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Efficient access to fluorescent benzofuro[3,2-*b*]carbazoles *via* TFA-promoted cascade annulations of sulfur ylides, 2-hydroxy-β-nitrostyrenes and indoles

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Supporting Information

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General information. Unless otherwise noted, all reagents and solvents were purchased from commercial sources and used without purification. Purifications of reaction products were carried out by chromatography using silica gel (200-300 mesh). Melting points were recorded on a BÜCHI B-540 melting point apparatus. NMR spectra were recorded for ^{1}H NMR at 500 MHz and for ^{13}C NMR at 125 MHz. For ^{1}H NMR, tetramethylsilane (TMS) served as internal standard (δ=0) and data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), and coupling constant(s) in Hz. For ^{13}C NMR, TMS (δ=0) or $CDCl_3$ (δ=77.26) was used as internal standard and spectra were obtained with complete proton decoupling. HPLC analysis and the HRMS of all final products were confirmed on a Agilent 1290 HPLC-6224 Time of Fight Mass Spectrometer using PhenomenexLuna 5μ C18, 100 Å, 150 X 4.60 mm 5 micron column at a flow rate of 0.5 mL/min using liner gradients buffer B in A (B: CH_3OH containing 0.1 % formic acid, A: H_2O containing 0.1% formic acid). Mobile phase B was increased linearly from 5% to 95% over 7 min and 95% over the next 2 min, after which the column was equilibrated to 5% for 1 min. α-Keto sulfur ylides **1** were readily prepared from the corresponding α-bromoketone with methyl sulfide. [1] 2-hydroxy-β-nitrostyrenes **2** were prepared from the corresponding salicylaldehyde and nitromethane. [2]

Reference:

1. S. J. Sabounchei, M. Ahmadianpoor, A. Yousefi, M. Bayat, A. Sedghi, F. A. Bagherjeri, R. W. Gable, *RSC Adv.* **2016**, 28308-28315.
2. V. T. Pérez, A. L. Fuentes de Arriba, L. M. Monleón, L. Simón, O. H. Rubio, F. Sanz, J. R. Morán, *Eur. J. Org. Chem.* **2014**, 3242-3248.

General procedure for the synthesis of dihydrobenzofuran. A mixture of 2-(dimethyl-λ^4-sulfanylidene)-1-phenylethan-1-one (1.0 mmol) and (*E*)-4-chloro-2-(2-nitrovinyl) phenol (1.0 mmol, 1.0 equiv) was stirred in $ClCH_2CH_2Cl$ (4 mL) at 35 ^{o}C for 10 min. Upon the completion *via* TLC detection, the reaction was extracted three times with DCM. The combined organic extracts were washed with brine, dried over $MgSO_4$ and concentrated. Purification of the crude product by chromatography (silica gel, petroleum: EtOAc = 25:1) to afford target products.

(5-chloro-3-(nitromethyl)-2, 3-dihydrobenzofuran-2-yl)(phenyl)methanone (**III**): Light yellow 1iquid (332 mg, 98 %). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07-8.05 (m, 2H), 7.66-7.62 (m, 1H), 7.54-7.50 (m, 2H), 7.18-7.16 (m, 2H), 6.79 (d, *J* = 8.5 Hz, 1H), 5.90 (d, *J* = 4.5 Hz, 1H), 4.79-4.67 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.0, 157.3, 134.4, 134.2, 130.2, 129.6, 129.0, 126.8, 125.7, 124.9, 111.6, 85.7, 76.9, 41.7. HRMS (ESI): m/z calcd for $[M+Na]^+$: 340.0341, found:340.0345.

Typical procedure for the synthesis of benzofuro[3,2-b]carbazoles. A mixture of α-keto sulfur ylides **1** (1.0 mmol) and 2-hydroxy-β-nitrostyrenes **2** (1.0 mmol, 1.0 equiv) was stirred in $ClCH_2CH_2Cl$ (4.0 mL) for 10 min. And the indoles **3** (1.0 mmol, 1.0 equiv) and TFA (2.0 mmol, 2.0 equiv) were added to the above mixture. The reaction mixture was stirred at 25 ^{o}C for another 12 h. Upon the completion *via* TLC detection, the reaction was quenched with aqueous $NaHCO_3$ (5 mL), and then extracted three times with DCM. The combined organic extracts were washed with brine, dried over

$MgSO_4$ and concentrated. Purification of the crude product by chromatography using PE/EtOAc to afford benzofuro[3,2-*b*]carbazoles **4**, **5** and **6**.

11-methyl-6-phenyl-11H-benzofuro[3,2-*b*]carbazole (4a): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), yellow solid (339 mg, 88 %), m.p. 184.2-185.0 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.5 Hz, 1H), 7.88 (s, 1H), 7.79-7.77 (m, 2H), 7.66 (t, *J* = 7.5 Hz, 2H), 7.62-7.59 (m, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.46-7.41 (m, 4H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.00-6.97 (m, 1H), 3.98 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 148.9, 142.4, 138.6, 135.1, 130.3, 128.8, 128.3, 127.0, 125.9, 125.0, 123.0, 122.6, 122.4, 122.3, 120.9, 120.5, 120.0, 118.3, 111.9, 108.2, 97.9, 77.3, 77.1, 76.8, 29.4. HRMS (ESI): m/z calcd for $(C_{25}H_{17}NO+K)^+$: 386.0942; found: 386.0943.

11-methyl-6-(*p*-tolyl)-11H-benzofuro[3,2-*b*]carbazole (4b): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (343 mg, 86 %), m.p. 189.2-190.0 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.0 Hz, 1H), 7.85 (s, 1H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.52-7.40 (m, 6H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.01 (t, *J* = 7.5 Hz, 1H), 3.96 (s, 3H), 2.58 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.3, 149.1, 142.4, 138.7, 138.1, 132.1, 130.2, 129.7, 127.1, 125.9, 125.1, 123.1, 122.7, 122.5, 122.3, 121.0, 120.6, 120.2, 118.4, 112.0, 108.3, 97.8, 29.5, 21.7. HRMS (ESI): m/z calcd for $(C_{26}H_{19}NO+K)^+$: 400.1098; found: 400.1095.

6-(3-methoxyphenyl)-11-methyl-11*H*-benzofuro[3,2-*b*]carbazole (4c): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Red solid (340 mg, 98 %)， m.p. 170.4-171.5℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09-8.07 (m, 1H), 7.88 (s, 1H), 7.60-7.55 (m, 2H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.48-7.44 (m, 2H), 7.42-7.34 (m, 4H), 7.21 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.04-7.01 (m, 1H), 3.96 (s, 3H), 3.90 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 157.3, 148.8, 142.4, 138.6, 136.5, 129.9, 127.1, 126.0, 125.0, 123.1, 122.7, 122.6, 122.6, 122.4, 120.9, 120.6, 119.9, 118.5, 115.5, 114.4, 112.0, 108.3, 98.0, 55.5, 29.5. HRMS (ESI): m/z calcd for $(C_{26}H_{19}NO_2+K)^+$: 416.1047; found: 416.1048.

6-(4-chlorophenyl)-11-methyl-11*H*-benzofuro[3,2-*b*]carbazole (4d): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Red solid (347 mg, 98 %), m.p. 216.3-216.9 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.86 (s, 1H), 7.72-7.70 (m, 2H), 7.63-7.61 (m, 2H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.49 -7.41 (m, 4H), 7.37 (td, *J* = 7.5, 1.0 Hz, 1H), 7.04-7.01 (m, 1H), 3.95 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 148.8, 142.4, 138.6, 134.3, 133.6, 131.9, 129.2, 127.2, 126.2, 125.0, 123.1, 122.5, 122.4, 122.3, 120.7, 118.7, 118.5, 111.9, 108.5, 98.3, 29.5. HRMS (ESI): m/z calcd for $(C_{25}H_{16}ClNO+K)^+$: 420.0552; found: 420.0559.

11-methyl-6-(4-(trifluoromethyl)phenyl)-11*H*-benzofuro[3,2-*b*]carbazole (4e): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (323 mg, 74 %), m.p. 204.5-205.8 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (d, *J* = 7.0 Hz, 1H), 7.92-7.91 (m, 5H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.48-7.44 (m, 3H), 7.40-7.36 (m, 2H), 7.02-6.99 (m, 1H), 4.00 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.3, 148.8, 142.6, 139.1, 138.7, 131.0, 130.4 (d, *J* = 32.5 Hz), 127.4, 126.3, 125.8 (q, *J* = 3.75 Hz), 124.9, 124.6 (d, *J* = 270.0 Hz), 123.3, 122.6, 122.3, 122.2, 120.7, 120.6, 118.7, 118.4, 111.9, 108.6, 98.7, 29.5. HRMS (ESI): m/z calcd for $(C_{26}H_{16}F_3NO+Na)^+$: 438.1076;

found: 438.1084.

11-methyl-6-(4-nitrophenyl)-11*H*-benzofuro[3,2-*b*]carbazole (4f): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (227 mg, 53 %), m.p. >250 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.5 Hz, 2H), 8.08 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 9.0 Hz, 2H), 7.92 (s, 1H), 7.53-7.44 (m, 4H), 7.42 -7.39 (m, 2H), 7.02 (s, 1H), 3.98 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 148.5, 147.8, 142.5, 142.3, 138.7, 131.6, 127.5, 126.5, 124.7, 124.1, 123.3, 122.7, 122.0, 121.9, 120.8, 120.1, 118.7, 117.4, 111.9, 108.8, 99.3, 29.6. HRMS (ESI): m/z calcd for $(C_{25}H_{16}N_2O_3+K)^+$: 431.0793; found: 431.0798.

4-(11-methyl-11*H*-benzofuro[3,2-*b*]carbazol-6-yl)benzonitrile (4g): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (323 mg, 82 %), m.p. 192.3-193.0 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09-8.07 (m, 1H), 7.92-7.87 (m, 5H), 7.53-7.45 (m, 4H), 7.39-7.37 (m, 2H), 7.02 (td, *J* = 8.0, 1.0 Hz, 1H), 3.97 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 148.5, 142.5, 140.3, 138.6, 132.6, 131.4, 127.5, 126.4, 124.8, 123.3, 122.7, 122.0, 122.0, 120.8, 120.2, 119.2, 118.7, 117.8, 112.1, 111.9, 108.70, 99.1, 29.6. HRMS (ESI): m/z calcd for $(C_{26}H_{16}N_2O+Na)^+$: 395.1155; found: 395.1153.

4-(11-methyl-11*H*-benzofuro[3,2-*b*]carbazol-6-yl)phenol (4h): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (206 mg, 57 %), m.p. 201.6-202.8 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.5 Hz, 1H), 7.85 (s, 1H), 7.65 (d, *J* = 8.5 Hz, 2H), 7.54-7.51 (m, 2H), 7.46-7.42 (m, 3H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.00 (t, *J* = 7.5 Hz, 1H), 3.97 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.3, 155.7, 149.1, 142.4, 138.7, 131.8, 127.5, 127.1, 125.9, 125.1, 123.1, 122.7, 122.5, 122.4, 121.1, 120.6, 119.8, 118.4, 115.9, 112.0, 108.3, 97.7, 29.5. HRMS (ESI): m/z calcd for $(C_{25}H_{17}NO_2+H)^+$: 364.1332; found: 364.1335.

11-methyl-6-(naphthalen-2-yl)-11*H*-benzofuro[3,2-*b*]carbazole (4i): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (374 mg, 86 %)，m.p. 130.6-131.2 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.14 (d, *J* = 8.0 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 1H), 8.05 (d, *J* = 7.5 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.91-7.90 (m, 2H), 7.65-7.59 (m, 2H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.47-7.42 (m, 4H), 7.40-7.37 (m, 1H), 6.93 (t, *J* = 7.0 Hz, 1H), 3.99 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.3, 149.1, 142.5, 138.8, 133.8, 133.3, 132.7, 129.5, 128.6, 128.5, 128.1, 127.1, 126.5, 126.4, 126.0, 125.1, 123.2, 122.6, 122.5, 122.4, 121.6, 121.0, 120.6, 120.2, 120.0, 118.8, 118.5, 112.0, 108.3, 98.1,29.5. HRMS (ESI): m/z calcd for $(C_{29}H_{19}NO+K)^+$: 436.1098; found: 436.1093.

4-methoxy-11-methyl-6-(thiophen-2-yl)-11H-benzofuro[3,2-b]carbazole (4j): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (307 mg, 80 %), m.p. 200.6-201.8 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.66 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.64 (dd, *J* = 5.5, 1.5 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.47-7.44 (m, 2H), 7.41-7.40 (m, 1H), 7.33(dd, *J* =5.0, 3.5 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.05-7.02 (m, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 4.03 (s, 3H), 3.94 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 146.2, 145.7, 142.4, 138.5, 135.1, 128.7, 127.5, 127.0, 126.5, 126.2, 123.2, 122.5, 122.4, 122.1, 118.5, 112.8, 110.0, 108.4, 98.9, 56.5, 29.5. HRMS (ESI): m/z calcd for $(C_{24}H_{17}NO_2S+H)^+$: 384.1053; found: 384.1050.

6-(2-bromophenyl)-11-methyl-11*H*-benzofuro[3,2-*b*]carbazole (4k): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), White solid (351 mg, 76 %), m.p. 224.5-225.8 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.5 Hz, 1H), 7.94 (t, *J* = 1.5 Hz, 1H), 7.89 (s, 1H), 7.74-7.70 (m, 2H), 7.56-7.50 (m, 2H), 7.48 -7.42 (m, 4H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.04-7.01 (m, 1H), 3.98 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.3, 148.8, 142.5, 138.6, 137.3, 133.4, 131.4, 130.4, 129.2, 127.3, 126.2, 124.9, 123.2, 122.7, 122.5, 122.3, 120.7, 120.7, 118.6, 118.4, 112.0, 108.5, 98.5, 29.6. HRMS (ESI): m/z calcd for $(C_{25}H_{16}BrNO+K)^+$: 464.0047; found: 464.0039.

6-(3-bromophenyl)-11-methyl-11*H*-benzofuro[3,2-*b*]carbazole (4l): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (384 mg, 83 %), m.p. 189.2-190.1 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 7.5, 0.5 Hz, 1H), 7.95 (t, *J* = 1.5 Hz, 1H), 7.89 (s, 1H), 7.74-7.71 (m, 2H), 7.56-7.50 (m, 2H), 7.48-7.41 (m, 4H), 7.39-7.35 (m, 1H), 7.04-7.01 (m, 1H), 3.98 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.3, 148.8, 142.5, 138.7, 137.4, 133.4, 131.4, 130.4, 129.2, 127.3, 126.2, 125.0, 123.3, 122.9, 122.5, 122.4, 122.4, 120.8, 120.7, 118.7, 118.4, 112.0, 108.5, 98.5, 29.6. HRMS (ESI): m/z calcd for $(C_{25}H_{16}BrNO+K)^+$: 464.0047; found: 464.0046.

4-methoxy-11-methyl-6-(3-phenylethyl)-11H-benzofuro[3,2-b]carbazole (4m): Purification by column chromatography (silica gel, petroleum: EtOAc = 30:1), Green solid (138 mg, 33 %), m.p. 189.2-190.0℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (d, *J* = 7.8 Hz, 1H), 7.74 (s, 1H), 7.65 (d, *J* = 7.3 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.46 (d, *J* = 7.4 Hz, 3H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.30-7.24 (m, 3H), 7.02 (d, *J* = 7.9 Hz, 1H), 4.12 (s, 3H), 3.98-3.93 (m, 5H), 3.28-3.22 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.8, 146.2, 145.8, 142.3, 142.1, 138.9, 128.6, 127.0, 126.2, 125.7, 123.0, 122.9, 122.8, 122.5, 121.1, 120.2, 118.9, 113.0, 110.0, 108.5, 96.7, 56.6, 35.3, 29.5, 29.0. HRMS (ESI): m/z calcd for $(C_{28}H_{24}NO)^+$: 406.1802; found: 406.1810.

3-methoxy-11-methyl-6-phenyl-11*H*-benzofuro[3,2-*b*]carbazole (5a): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (282 mg, 75 %), m.p. 185.2-186.0 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.5 Hz, 1H), 7.77-7.75 (m, 3H), 7.66-7.63 (m, 2H), 7.60-7.57 (m, 1H), 7.44-7.39 (m, 3H), 7.07 (d, *J* = 2.5 Hz, 1H), 6.98-6.95 (m, 2H), 3.96 (s, 3H), 3.87 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 158.7, 149.1, 142.2, 138.8, 135.3, 130.4, 128.9, 128.3, 125.6, 123.4, 122.8, 122.2, 120.9, 120.0, 119.6, 118.3, 118.1, 110.8, 108.3, 97.2, 96.8, 55.8, 29.5. HRMS (ESI): m/z calcd for $(C_{26}H_{19}NO_2+H)^+$: 378.1489; found: 378.1485.

2-fluoro-11-methyl-6-phenyl-11*H*-benzofuro[3,2-*b*]carbazole (5b): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (321 mg, 88 %), m.p. 106.2-108.5 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.76-7.71 (m, 3H), 7.65 (t, *J* = 7.5 Hz, 2H), 7.61-7.58 (m, 1H), 7.47-7.39 (m 4H), 7.14 (td, *J* = 9.0, 3.0 Hz, 1H), 6.98 (t, *J* = 7.5 Hz, 1H), 3.98 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.8 (d, *J* = 237.5 Hz), 153.3, 149.9, 142.6, 138.6, 135.0, 130.3, 128.9, 128.8 (d, *J* = 10 Hz), 128.5, 126.3, 125.9 (d, *J* = 10 Hz), 122.7 (d, *J* = 3.75 Hz), 122.6, 121.5, 120.3, 118.5, 114.3 (d, *J* = 25 Hz), 112.5 (d, *J* = 8.75 Hz), 108.4, 106.6 (d, *J* = 25 Hz), 98.1, 29.5. HRMS (ESI): m/z calcd for $(C_{25}H_{16}FNO+H)^+$: 366.1289; found: 366.1285.

2-chloro-11-methyl-6-phenyl-11*H*-benzofuro[3,2-*b*]carbazole (5c): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), White solid (342 mg,

90 %), m.p. 236.3-236.8 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, *J* = 2.0 Hz, 1H), 7.83 (s, 1H), 7.75-7.74 (m, 2H), 7.66-7.63 (m, 2H), 7.61-7.582 (m, 1H), 7.47-7.36 (m, 6H), 6.98 (d, *J* = 7.0 Hz, 1H), 3.97 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 149.5, 142.6, 138.7, 134.9, 130.3, 128.9, 128.5, 127.8, 127.0, 126.5, 126.3, 122.6, 122.5, 122.1, 121.6, 120.4, 120.3, 118.5, 113.0, 108.4, 98.1, 29.5. HRMS (ESI): m/z calcd for $(C_{25}H_{16}ClNO+H)^+$: 382.0993; found: 382.1000.

