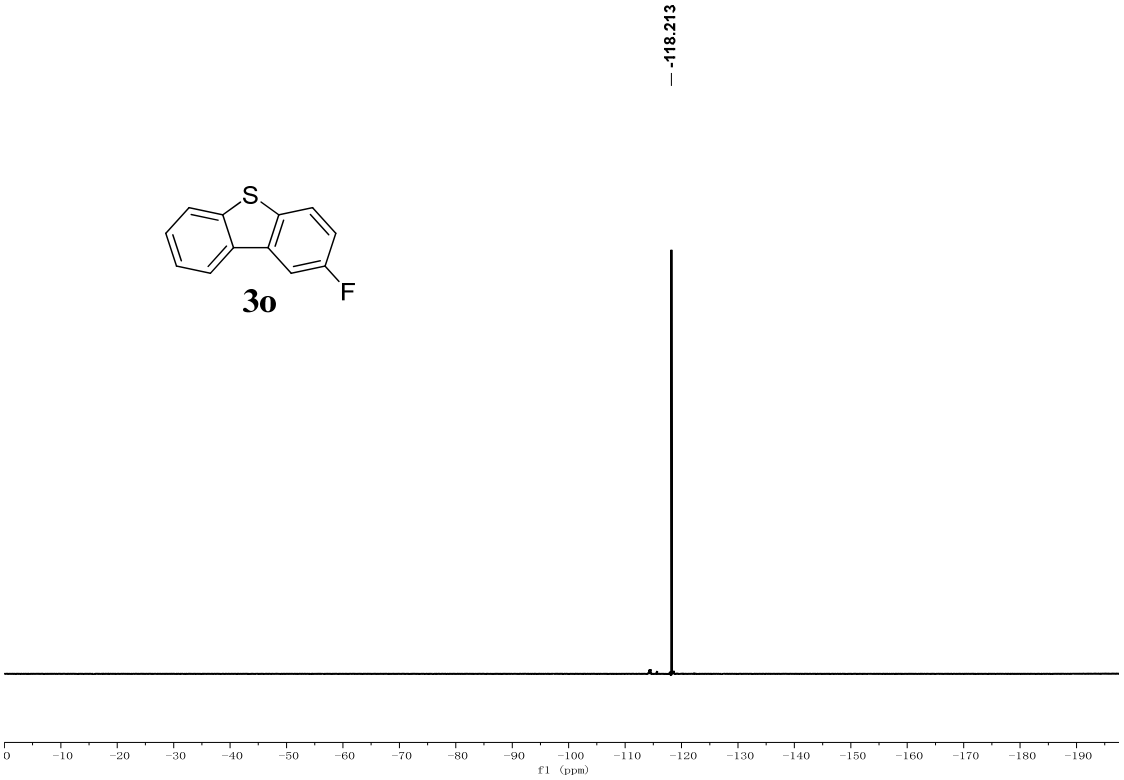
114.79
107.89
107.66
77.32
77.00
76.68

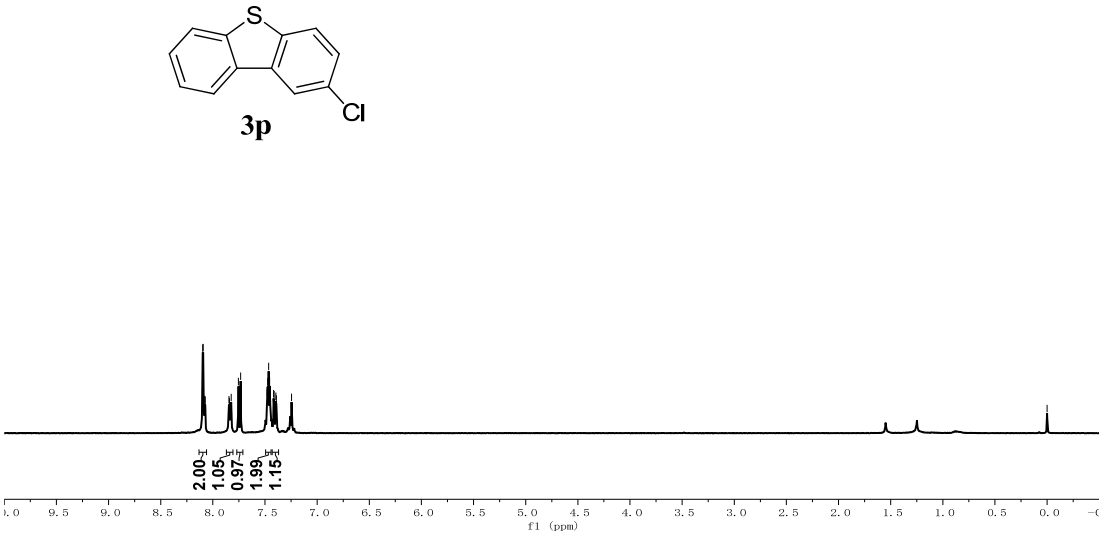

S
F

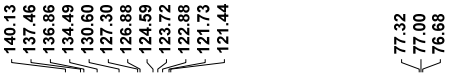
3o

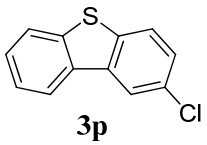

f1 (ppm)


-118.213
S
F
3o
f1 (ppm)