2-bromo-11-methyl-6-phenyl-11*H*-benzofuro[3,2-*b*]carbazole (5d): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (391 mg, 92 %), m.p. 224.2-225.7 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (d, *J* = 2.0 Hz, 1H), 7.82 (s, 1H), 7.74 (d, *J* = 6.5 Hz, 2H), 7.66-7.63 (m, 2H), 7.61-7.58 (m, 1H), 7.51 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.47-7.44 (m, 1H), 7.42-7.38 (m, 3H), 6.99-6.96 (m, 1H), 3.96 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.1, 149.4, 142.7, 138.8, 134.9, 130.4, 129.8, 128.9, 128.5, 127.2, 126.4, 123.5, 122.6, 122.6, 122.0, 121.8, 120.4, 118.6, 115.2, 113.5, 108.4, 98.1, 29.6. HRMS (ESI): m/z calcd for $(C_{25}H_{16}BrNO+H)^+$: 426.0488; found: 426.0489.

methyl 11-methyl-6-phenyl-11*H*-benzofuro[3,2-*b*]carbazole-2-carboxylate (5e): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (356 mg, 88 %), m.p. 173.5-174.3℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.77 (m, 1H), 8.13 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.86 (s, 1H), 7.77-7.75 (m, 2H), 7.68-7.64 (m, 2H), 7.63-7.60 (m, 1H), 7.51 (d, *J* = 8.5 Hz, 1H), 7.47-7.44 (m, 1H), 7.41 (dd, *J* = 12.5, 8.0 Hz, 2H), 6.99 (td, *J* = 8.0, 1.0 Hz, 1H), 3.99 (s, 3H), 3.93 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.3, 160.0, 149.4, 142.5, 138.8, 134.8, 130.3, 128.9, 128.8, 128.5, 126.3, 125.3, 124.5, 122.8, 122.5, 122.4, 122.3, 121.4, 120.3, 118.5, 111.7, 108.4, 98.2, 52.3, 29.5. HRMS (ESI): m/z calcd for $(C_{27}H_{19}NO_3+H)^+$: 406.1438; found: 406.1445.

11-benzyl-6-phenyl-11*H*-benzofuro[3,2-*b*]carbazole (6a): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (281 mg, 61 %), m.p. 200.4-201.2 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.5 Hz, 1H), 7.83 (s, 1H), 7.80 (d, *J* = 7.0 Hz, 2H), 7.68-7.65 (m, 2H), 7.62-7.59 (m, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.45-7.38 (m, 4H), 7.33-7,28 (m, 4H), 7.23 (d, *J* = 7.5 Hz, 2H), 7.00-6.98 (m, 1H), 5.67 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.3, 149.1, 142.1, 138.3, 137.2, 135.2, 130.4, 129.0, 128.9, 128.4, 127.7, 127.2, 126.5, 126.2, 124.9, 123.3, 122.9, 122.6, 122.3, 121.2, 120.7, 120.3, 118.8, 112.0, 108.7, 98.4, 46.9. HRMS (ESI): m/z calcd for $(C_{31}H_{21}NO+K)^+$: 462.1255; found: 462.1253.

10,13-dimethyl-8-phenyl-13*H*-naphtho[1',2':4,5]furo[3,2-*b*]carbazole (6c): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (381 mg, 88 %), m.p. 239.6-240.5 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (d, *J* = 8.5 Hz, 1H), 8.24 (s, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.91 (d, *J* = 9.0 Hz, 1H), 7.83-7.78 (m, 3H), 7.73 (d, *J* = 9.0 Hz, 1H), 7.69-7.66 (m, 2H), 7.63-7.61 (m, 1H), 7.59-7.56 (m, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.22 (s, 1H), 4.05 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 148.7, 140.9, 139.4, 135.4, 130.6, 130.5, 129.5, 129.4, 128.8, 128.4, 127.6, 127.3, 127.1, 124.2, 123.7, 123.4, 122.7, 122.5, 120.3, 119.9, 117.9, 113.2, 108.0, 99.0, 29.6, 21.6. HRMS (ESI): m/z calcd for $(C_{30}H_{21}NO+Na)^+$: 434.1515; found: 434.1511.

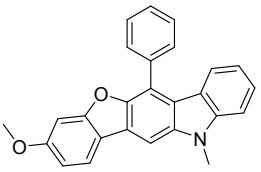
8-methoxy-11-methyl-6-phenyl-11*H*-benzofuro[3,2-*b*]carbazole (6d): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Yellow solid (359 mg, 90 %), m.p. 144.9-145.6 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.0 Hz, 1H), 7.84 (s, 1H), 7.78-7.77 (m, 2H), 7.65 (t, *J* = 7.5 Hz, 2H), 7.59-7.56 (m, 1H), 7.53 (d, *J* = 8.5 Hz, 1H), 7.44 (td, *J* = 7.0, 1.0 Hz, 1H), 7.37-7.34 (m, 1H), 7.30 (d, *J* = 8.5 Hz, 1H), 7.08 (dd, *J* = 9.0, 2.5 Hz, 1H), 6.88 (d, *J* = 2.5 Hz, 1H), 3.95 (s, 3H), 3.61 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 152.9, 148.6, 139.3, 137.6, 135.2, 130.6, 128.8, 128.4, 127.1, 125.1, 123.2, 122.9, 122.3, 120.7, 120.6, 119.9, 115.2, 111.9, 108.9, 105.5, 98.0, 55.8, 29.6. HRMS (ESI): m/z calcd for $(C_{26}H_{19}NO_2+Na)^+$: 400.1308; found: 400.1298.

8-bromo-11-methyl-6-phenyl-11*H*-benzofuro[3,2-*b*]carbazole (6e): Purification by column chromatography (silica gel, petroleum: EtOAc = 20:1), Brown solid (323 mg, 76 %), m.p. 230.1-231.0 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.0 Hz, 1H), 7.86 (s, 1H), 7.75-7.73 (m, 2H), 7.66 (t, *J* = 7.5 Hz, 2H), 7.63-7.61 (m, 1H), 7.54 -7.50 (m, 3H), 7.47-7.44 (m, 1H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.28 (s, 1H), 3.95 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.5, 149.0, 141.1, 139.0, 134.6, 130.3, 129.0, 128.7, 128.6, 127.5, 125.0, 123.9, 122.5, 120.7, 120.4, 119.9, 112.1, 111.2, 109.7, 98.2, 29.6. HRMS (ESI): m/z calcd for $(C_{25}H_{16}BrNO+H)^+$: 426.0488; found: 426.0491.

4-methoxy-6-phenyl-11*H*-benzofuro[3,2-*b*]carbazole-8-carbonitrile (6f): Purification by column chromatography (silica gel, petroleum: EtOAc = 10:1), Yellow solid (225 mg, 58 %), m.p. 243.7-244.2 ℃. ^{1}H NMR (500 MHz, DMSO-d6) δ 12.18 (s, 1H), 8.25 (s, 1H), 7.87 (d, *J* = 7.5 Hz, 1H), 7.74-7.66 (m, 7H), 7.38 (s, 1H), 7.34 (t, *J* = 8.0 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 1H), 3.92 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d6) δ 148.2, 145.4, 145.1, 143.4, 137.5, 134.0, 129.8, 129.2, 128.8, 128.7, 125.7, 125.3, 124.1, 123.6, 122.1, 120.4, 119.7, 119.4, 113.4, 112.2, 110.3, 101.9, 99.5, 55.7. HRMS (ESI): m/z calcd for $(C_{26}H_{16}N_2O_2+H)^+$: 389.1285; found: 389.1281.

X-ray Crystallography Data of 5a (CCDC No. 1914003)

Single crystals of compound **5a** were measured on a Rigaku RAXIS-RAPID single-crystal diffractometer. The recrystallization solvent of **5a** was EtOH.



5a

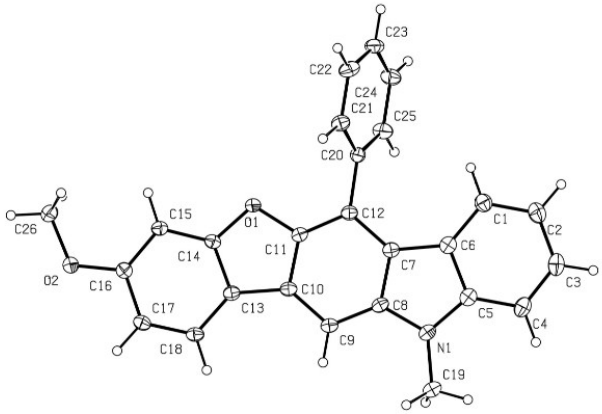


Table S1 X-ray crystallography data of **5a**

Formula moiety	$C_{26}H_{19}NO_2$
Formula sum	$C_{26}H_{19}NO_2$
Formula weight	377.42
Temperature	170 K
Crystal system	triclinic
Space group	P -1
Unit cell dimensions	a=8.3803(4)Å b=10.8364(7) Å c= 11.0444(6) Å alpha=77.127(2) deg. beta=89.613(2) deg. gamma=76.222(2) deg.
Volume	948.49(9) $Å^3$
Z	2
Calculated density	1.322 g/cm^3
Absorption coefficient	0.083 mm^{-1}
F(000)	396.0
Crystal size	0.449 x 0.357 x 0.25 mm
Theta range for data collection	3.19 to 26.36 deg
Reflections collected / unique	10918/ 3830 [R(int) = 0.0246]
Data / restraints / parameters	3830/ 0 / 264
Goodness-of-fit on F2	1.048

Final R indices [I>2sigma(I)]	R1 = 0.0419, wR2 = 0.1084
R indices (all data)	R1 = 0.0497, wR2 = 0.1154

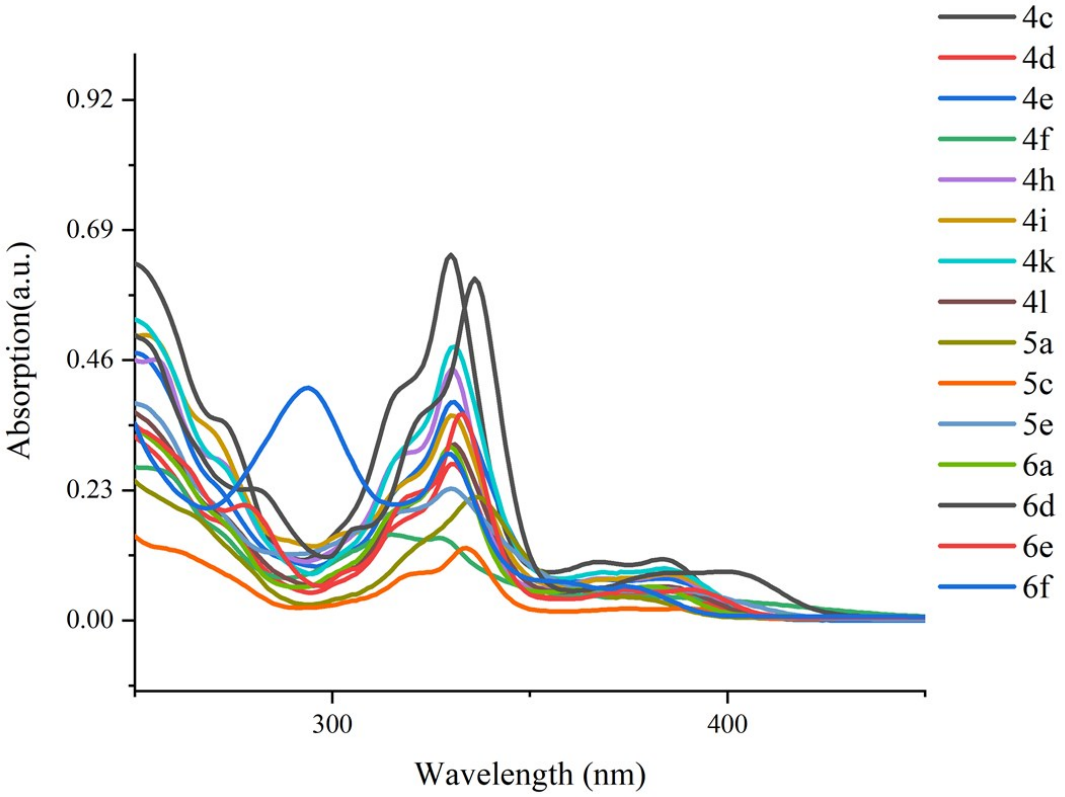


Figure S1. UV/Vis absorption profiles (c = 2.5 x 10^{-6} M in EtOH).

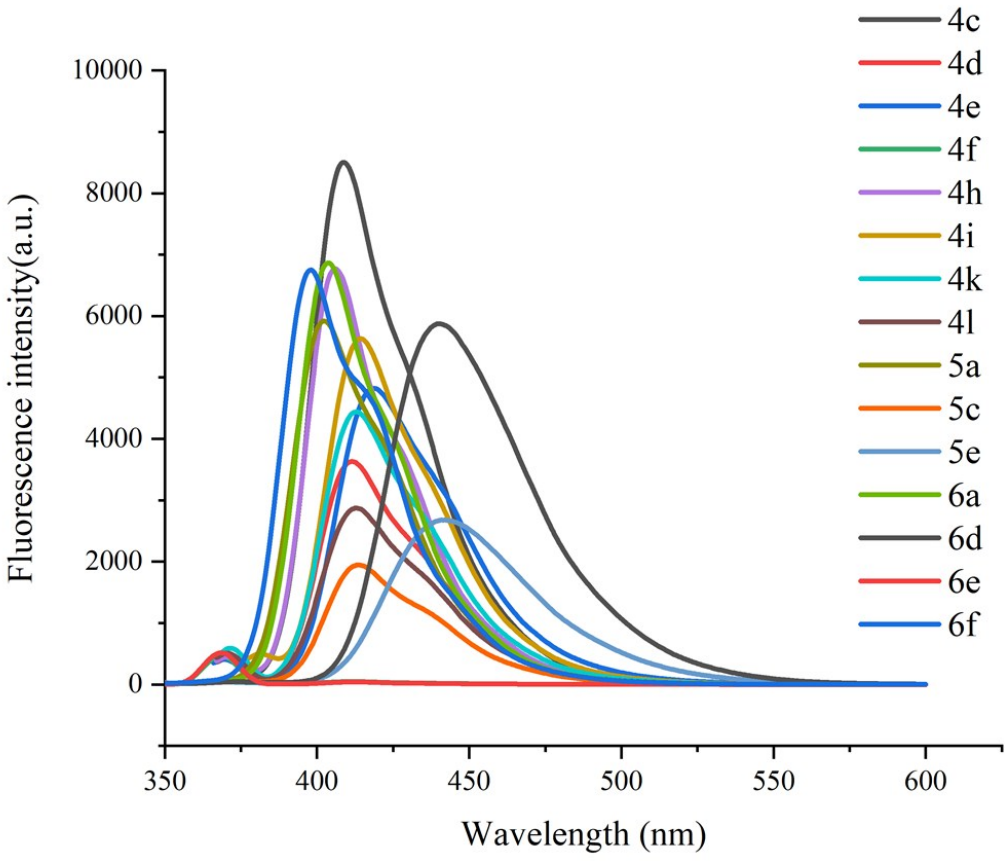
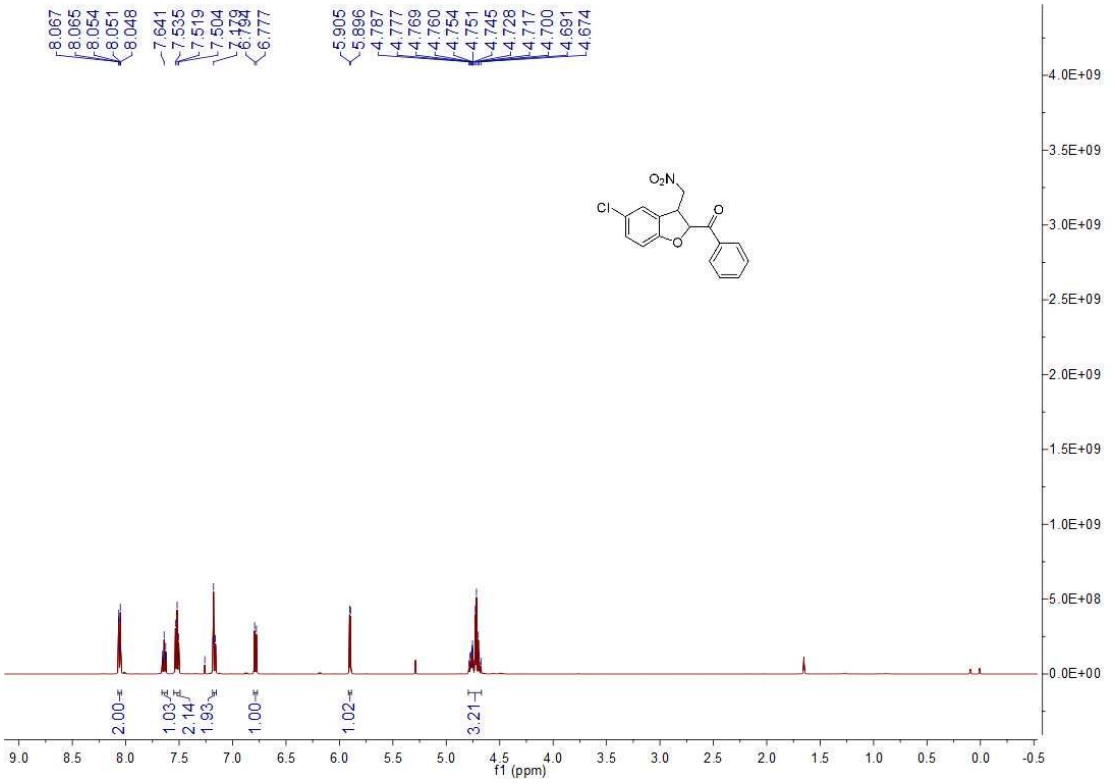
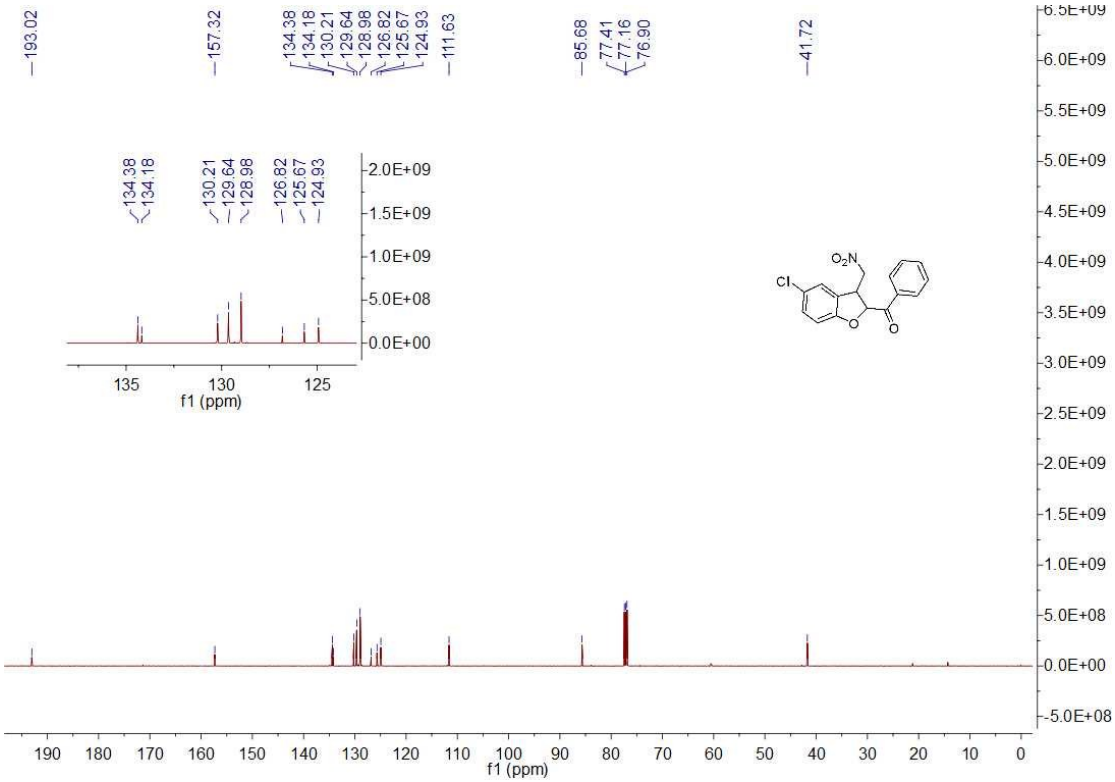
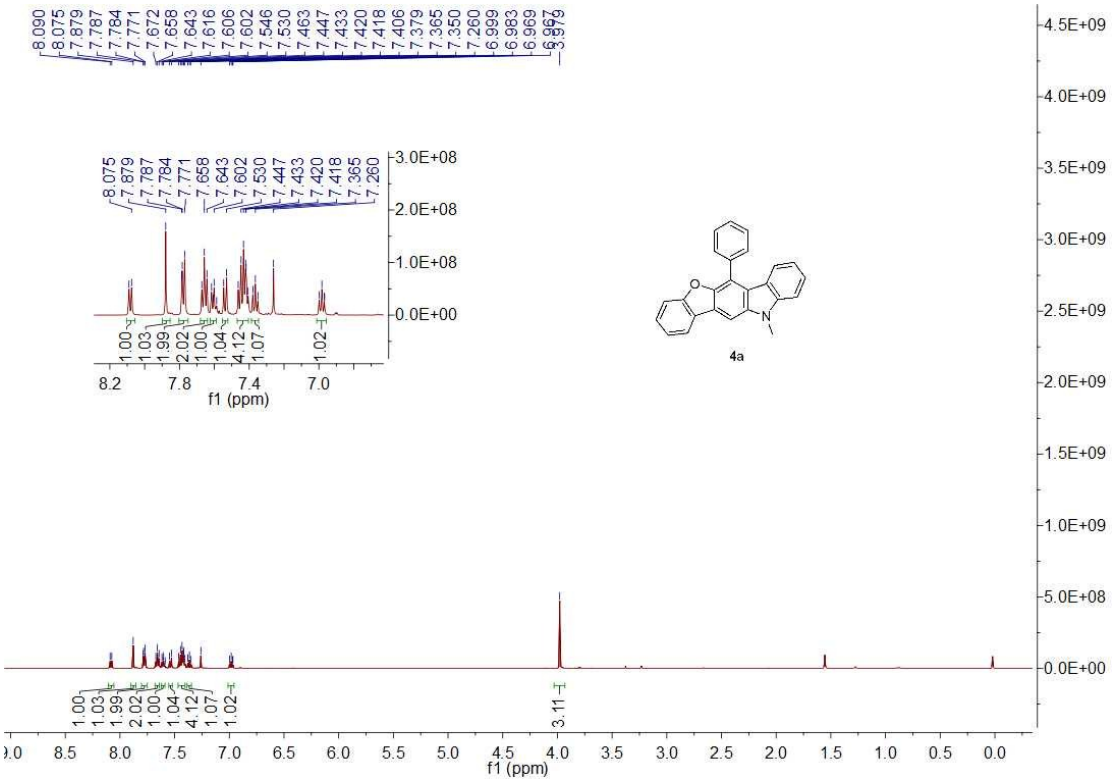