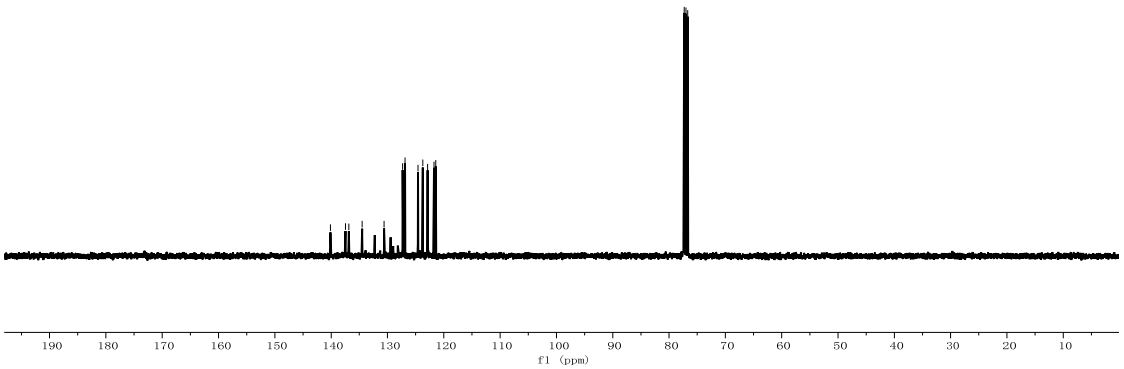

8.097
8.093
8.079
8.073
7.846
7.840
7.832
7.824
7.754
7.733
7.479
7.473
7.465
7.455
7.417
7.412
7.396
7.391
7.245
0.000

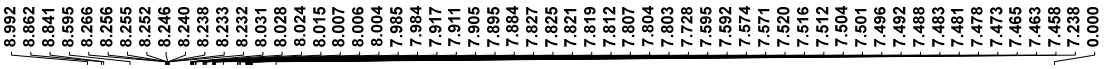

S
Cl
3p
2.00
1.05
0.97
1.99
1.15
f1 (ppm)


140.13
137.46
136.86
134.49
130.60
127.30
126.88
124.59
123.72
122.88
121.73
121.44
77.32
77.00
76.68


S
Cl

3p


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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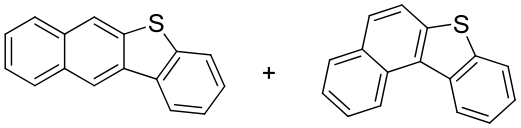
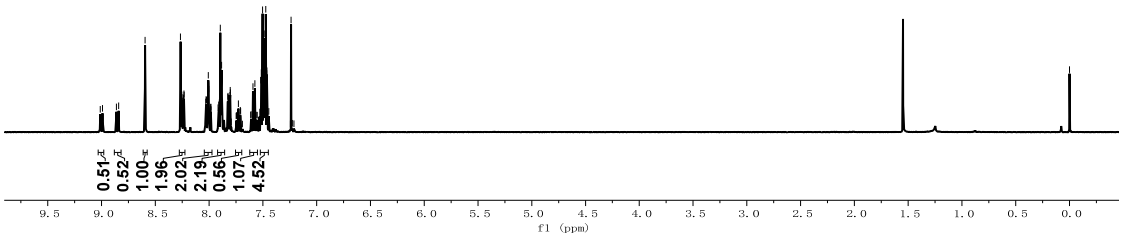
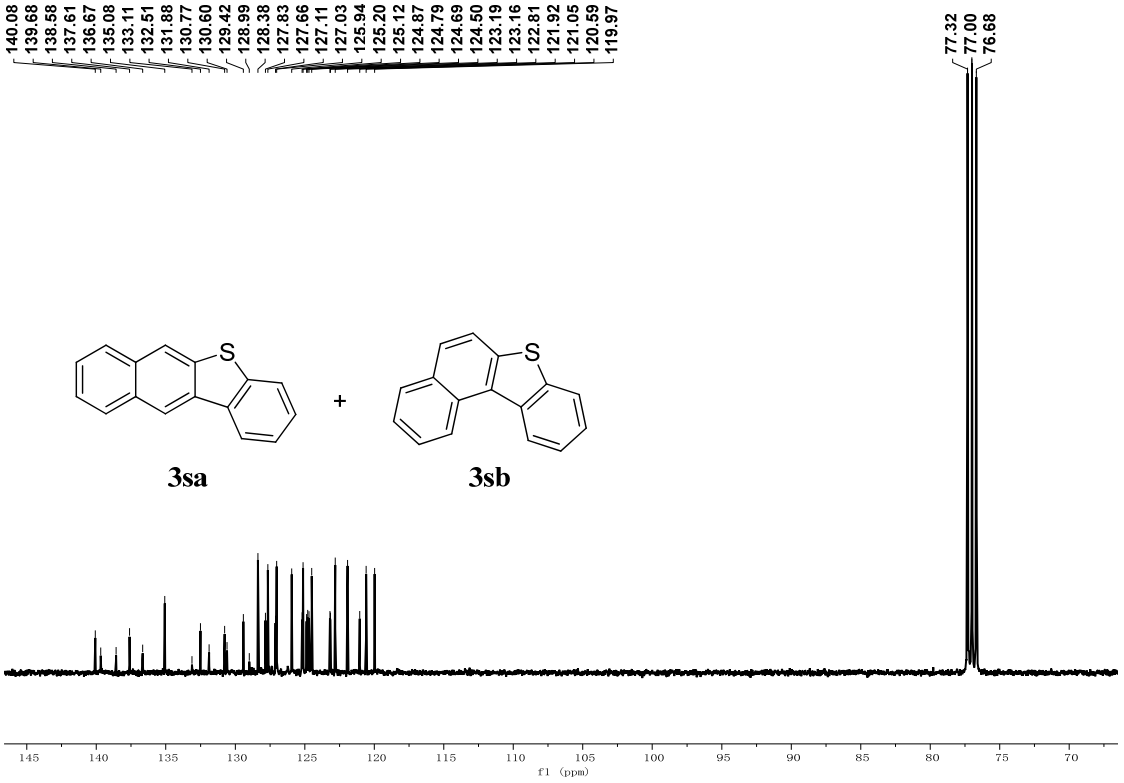
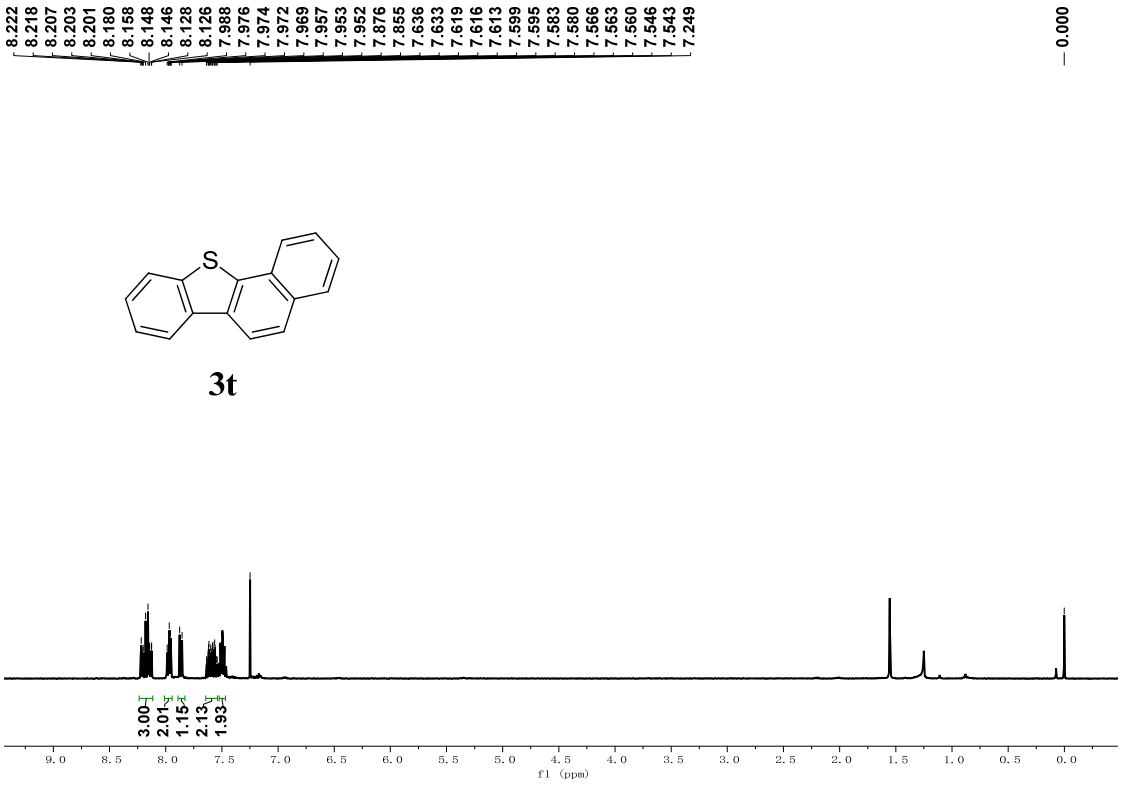
8.862
8.841
8.595
8.266
8.256
8.255
8.252
8.246
8.240
8.238
8.233
8.232
8.031
8.028
8.024
8.015
8.007
8.006
8.004
7.985
7.984
7.917
7.911
7.905
7.895
7.884
7.827
7.825
7.821
7.819
7.812
7.807
7.804
7.803
7.728
7.595
7.592
7.574
7.571
7.520
7.516
7.512
7.504
7.501
7.496
7.492
7.488
7.483
7.481
7.478
7.473
7.465
7.463
7.458
7.238
0.000