Figure S2. Fluorescent emission profiles (c = 2.5 x 10^{-6} M in EtOH)

NMR spectrum



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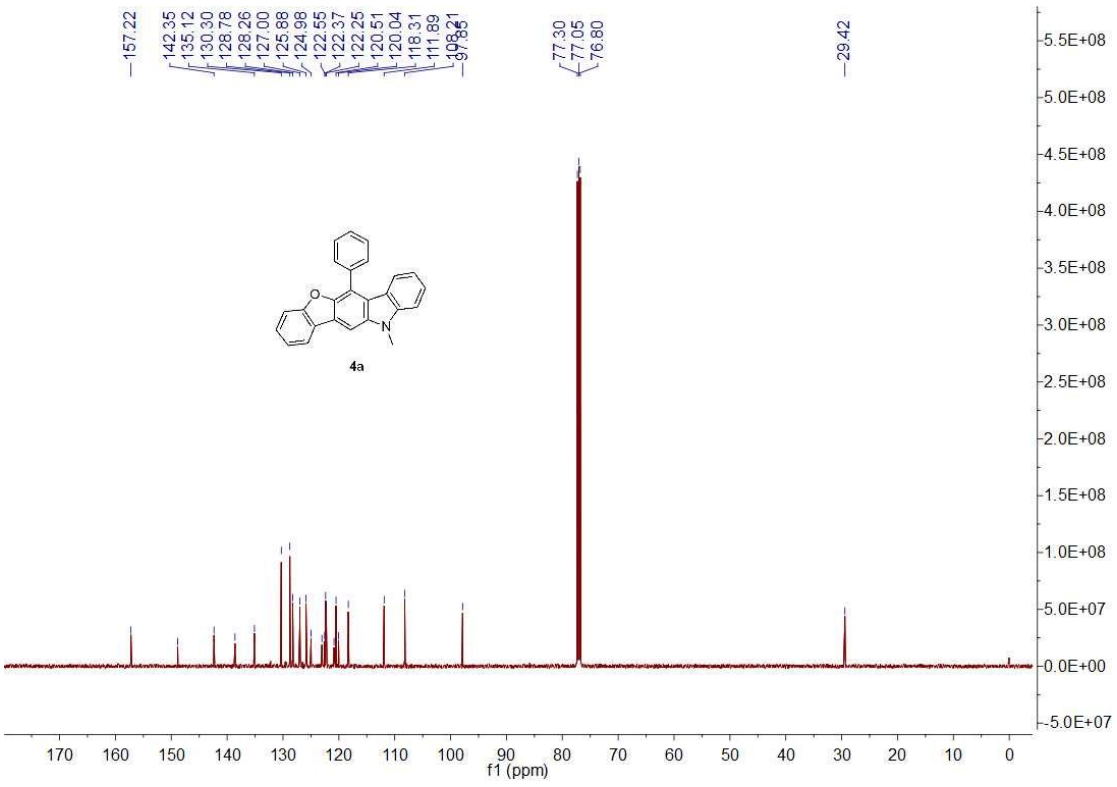
f1 (ppm)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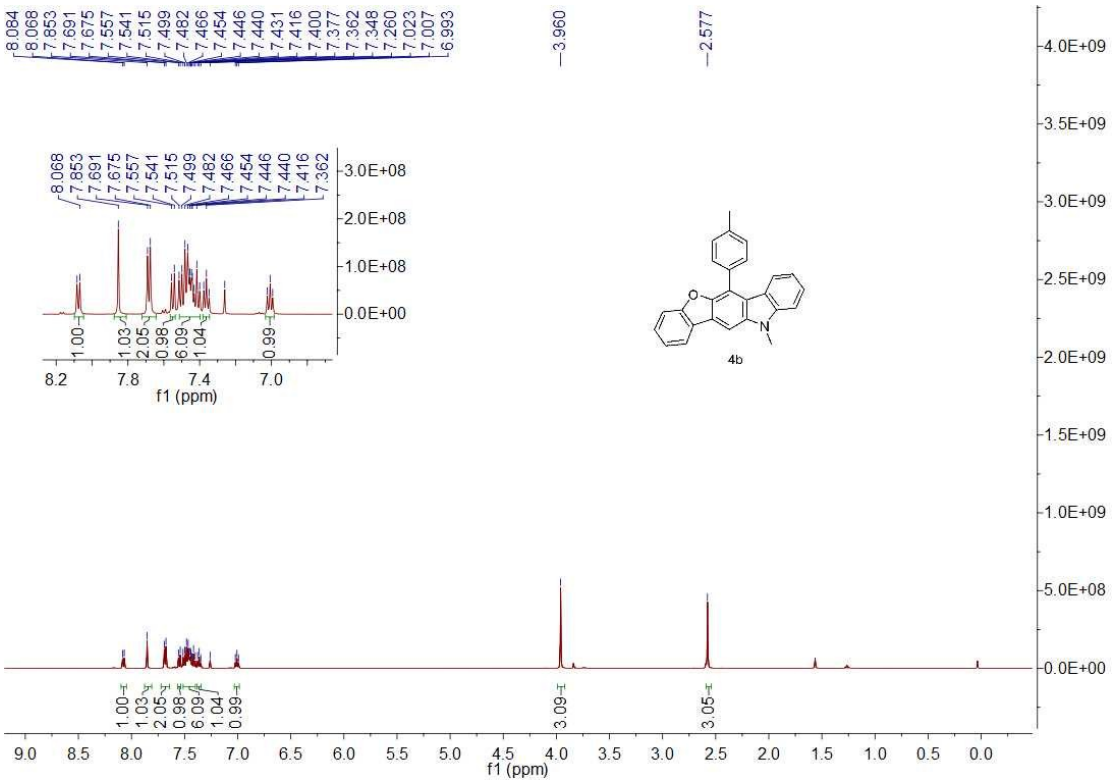
f1 (ppm)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f1 (ppm)
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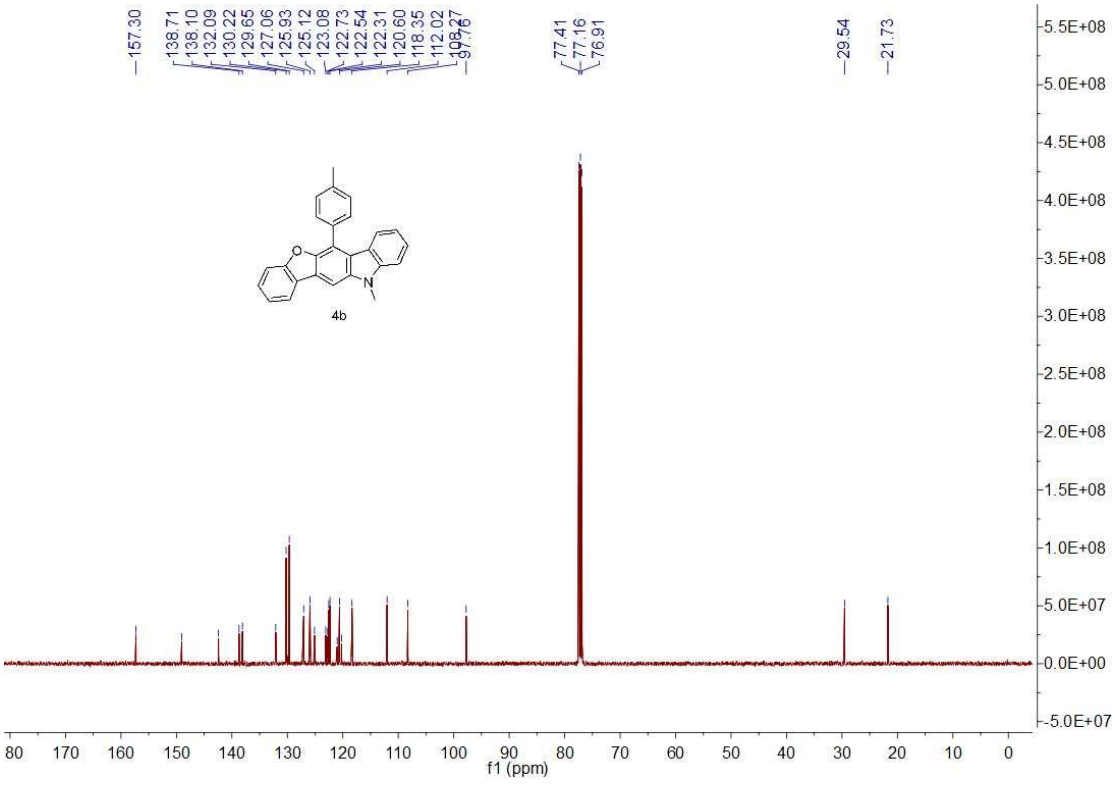
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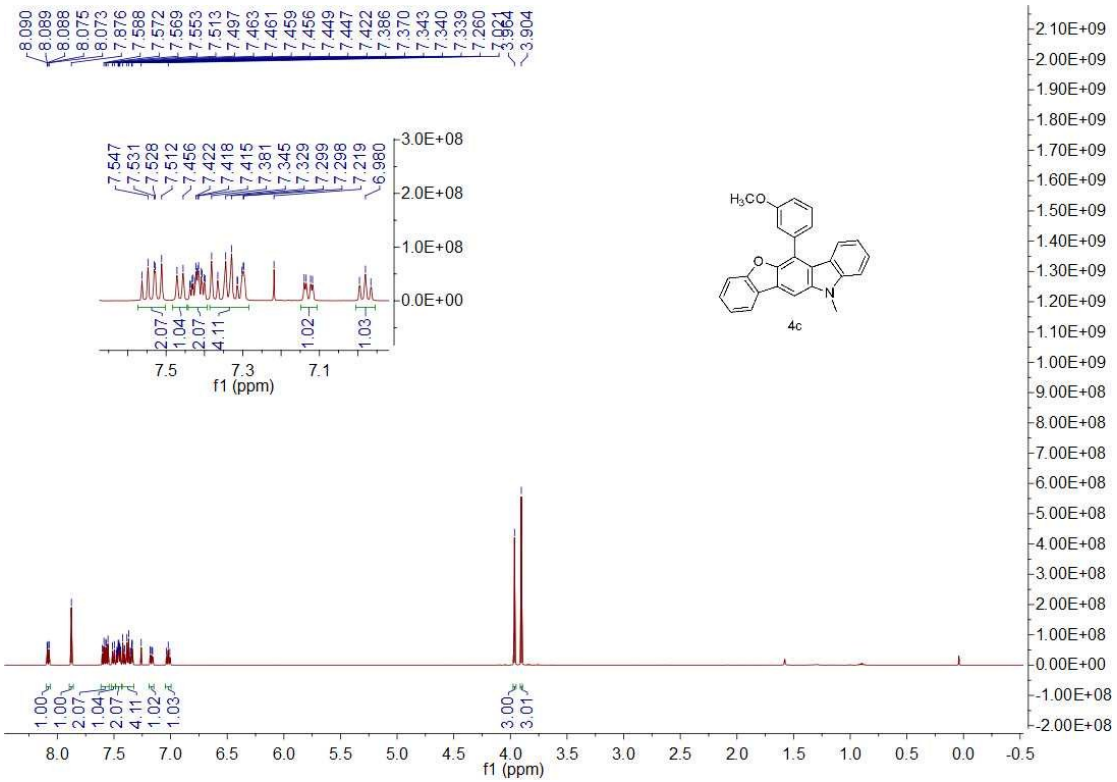
f1 (ppm)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1.03
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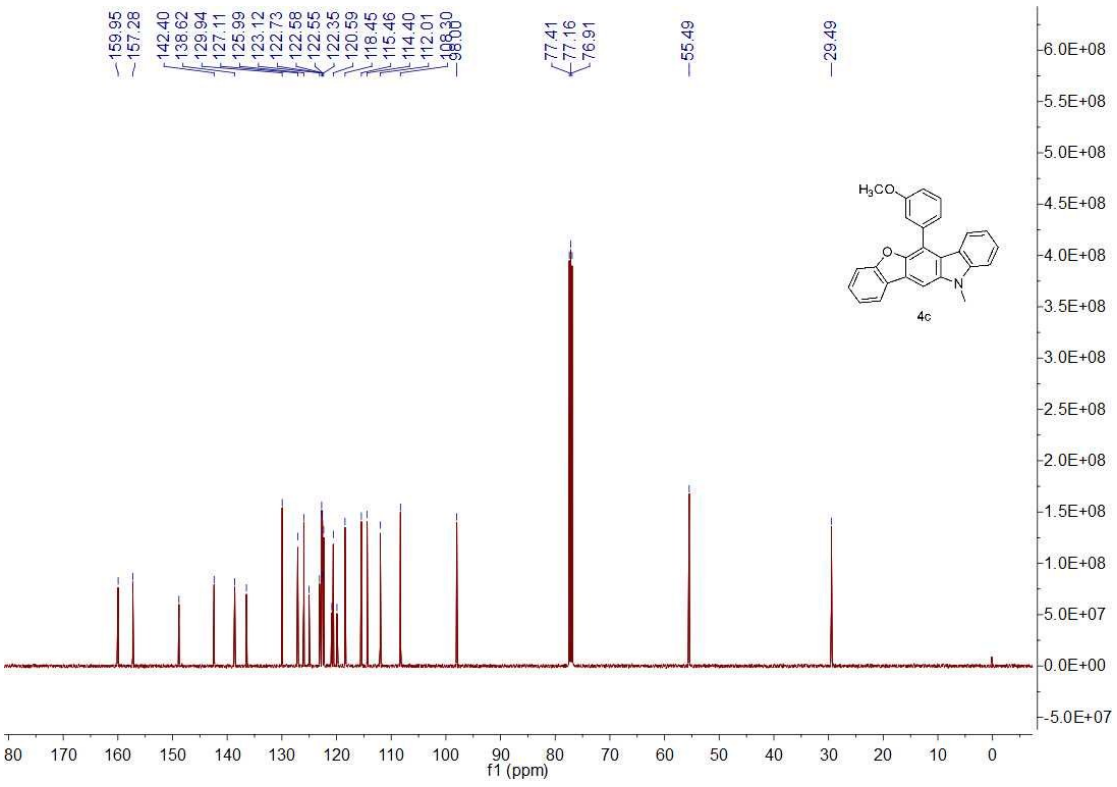
f1 (ppm)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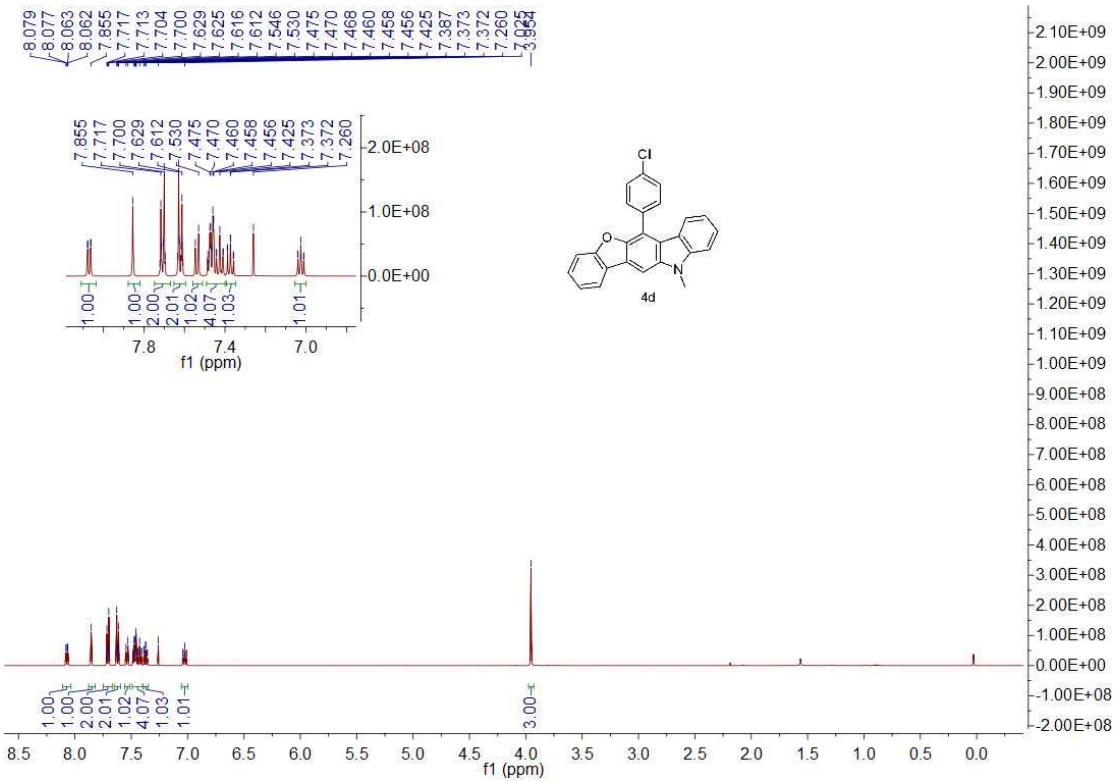
f1 (ppm)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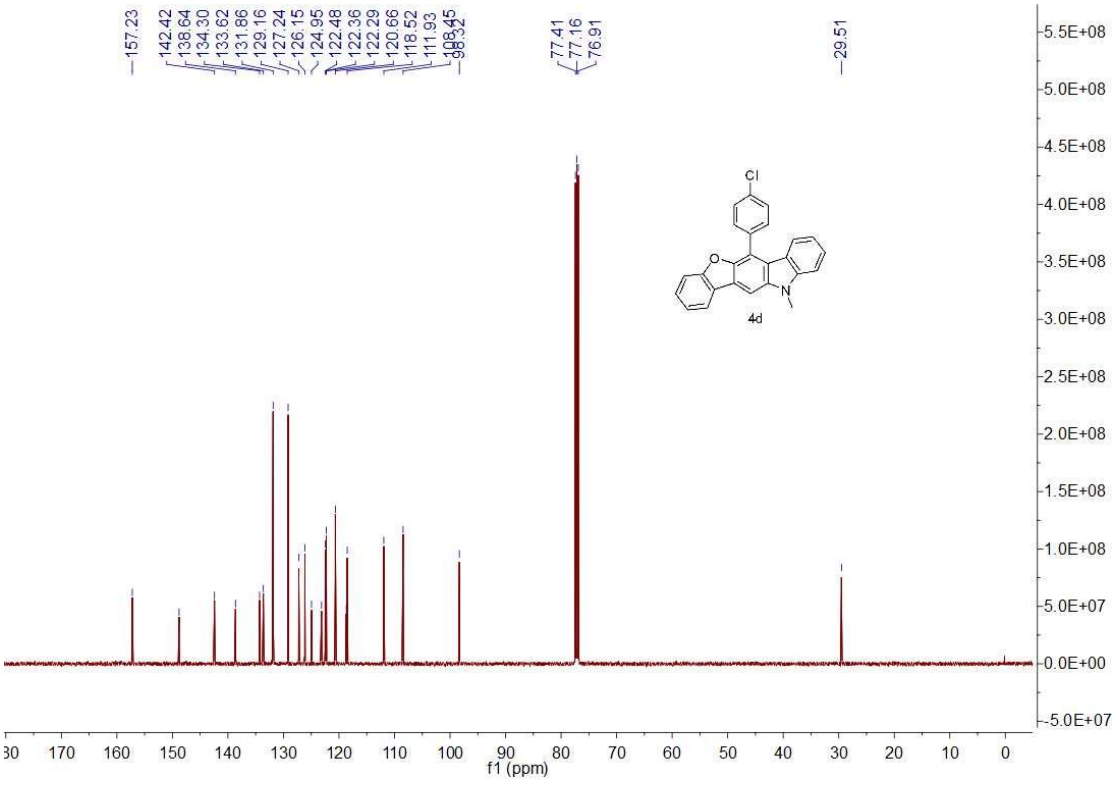