S
+
S

3sa **3sb**


0.51
0.52
1.00
1.96
2.02
2.19
0.56
1.07
4.52
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)


140.08
139.68
138.58
137.61
136.67
135.08
133.11
132.51
131.88
130.77
130.60
129.42
128.99
128.38
127.83
127.66
127.11
127.03
125.94
125.20
125.12
124.87
124.79
124.69
124.50
123.19
123.16
122.81
121.92
121.05
120.59
119.97
77.32
77.00
76.68
S
+
S
3sa
3sb
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
f1 (ppm)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8.218
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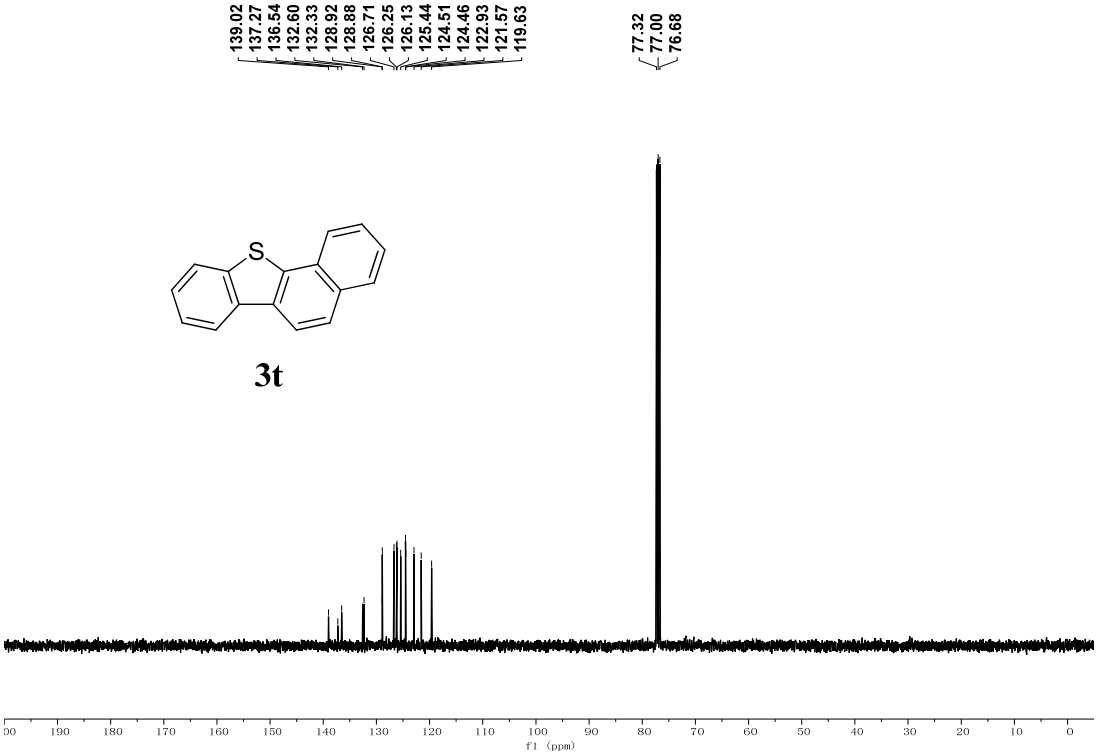
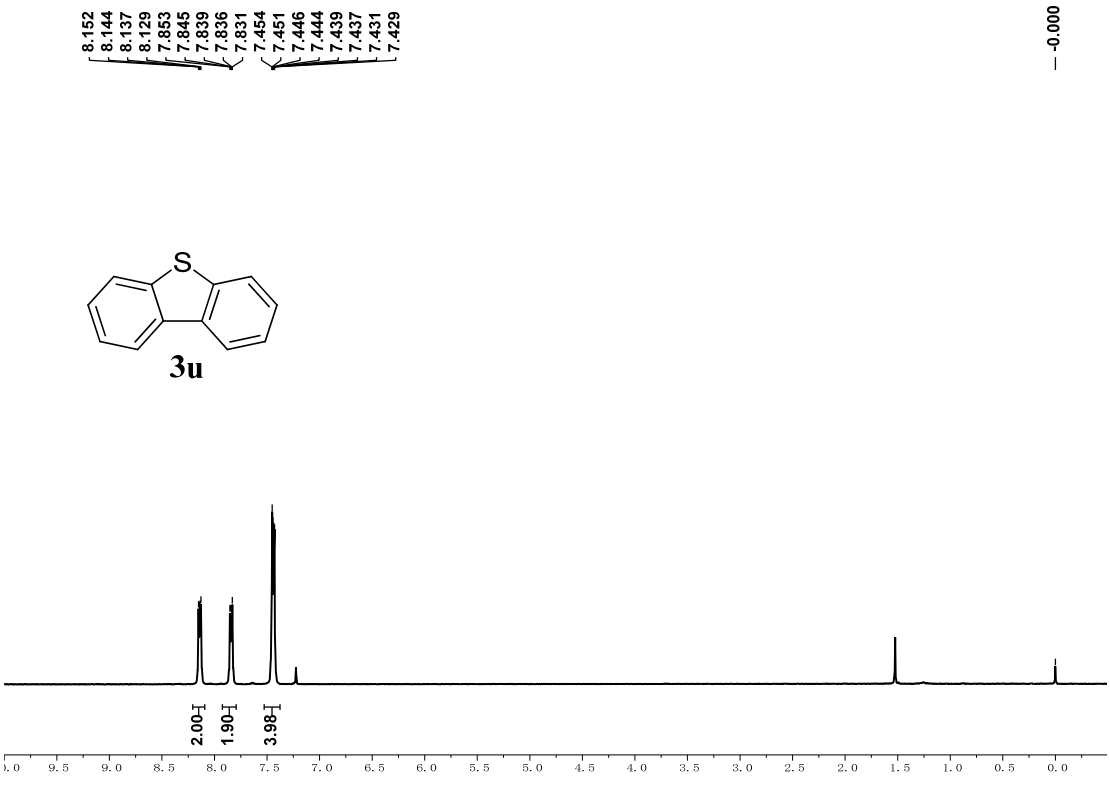
8.203
8.201
8.180
8.158
8.148
8.146
8.128
8.126
7.988
7.976
7.974
7.972
7.969
7.957
7.953
7.952
7.876
7.855
7.636
7.633
7.619
7.616
7.613
7.599
7.595
7.583
7.580
7.566
7.563
7.560
7.546
7.543
7.249
0.000
S
3t
3.00
2.01
1.15
2.13
1.93
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


139.02
137.27
136.54
132.60
132.33
128.92
128.88
126.71
126.25
126.13
125.44
124.51
124.46
122.93
121.57
119.63
77.32
77.00
76.68
S
f1 (ppm)

3t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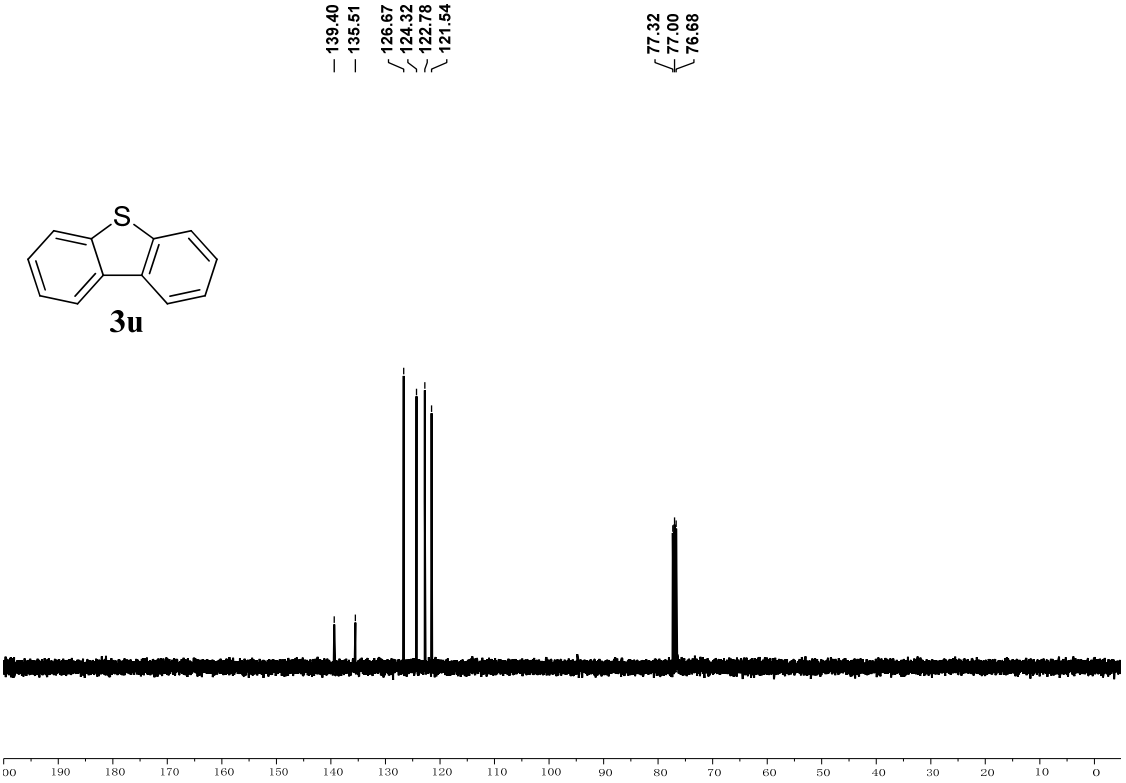
7.853
7.845
7.839
7.836
7.831
7.454
7.451
7.446
7.444
7.439
7.437
7.431
7.429
-0.000
S
2.00
1.90
3.98

3u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135.51
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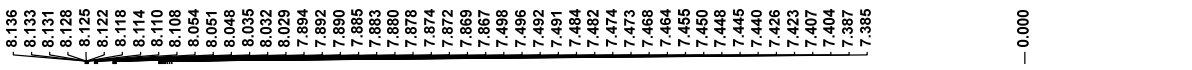
124.32
122.78
121.54
77.32
77.00
76.68
S

3u


8.136
8.133
8.131
8.128
8.125
8.122
8.118
8.114
8.110
8.108
8.054
8.051
8.048
8.035
8.032
8.029
7.894
7.892
7.890
7.885
7.883
7.880
7.878
7.874
7.872
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7.867
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7.496
7.492
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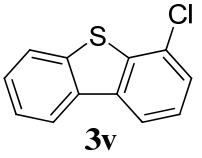
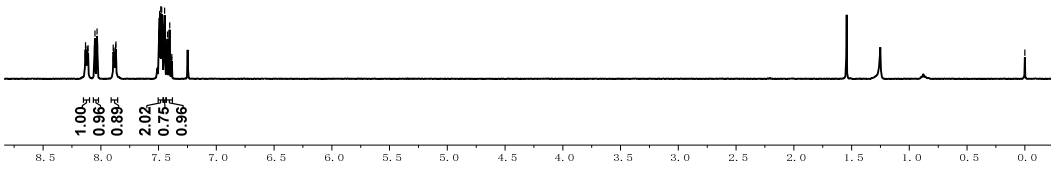
7.484
7.482
7.474
7.473
7.468
7.464
7.455
7.450
7.448
7.445
7.440
7.426
7.423
7.407
7.404
7.387
7.385
0.000