f1 (ppm)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O
N
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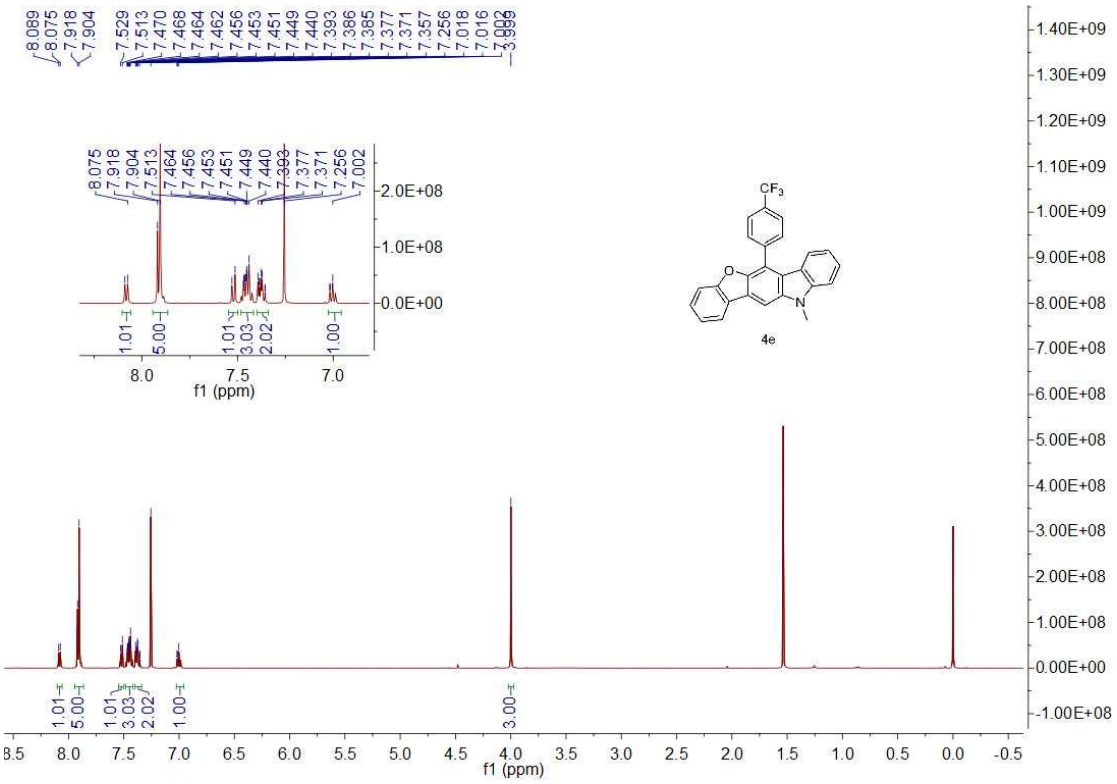
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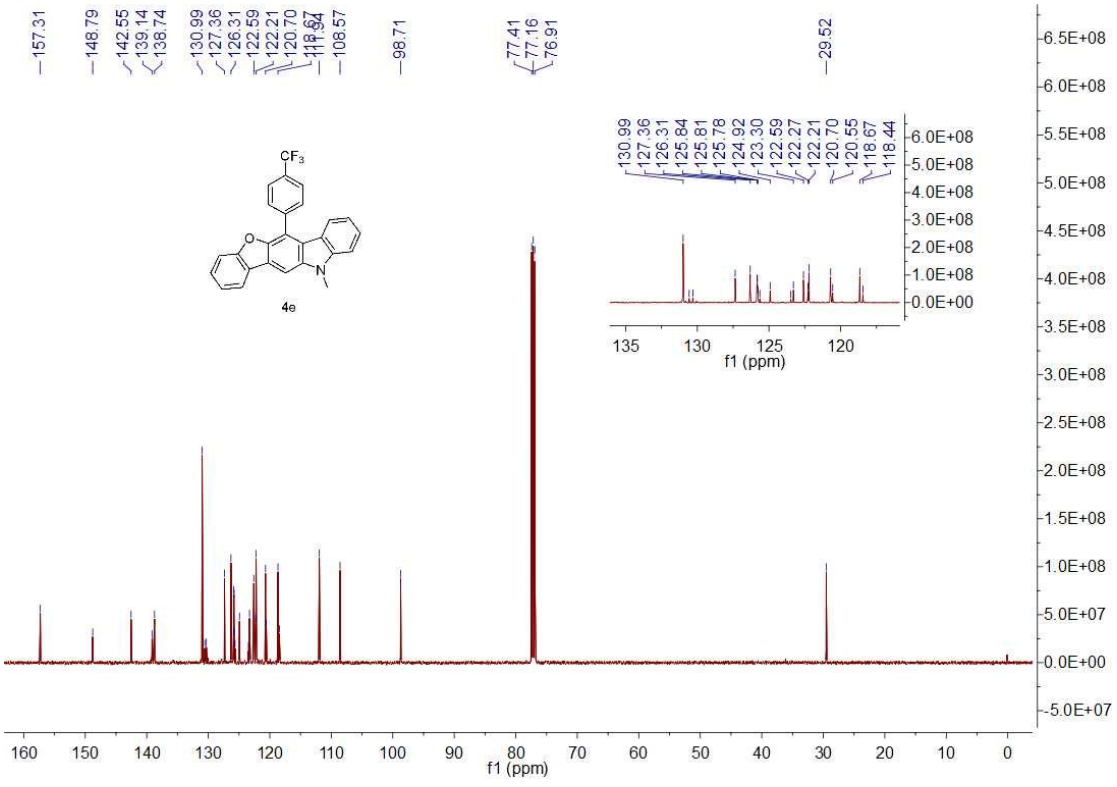
4e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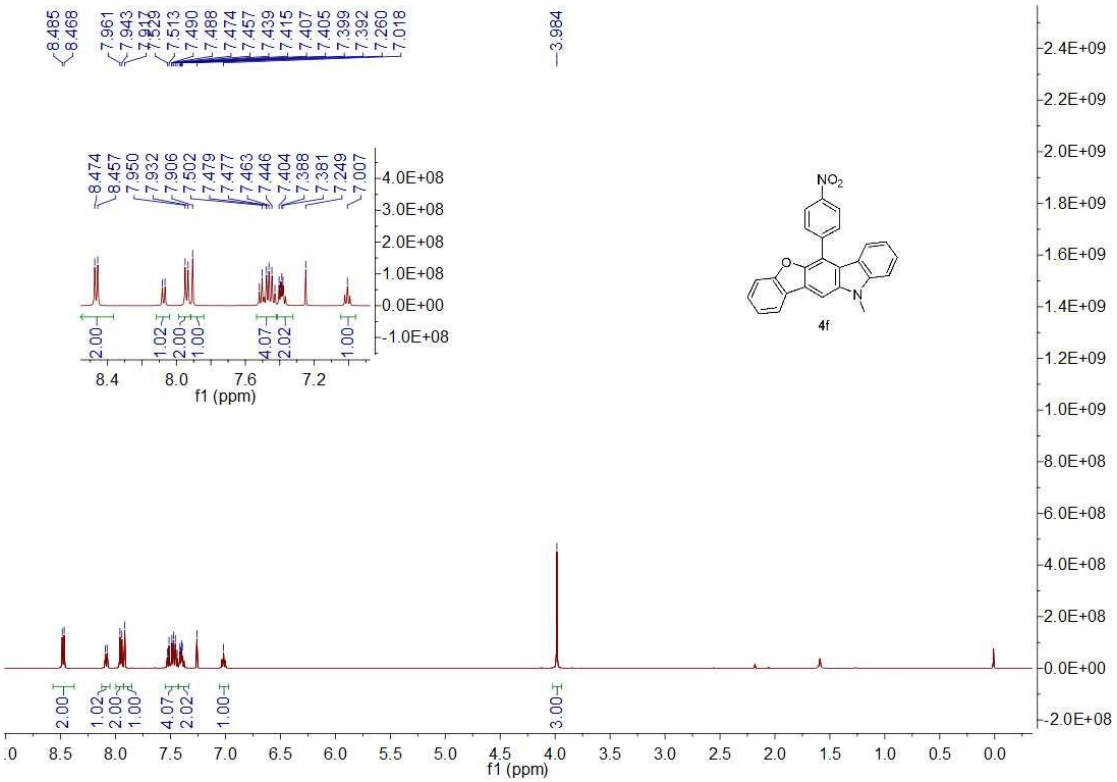
f1 (ppm)
4e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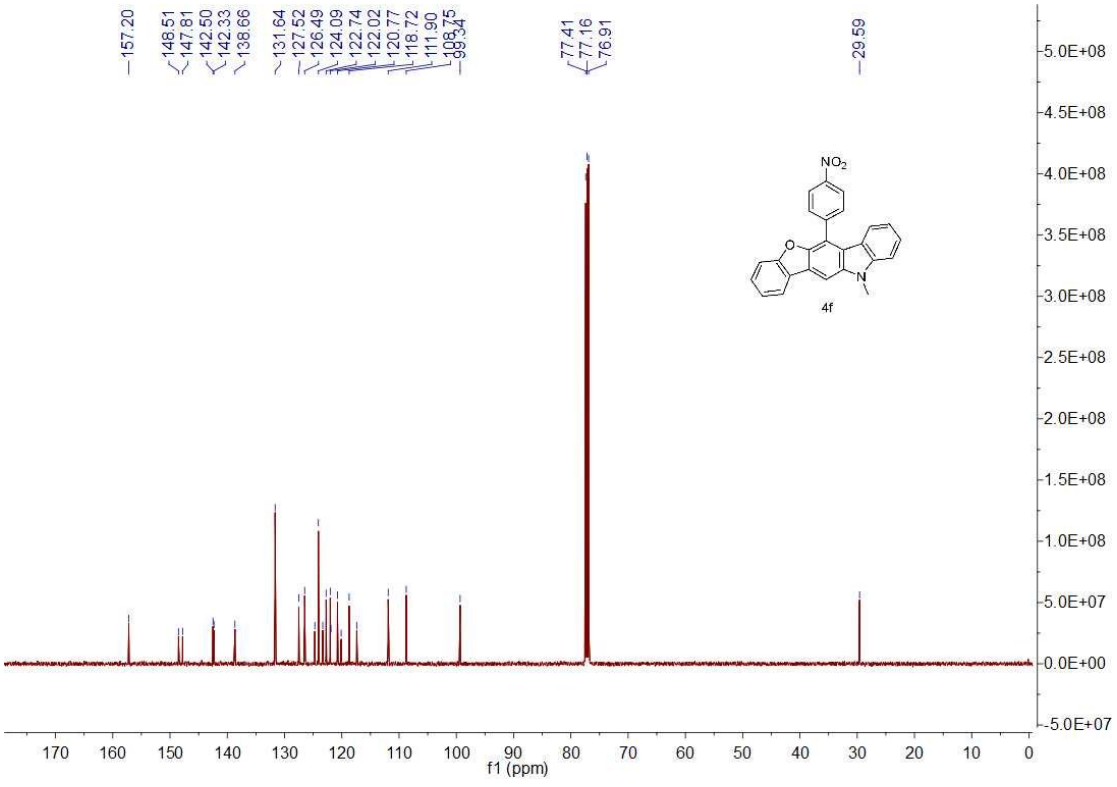
8.468
7.961
7.943
7.513
7.490
7.488
7.474
7.457
7.439
7.415
7.407
7.405
7.399
7.392
7.260
7.018
3.984
8.474
8.457
7.950
7.932
7.906
7.502
7.479
7.477
7.463
7.446
7.404
7.388
7.381
7.249
7.007
f1 (ppm)
NO2
4f
f1 (ppm)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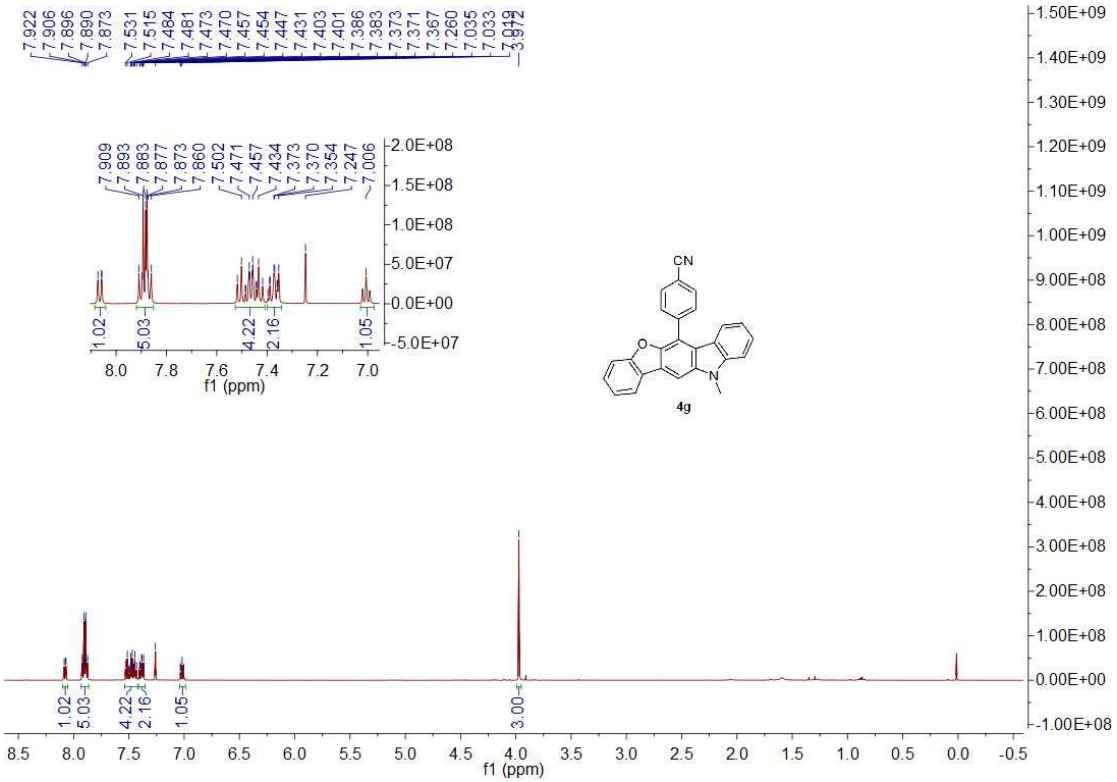
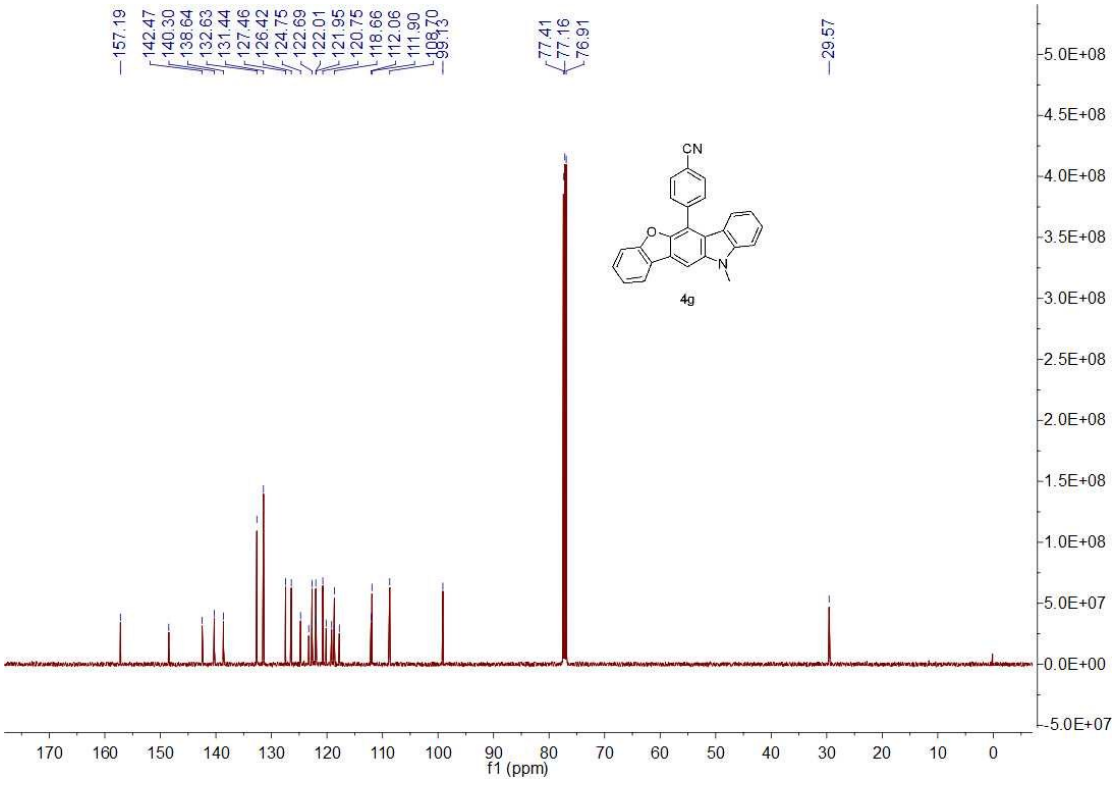
148.51
147.81
142.50
142.33
138.66
131.64
127.52
126.49
124.09
122.74
122.02
120.77
118.72
111.90
108.75
99.34
77.41
77.16
76.91
29.59
NO2
4f
f1 (ppm)