Cl
S

3v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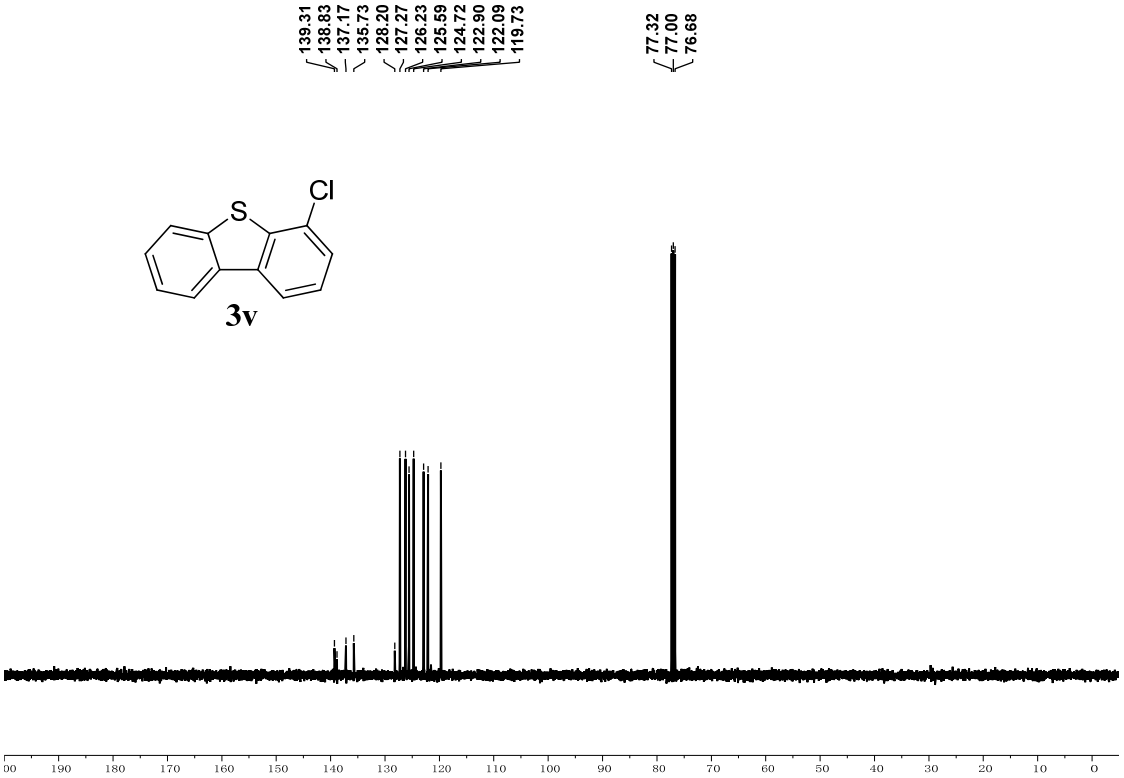
0.89
2.02
0.75
0.96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137.17
135.73
128.20
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125.59
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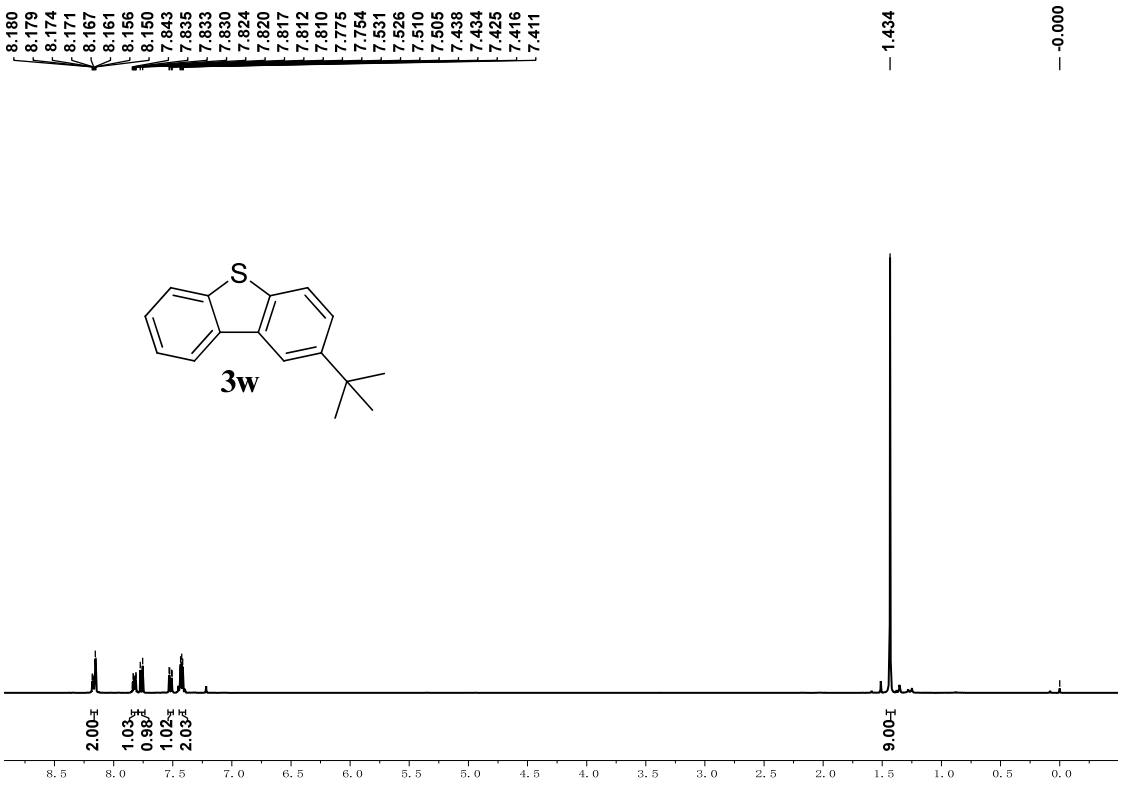
122.90
122.09
119.73
77.32
77.00
76.68
Cl
S
3v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8.161
8.156
8.150
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7.835
7.833
7.830
7.824
7.820
7.817
7.812
7.810
7.775
7.754
7.531
7.526
7.510
7.505
7.438
7.434
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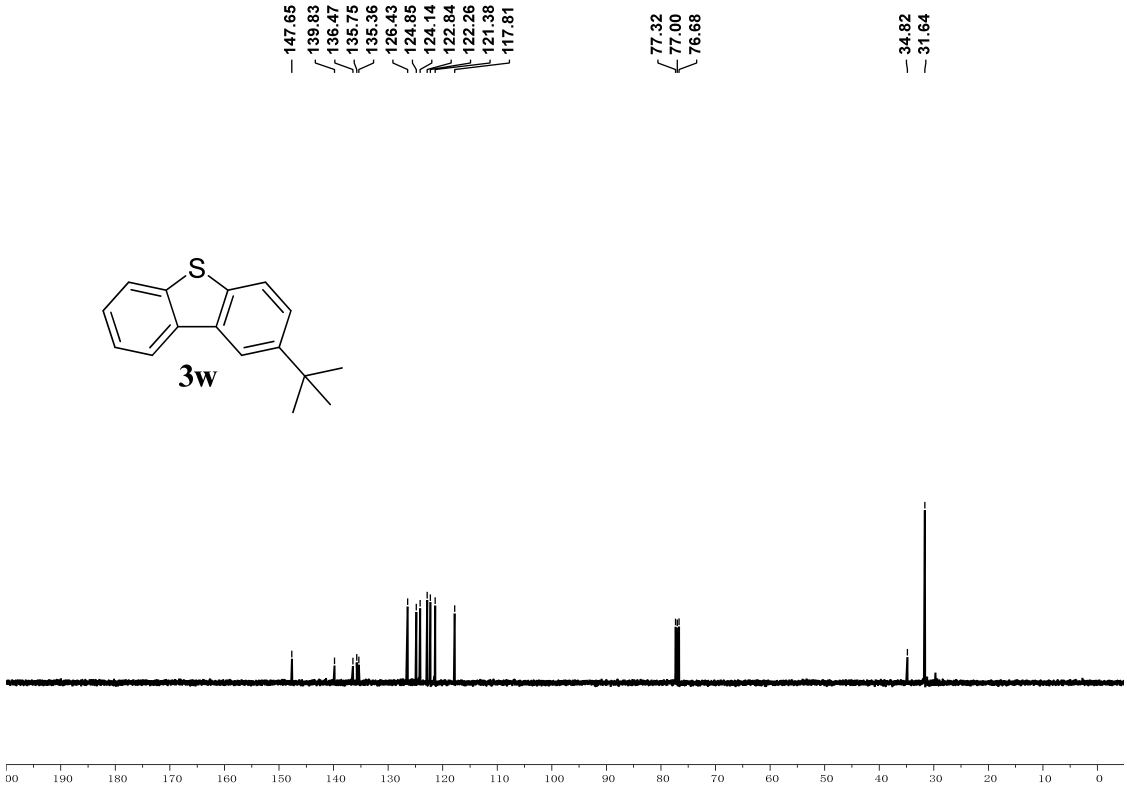
1.434
0.000
S
3w
2.00
1.03
0.98
1.02
2.03
9.00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124.14
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122.26
121.38
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77.00
76.68
34.82
31.64
S
3w
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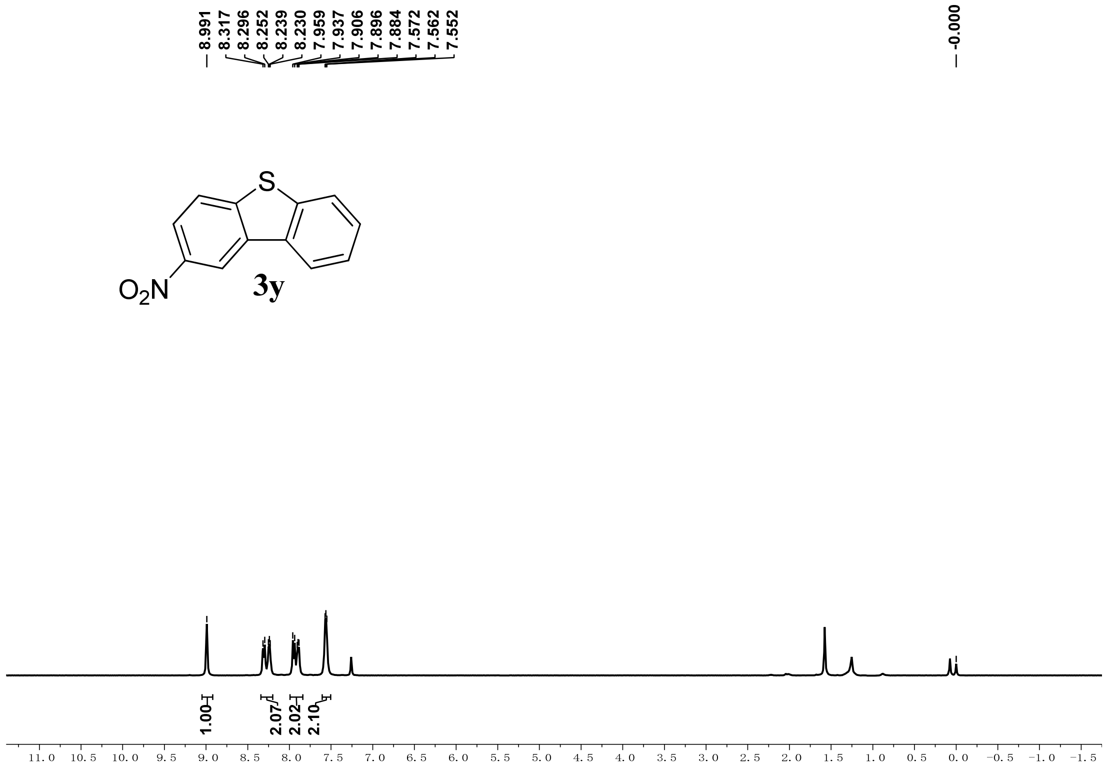
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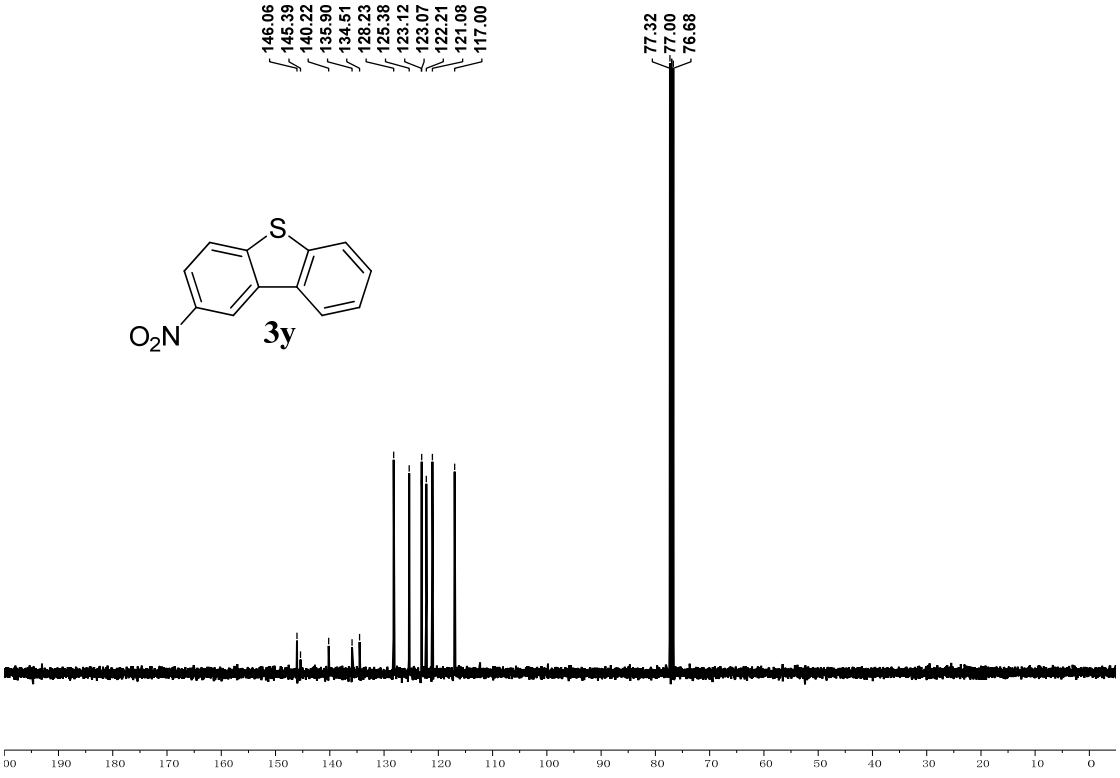
8.252
8.239
8.230
7.959
7.937
7.906
7.896
7.884
7.572
7.562
7.552
-0.000
S
O2N
3y
1.00
2.07
2.02
2.10