7.922
7.906
7.896
7.890
7.873
7.531
7.515
7.484
7.481
7.473
7.470
7.457
7.454
7.447
7.431
7.403
7.401
7.386
7.383
7.373
7.371
7.367
7.260
7.035
7.033
3.972
7.909
7.893
7.883
7.877
7.873
7.860
7.502
7.471
7.457
7.434
7.373
7.370
7.354
7.247
7.006
1.02
5.03
4.22
2.16
1.05
3.00
f1 (ppm)
CN
O
N
4g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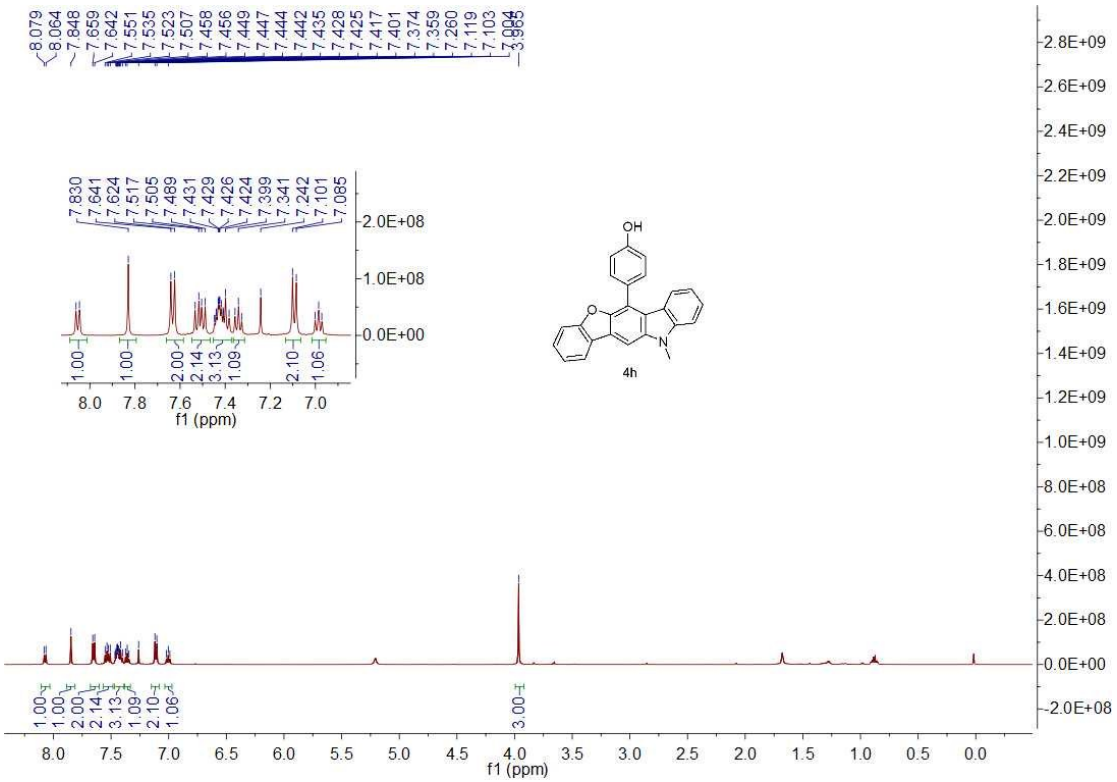
140.30
138.64
132.63
131.44
127.46
126.42
124.75
122.69
122.01
121.95
120.75
118.66
112.06
111.90
108.70
99.13
77.41
77.16
76.91
29.57
f1 (ppm)
CN
O
N
4g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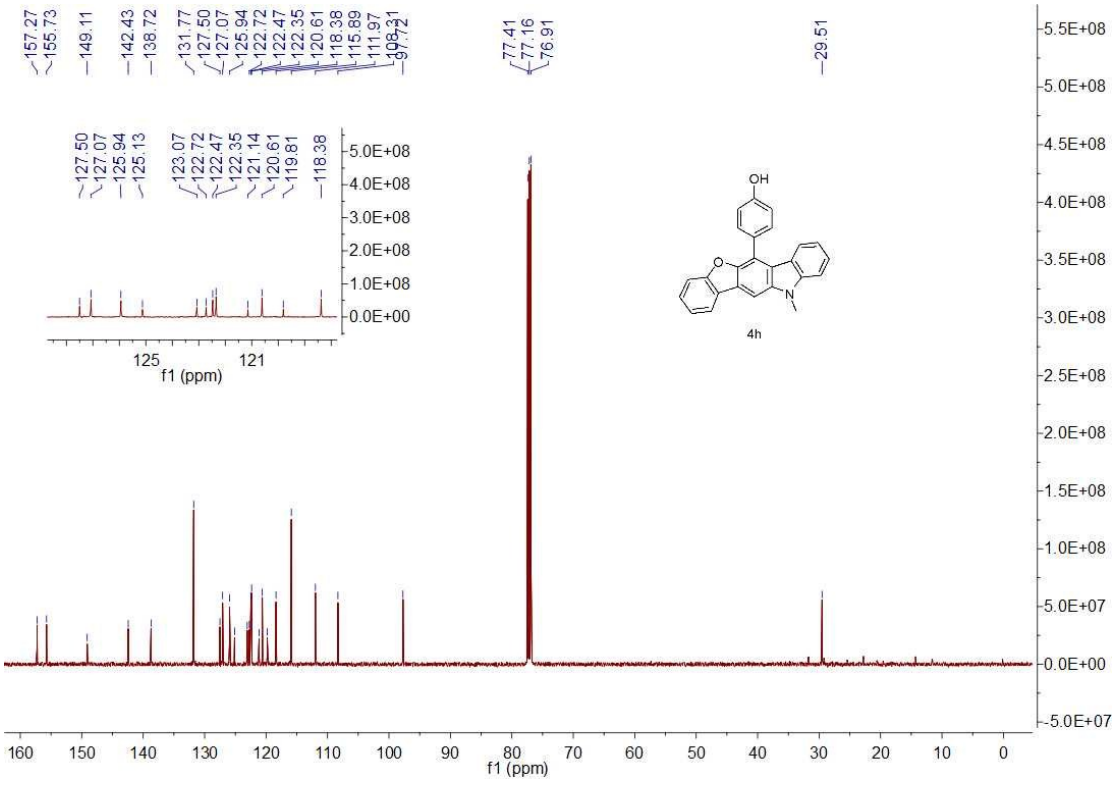
8.064
7.848
7.659
7.642
7.551
7.535
7.523
7.507
7.458
7.456
7.449
7.447
7.444
7.442
7.435
7.428
7.425
7.417
7.401
7.374
7.359
7.260
7.119
7.103
3.965
7.830
7.641
7.624
7.517
7.505
7.489
7.431
7.429
7.426
7.424
7.399
7.341
7.242
7.101
7.085
2.0E+08
1.0E+08
0.0E+00
1.00
1.00
2.00
2.14
3.13
1.09
2.10
1.06
8.0 7.8 7.6 7.4 7.2 7.0
f1 (ppm)
OH
O
N
4h
2.8E+09
2.6E+09
2.4E+09
2.2E+09
2.0E+09
1.8E+09
1.6E+09
1.4E+09
1.2E+09
1.0E+09
8.0E+08
6.0E+08
4.0E+08
2.0E+08
0.0E+00
-2.0E+08
1.00
1.00
2.00
2.14
3.13
1.09
2.10
1.06
3.00
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)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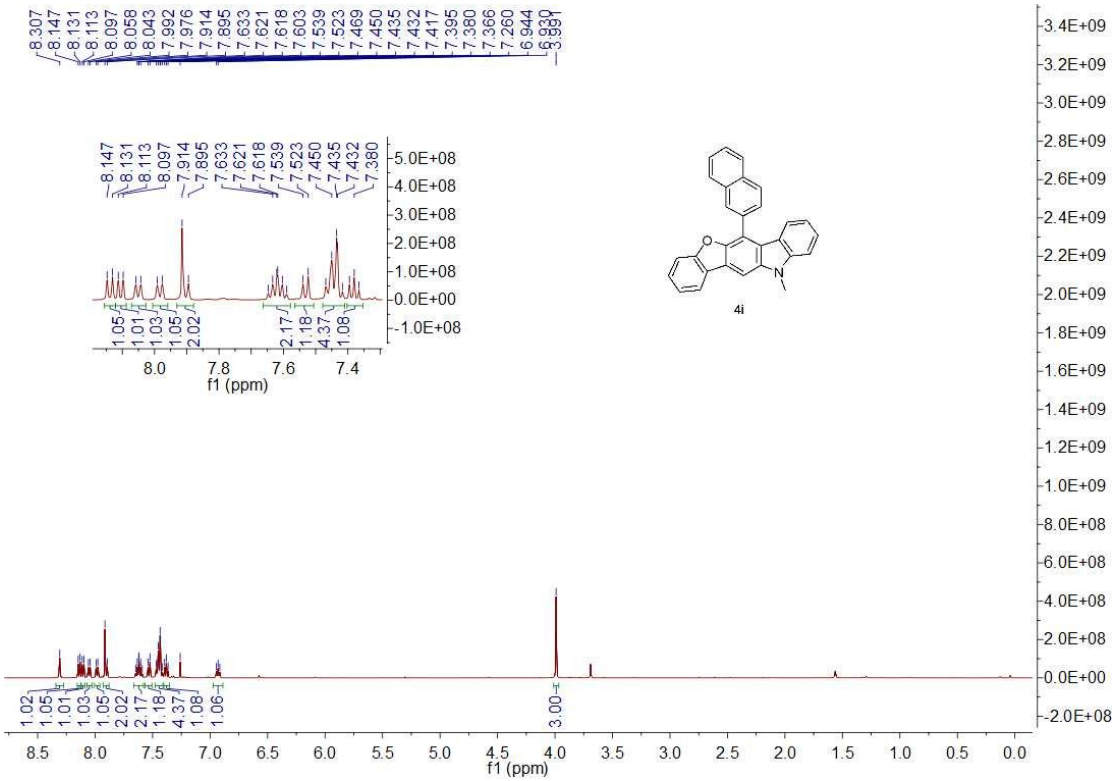
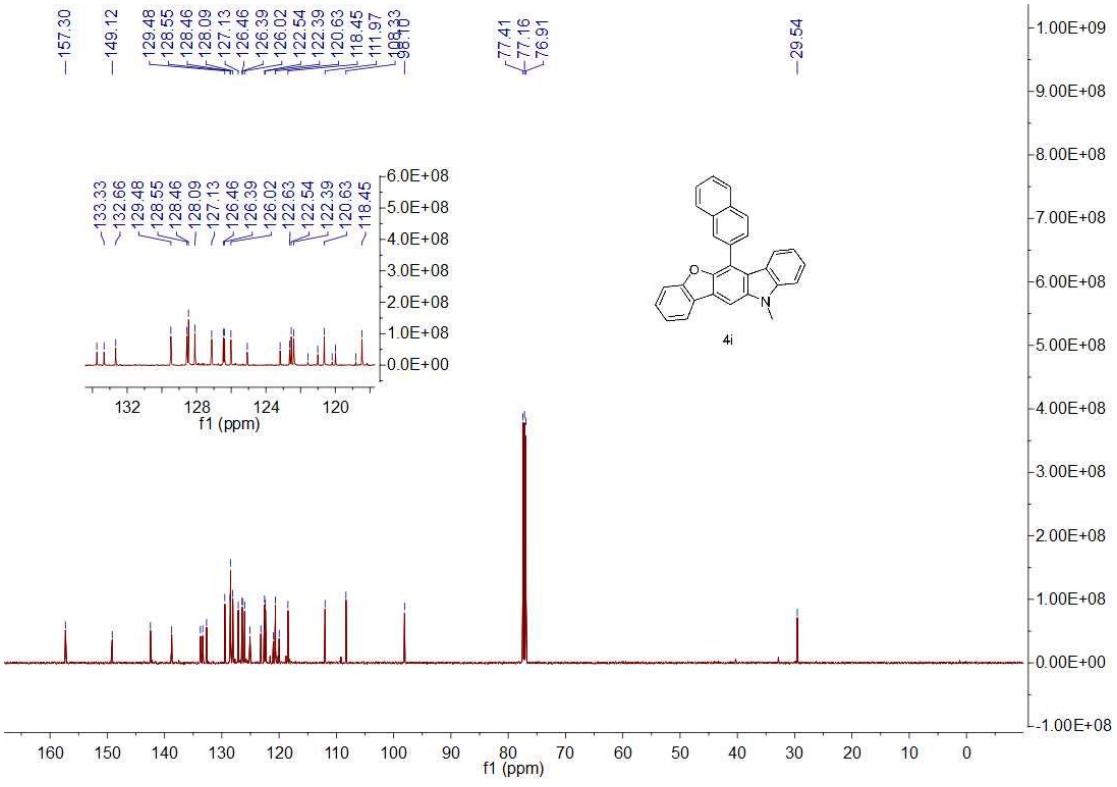
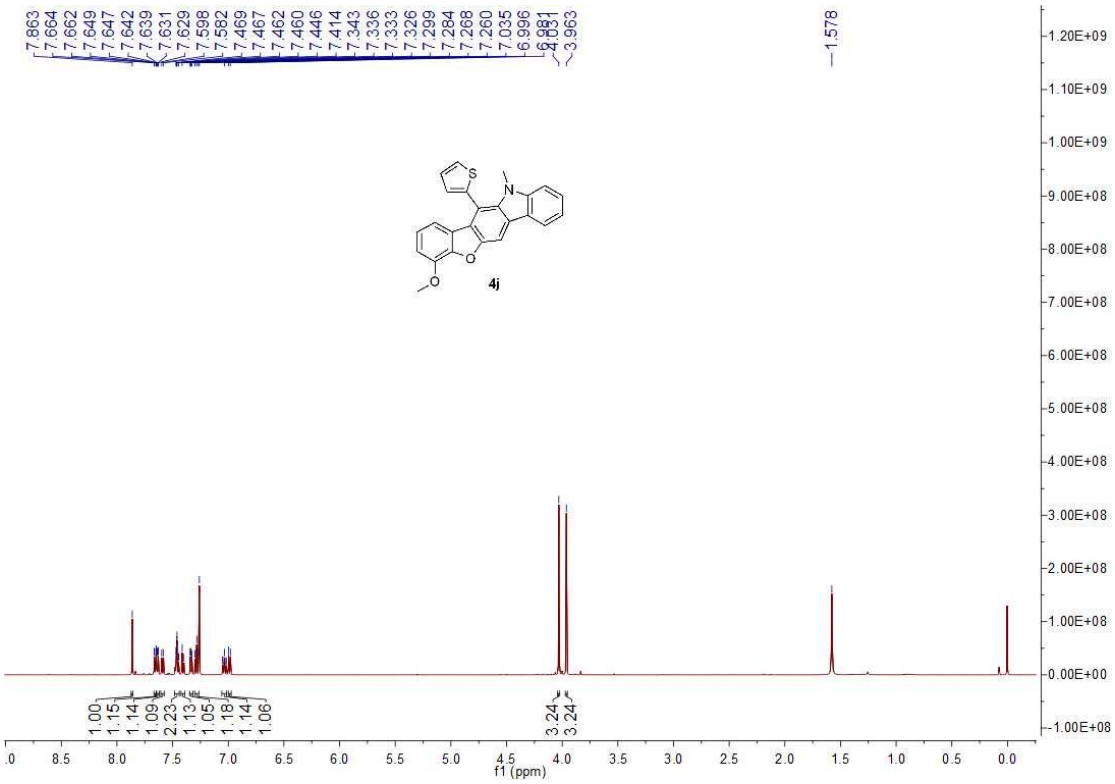
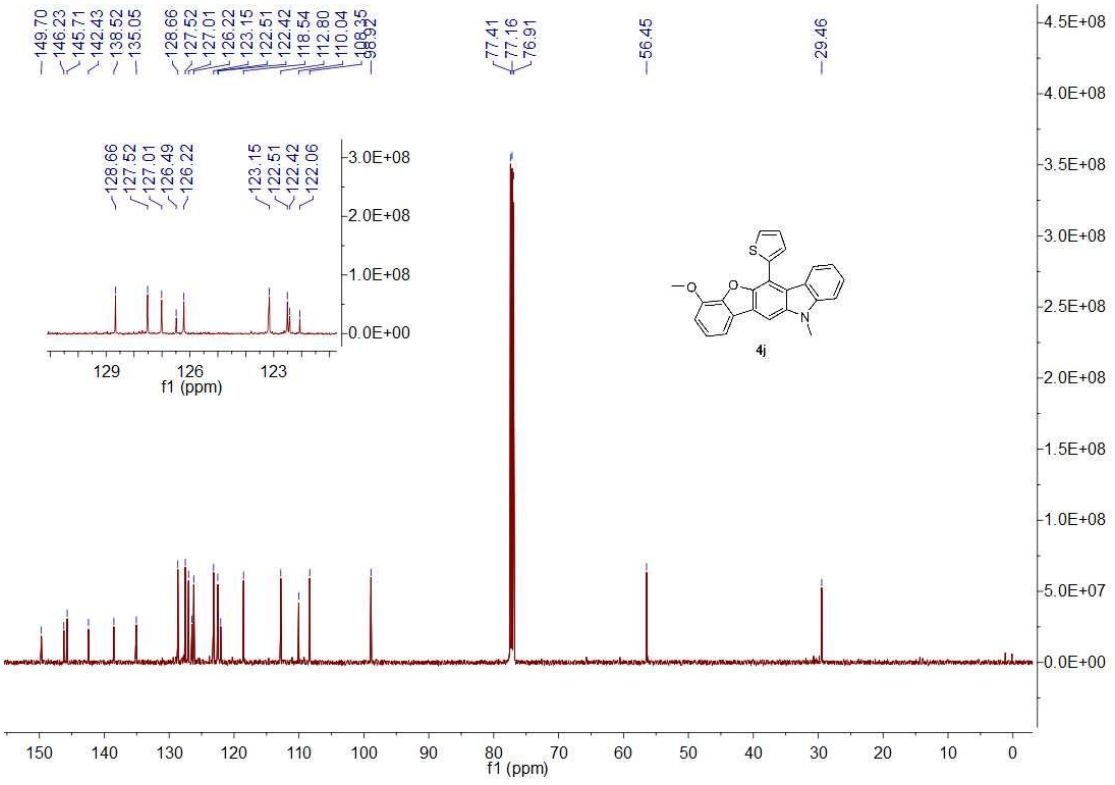
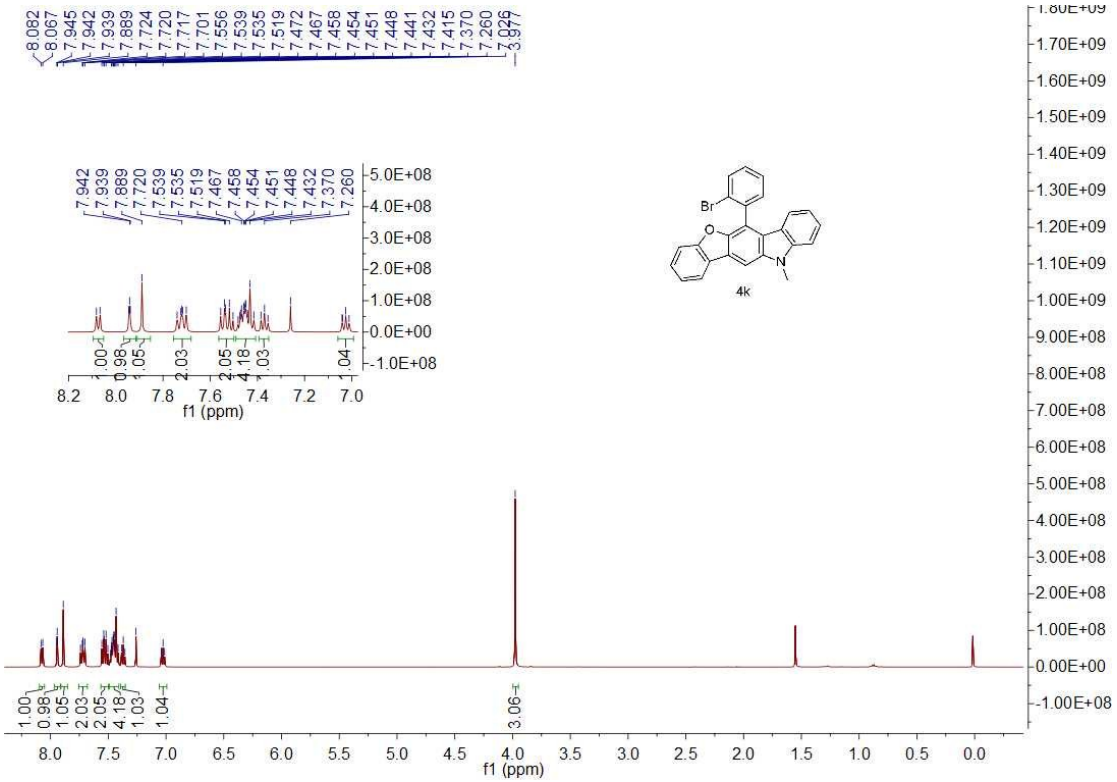
155.73
149.11
142.43
138.72
131.77
127.50
127.07
125.94
122.72
122.47
122.35
120.61
118.38
115.89
111.97
108.31
97.72
77.41
77.16
76.91
29.51
127.50
127.07
125.94
125.13
123.07
122.72
122.47
122.35
121.14
120.61
119.81
118.38
5.0E+08
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
125
121
f1 (ppm)
OH
O
N
4h
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