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5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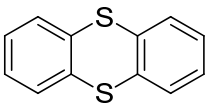
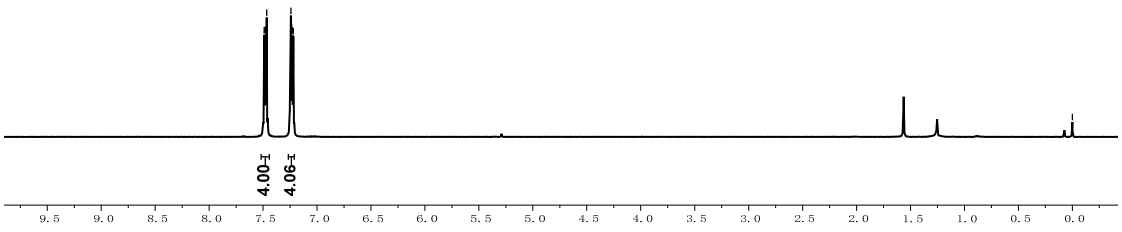
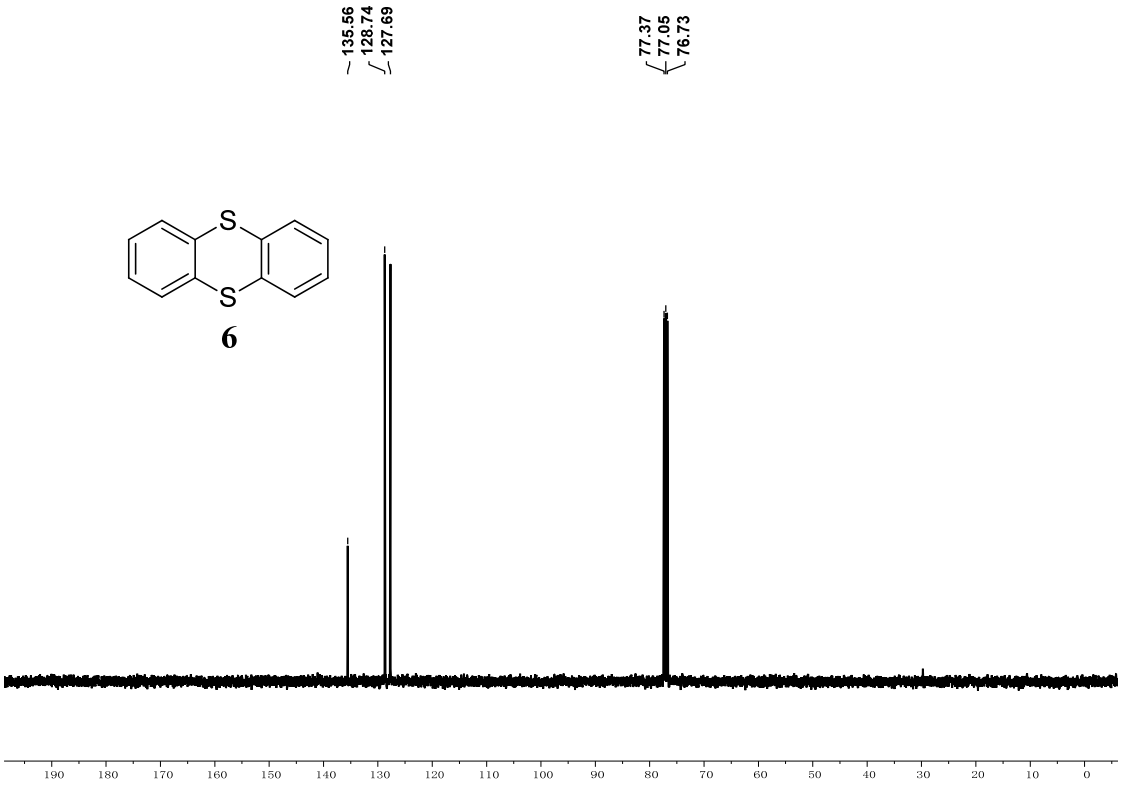
145.39
140.22
135.90
134.51
128.23
125.38
123.12
123.07
122.21
121.08
117.00
77.32
77.00
76.68
S
O2N
3y


7.490
7.481
7.475
7.467
7.253
7.250
7.243
7.235
7.228
7.220
-0.000


S
S

6


4.00
4.06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77.37
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76.73
S
S
6
190
180
170
160
150
140
130
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110
100
90
80
70
60
50
40
30
20
10
0

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