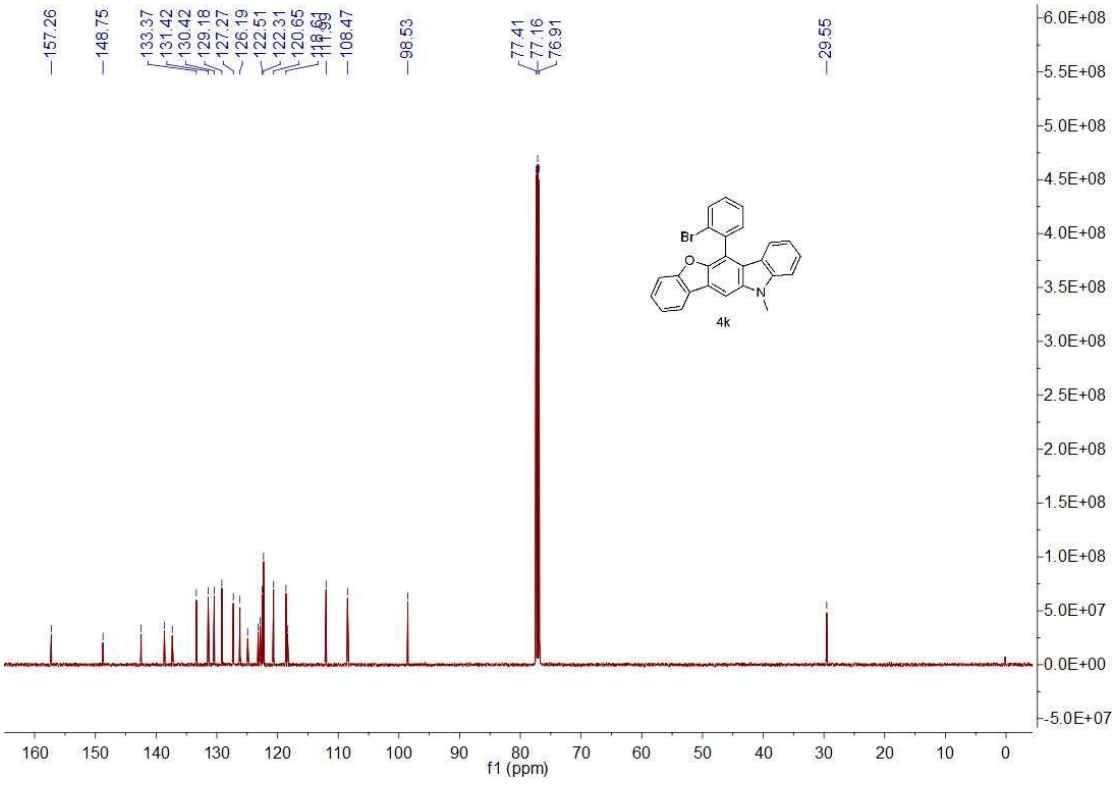

8.307
8.147
8.131
8.113
8.097
8.058
8.043
7.992
7.976
7.914
7.895
7.633
7.621
7.618
7.603
7.539
7.523
7.469
7.450
7.435
7.432
7.417
7.395
7.380
7.366
7.260
6.944
6.930
3.991
1.02
1.05
1.01
1.03
1.05
2.02
2.17
1.18
4.37
1.08
1.06
3.00
f1 (ppm)
4i

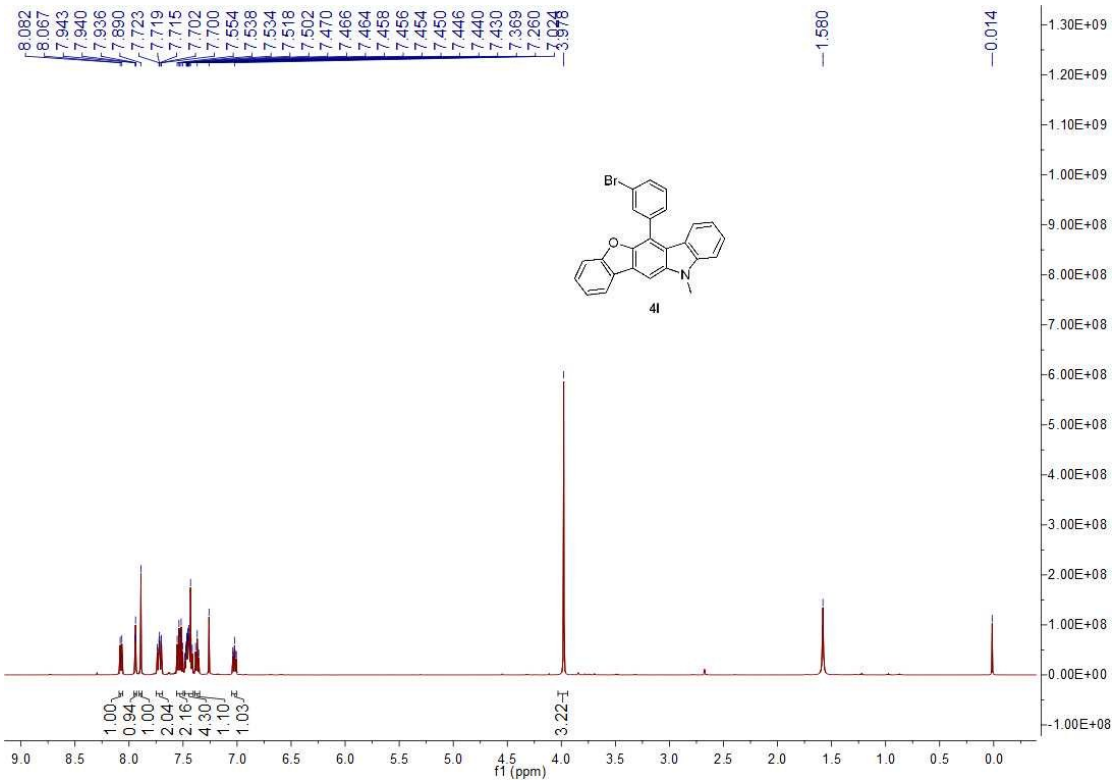

157.30
149.12
129.48
128.55
128.46
128.09
127.13
126.46
126.39
126.02
122.54
122.39
120.63
118.45
111.97
108.33
98.10
77.41
77.16
76.91
29.54
f1 (ppm)
4i

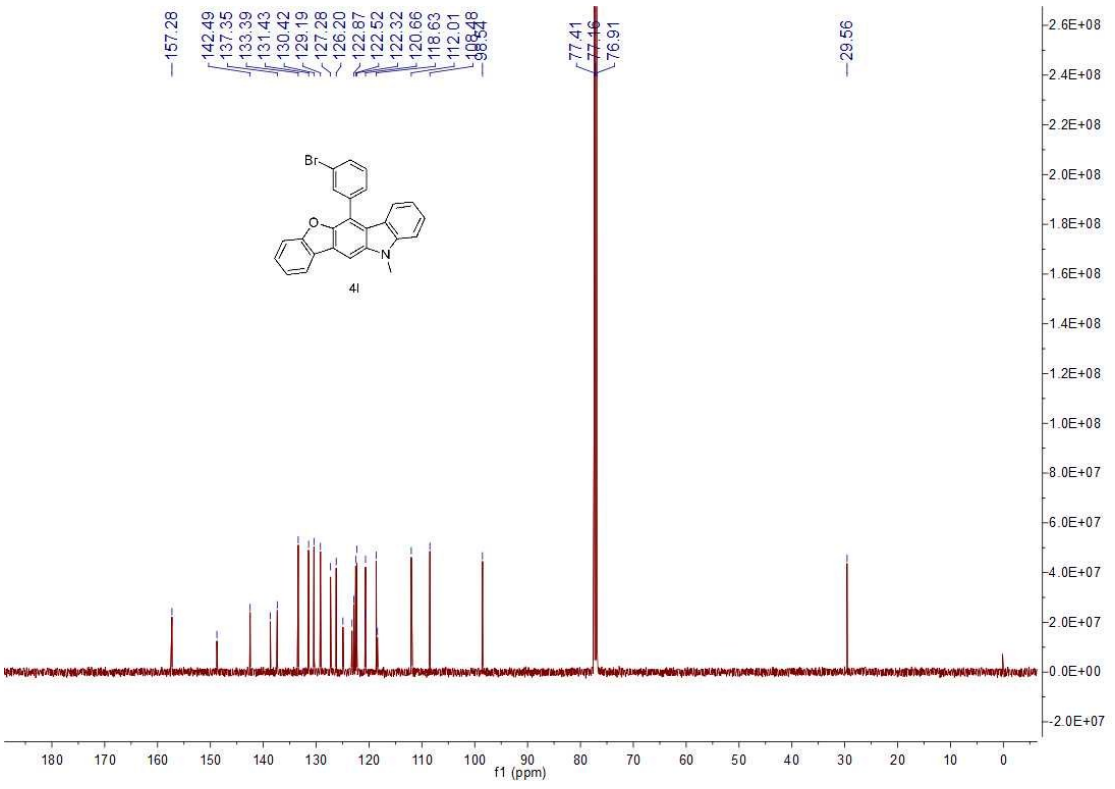

7.863
7.664
7.662
7.649
7.647
7.642
7.639
7.631
7.629
7.598
7.582
7.469
7.467
7.462
7.460
7.446
7.414
7.343
7.336
7.333
7.326
7.299
7.284
7.268
7.260
7.035
6.996
6.981
4.031
3.963
1.578
4j
1.00
1.15
1.14
1.09
2.23
1.13
1.05
1.18
1.14
1.06
3.24
3.24
f1 (ppm)

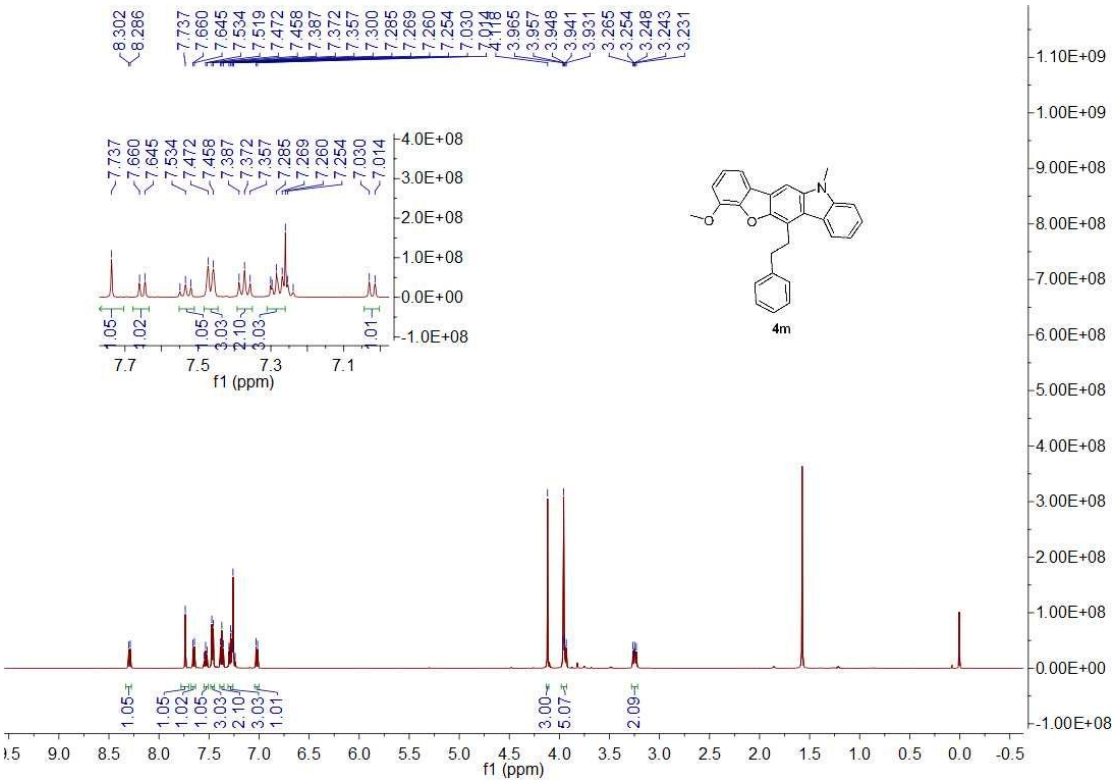

149.70
146.23
145.71
142.43
138.52
135.05
128.66
127.52
127.01
126.49
126.22
123.15
122.51
122.42
118.54
112.80
110.04
98.92
77.41
77.16
76.91
56.45
29.46
4j
f1 (ppm)

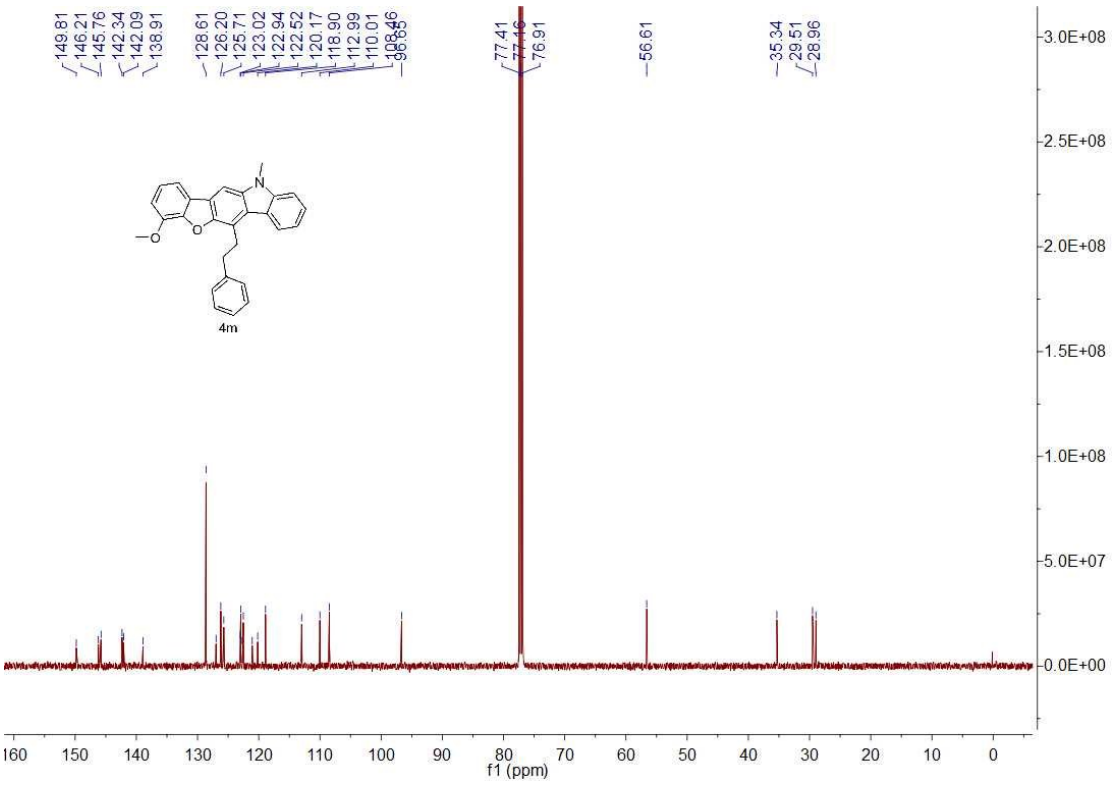

8.082
8.067
7.945
7.942
7.939
7.889
7.724
7.720
7.717
7.701
7.556
7.539
7.535
7.519
7.472
7.467
7.458
7.454
7.451
7.448
7.441
7.432
7.415
7.370
7.260
7.026
3.977
Br
O
N
4k
1.00
0.98
1.05
2.03
2.05
4.18
1.03
1.04
3.06
f1 (ppm)

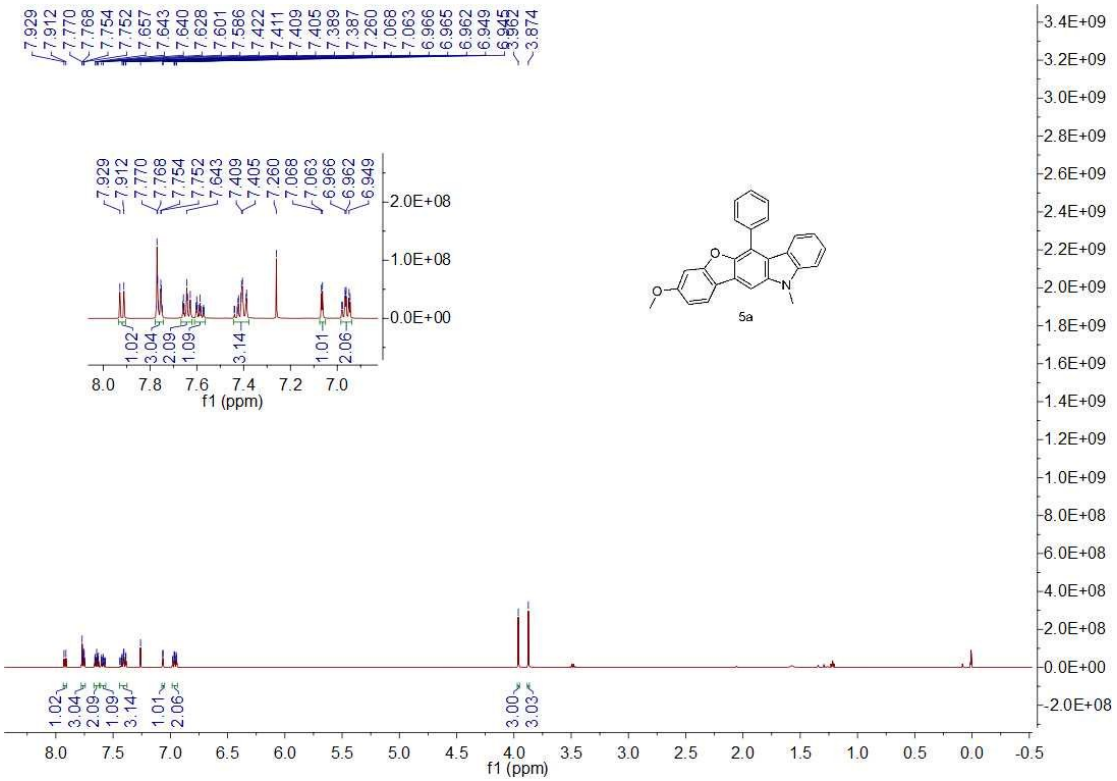

157.26
148.75
133.37
131.42
130.42
129.18
127.27
126.19
122.51
122.31
120.65
108.47
98.53
77.41
77.16
76.91
29.55
Br
O
N
4k
f1 (ppm)


8.082
8.067
7.943
7.940
7.936
7.890
7.723
7.719
7.715
7.702
7.700
7.554
7.538
7.534
7.518
7.502
7.470
7.466
7.464
7.458
7.456
7.454
7.450
7.446
7.440
7.430
7.369
7.260
3.978
1.580
0.014
Br
O
N
4l
1.00
0.94
1.00
2.04
2.16
4.30
1.10
1.03
3.22
f1 (ppm)


157.28
142.49
137.35
133.39
131.43
130.42
129.19
127.28
126.20
122.87
122.52
122.32
120.66
118.63
112.01
77.41
77.16
76.91
29.56
Br
O
N
4l
f1 (ppm)


8.302
8.286
7.737
7.660
7.645
7.534
7.519
7.472
7.458
7.387
7.372
7.357
7.300
7.285
7.269
7.260
7.254
7.030
7.014
4.118
3.965
3.957
3.948
3.941
3.931
3.265
3.254
3.248
3.243
3.231
4m
f1 (ppm)


4m
f1 (ppm)


7.929
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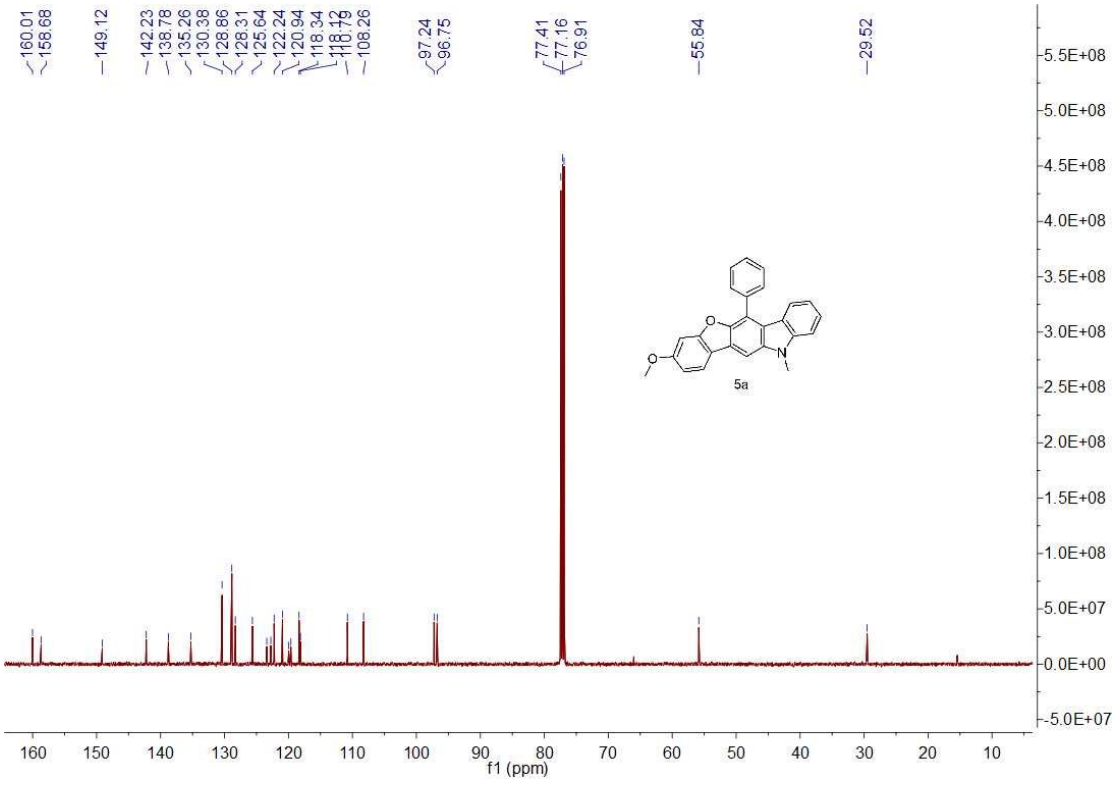
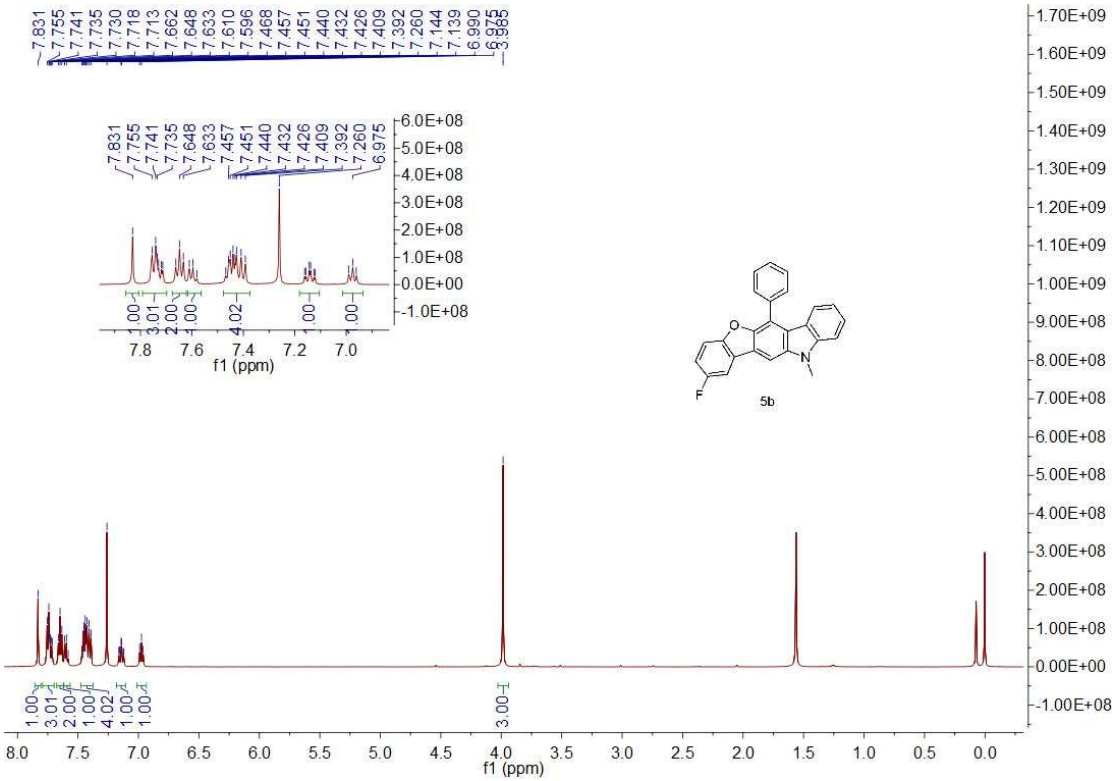
7.770
7.768
7.754
7.752
7.657
7.643
7.640
7.628
7.601
7.586
7.422
7.411
7.409
7.405
7.389
7.387
7.260
7.068
7.063
6.966
6.965
6.962
6.949
6.945
3.962
3.874
1.02
3.04
2.09
1.09
3.14
1.01
2.06
3.00
3.03
f1 (ppm)
5a


160.01
158.68
149.12
142.23
138.78
135.26
130.38
128.86
128.31
125.64
122.24
120.94
118.34
118.12
118.09
108.26
97.24
96.75
77.41
77.16
76.91
55.84
29.52
f1 (ppm)
5a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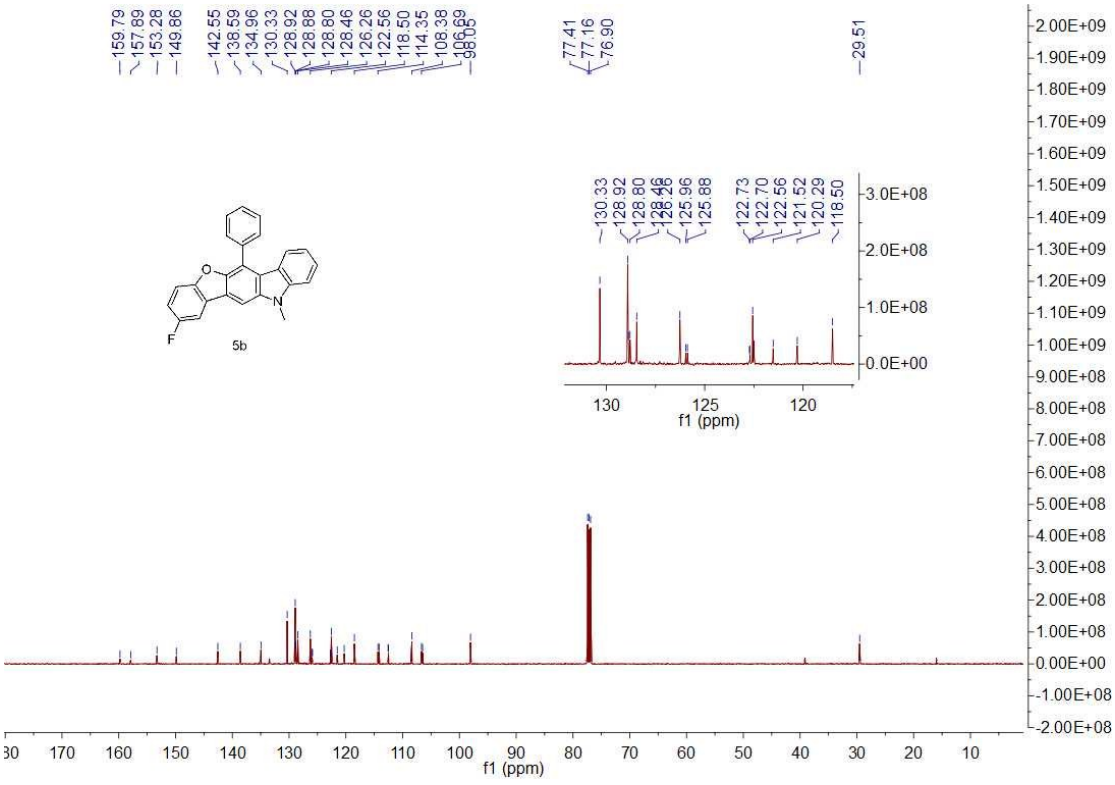
7.741
7.735
7.730
7.718
7.713
7.662
7.648
7.633
7.610
7.596
7.468
7.457
7.451
7.440
7.432
7.426
7.409
7.392
7.260
7.144
7.139
6.990
6.975
3.985
f1 (ppm)
5b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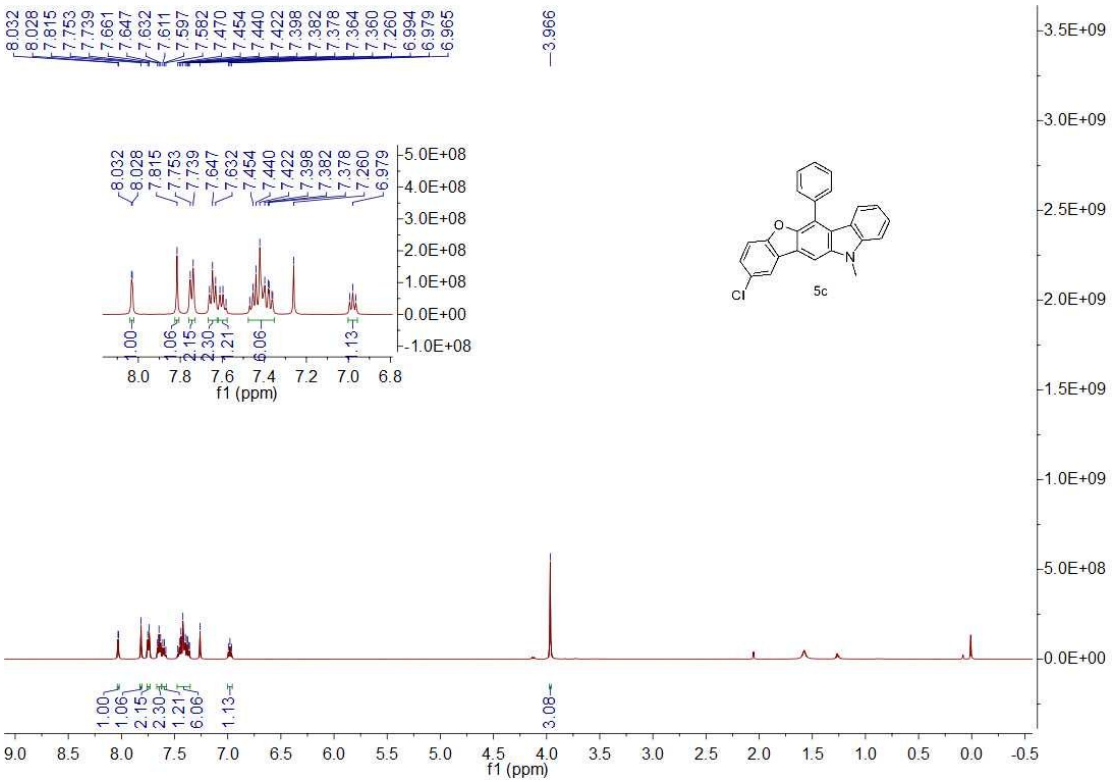
157.89
153.28
149.86
142.55
138.59
134.96
130.33
128.92
128.88
128.80
128.46
126.26
122.56
118.50
114.35
108.38
77.41
77.16
76.90
29.51
f1 (ppm)
5b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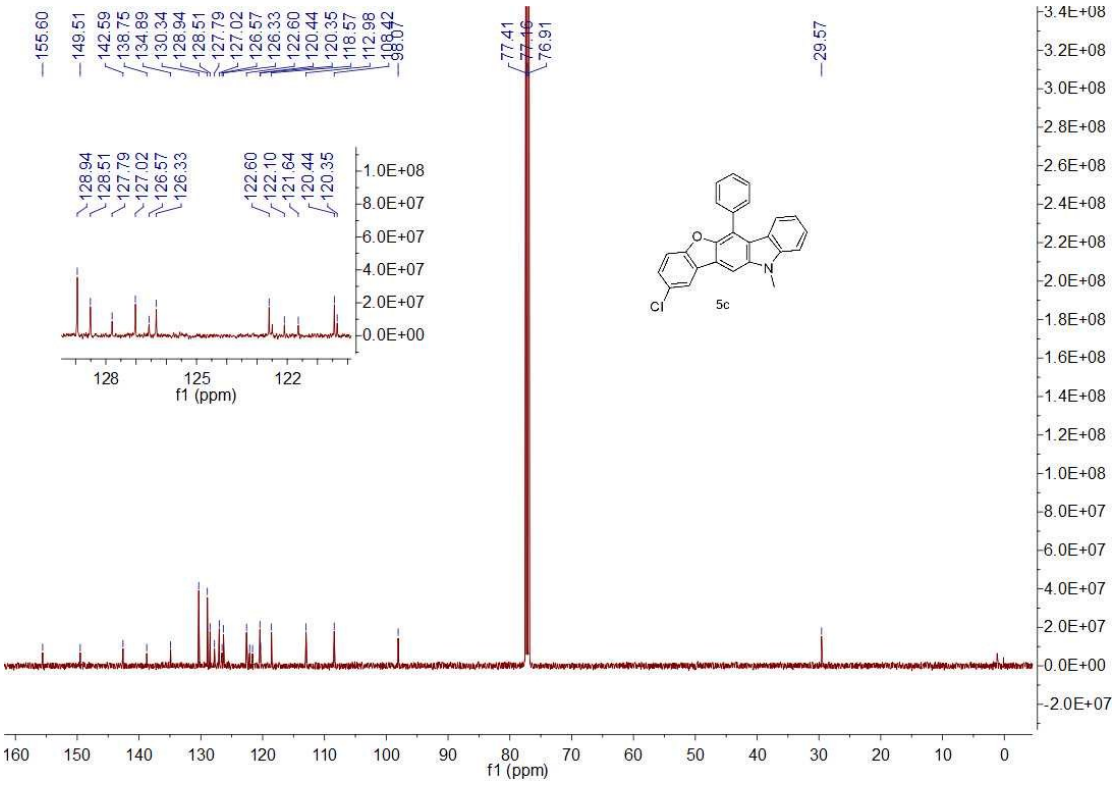
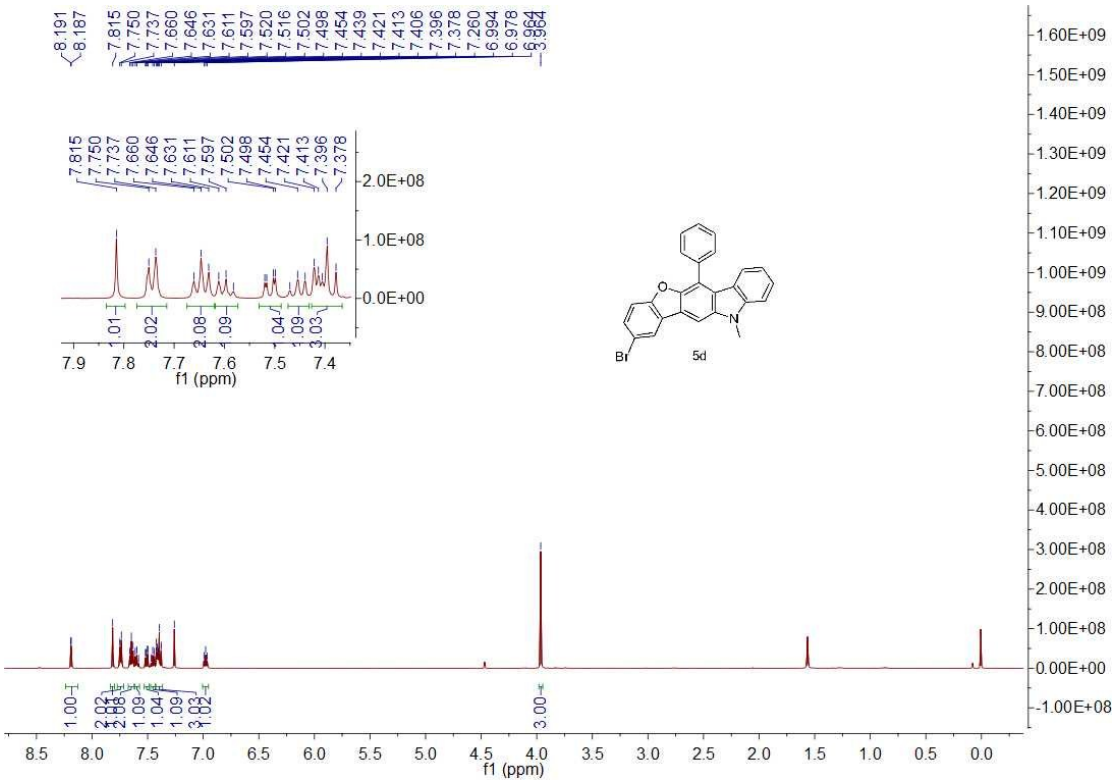
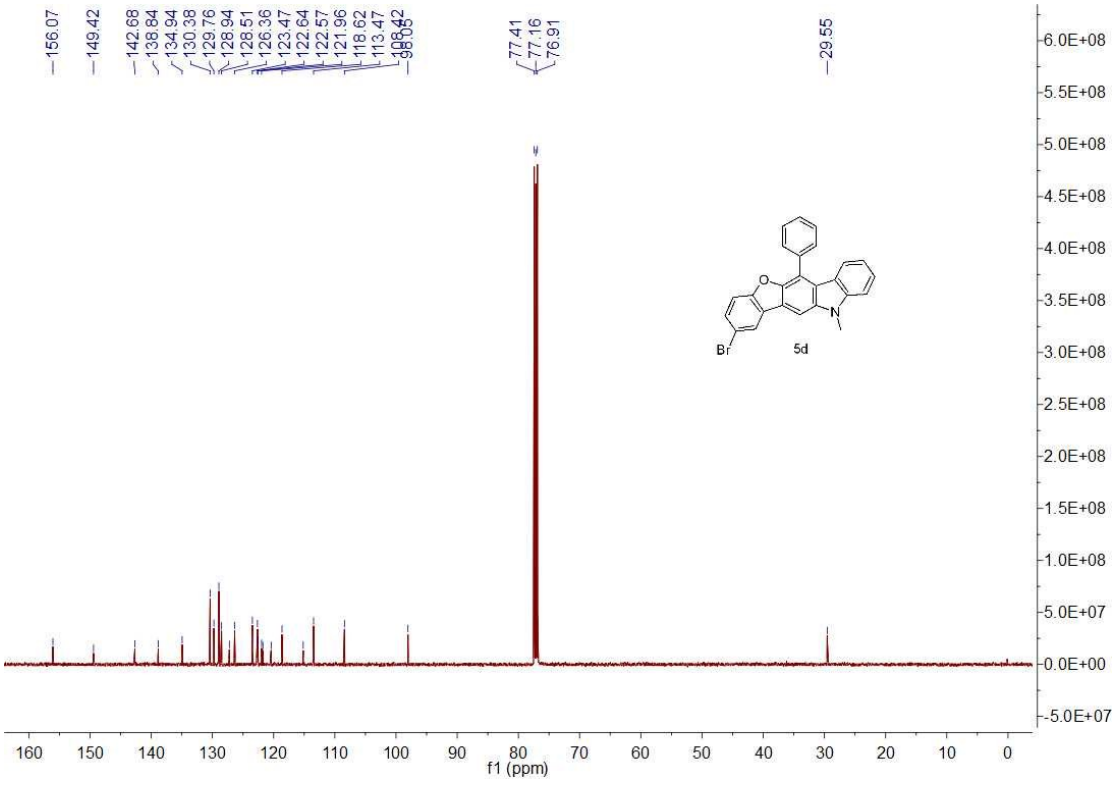
8.028
7.815
7.753
7.739
7.661
7.647
7.632
7.611
7.597
7.582
7.470
7.454
7.440
7.422
7.398
7.382
7.378
7.364
7.360
7.260
6.994
6.979
6.965
3.966
1.00
1.06
2.15
2.30
1.21
6.06
1.13
3.08
f1 (ppm)
Cl
O
N
5c


155.60
149.51
142.59
138.75
134.89
130.34
128.94
128.51
127.79
127.02
126.57
126.33
122.60
120.44
120.35
118.57
112.98
98.07
77.41
77.16
76.91
29.57
f1 (ppm)
Cl
O
N
5c


8.191
8.187
7.815
7.750
7.737
7.660
7.646
7.631
7.611
7.597
7.520
7.516
7.502
7.498
7.454
7.439
7.421
7.413
7.406
7.396
7.378
7.260
6.994
6.978
6.964
3.964
2.0E+08
1.0E+08
0.0E+00
1.01
2.02
2.08
1.09
1.04
1.09
3.03
7.9
7.8
7.7
7.6
7.5
7.4
f1 (ppm)
Br
O
N
5d
1.60E+09
1.50E+09
1.40E+09
1.30E+09
1.20E+09
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
1.00
2.02
2.08
1.09
1.04
1.09
3.02
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
f1 (ppm)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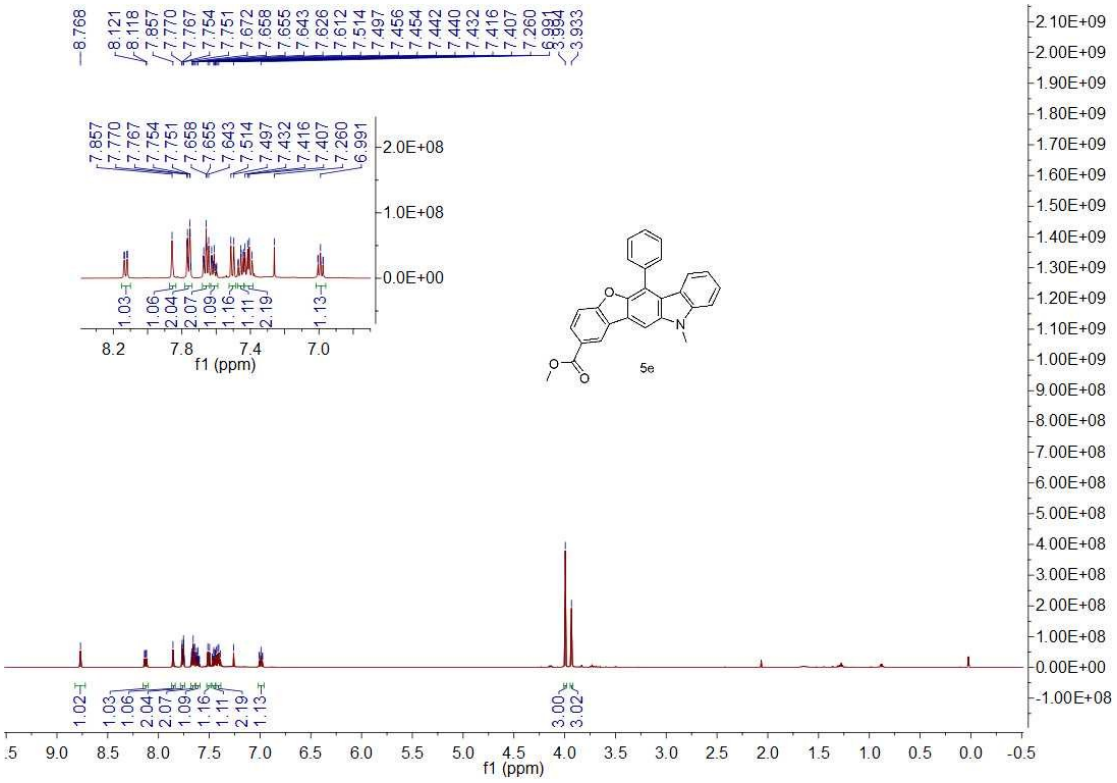
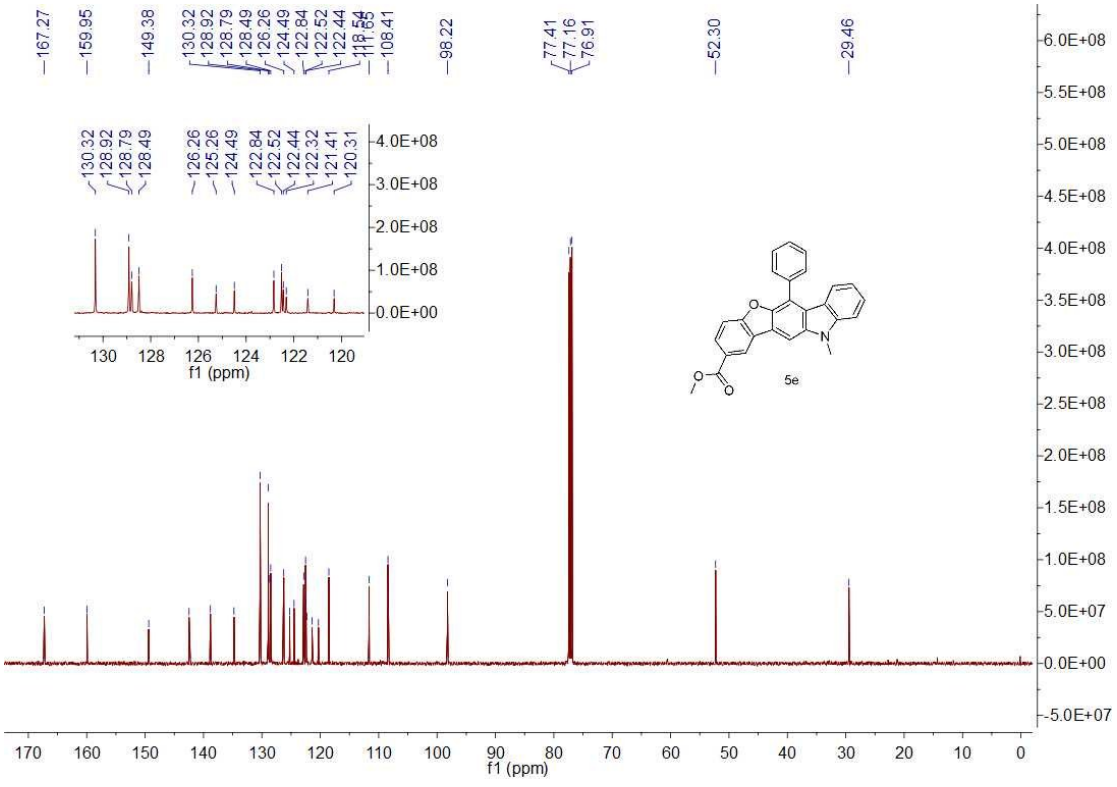
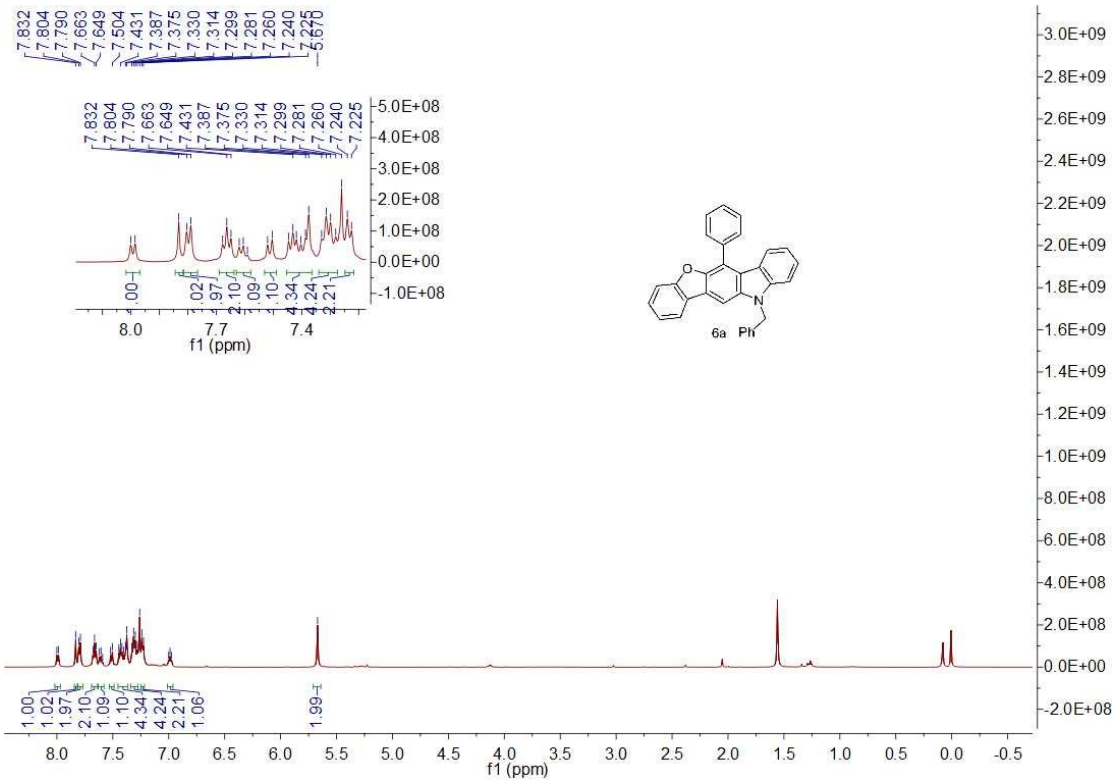
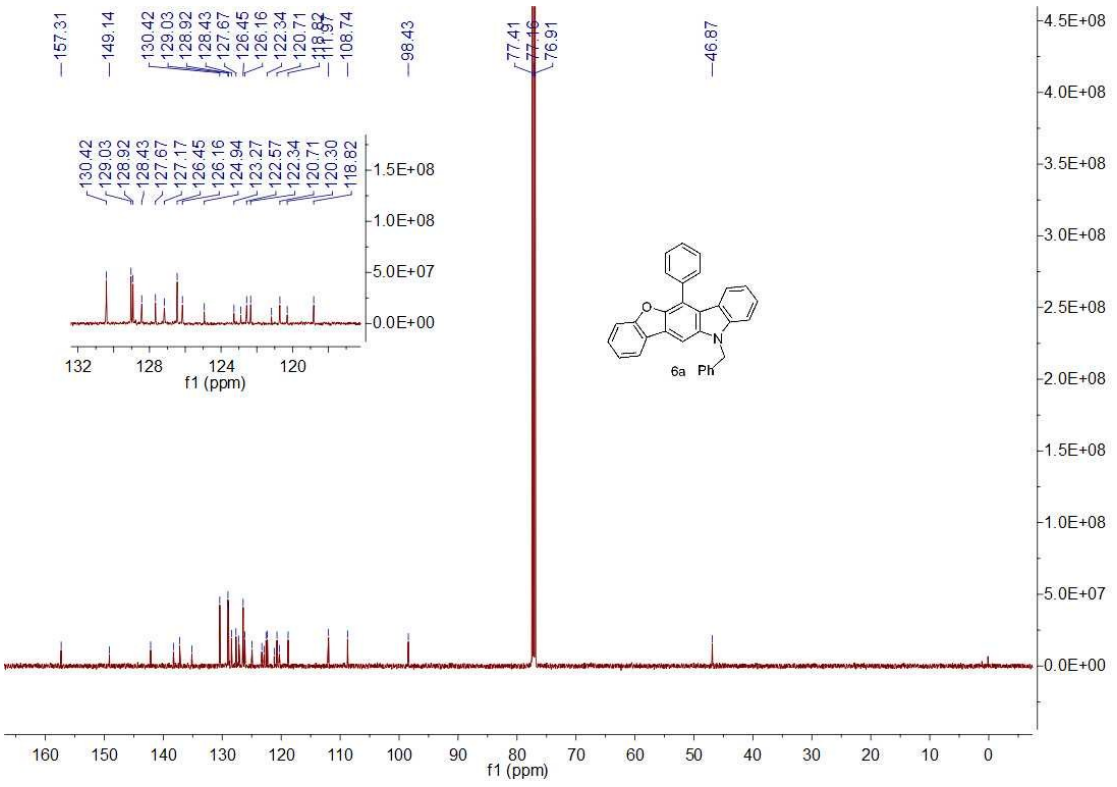
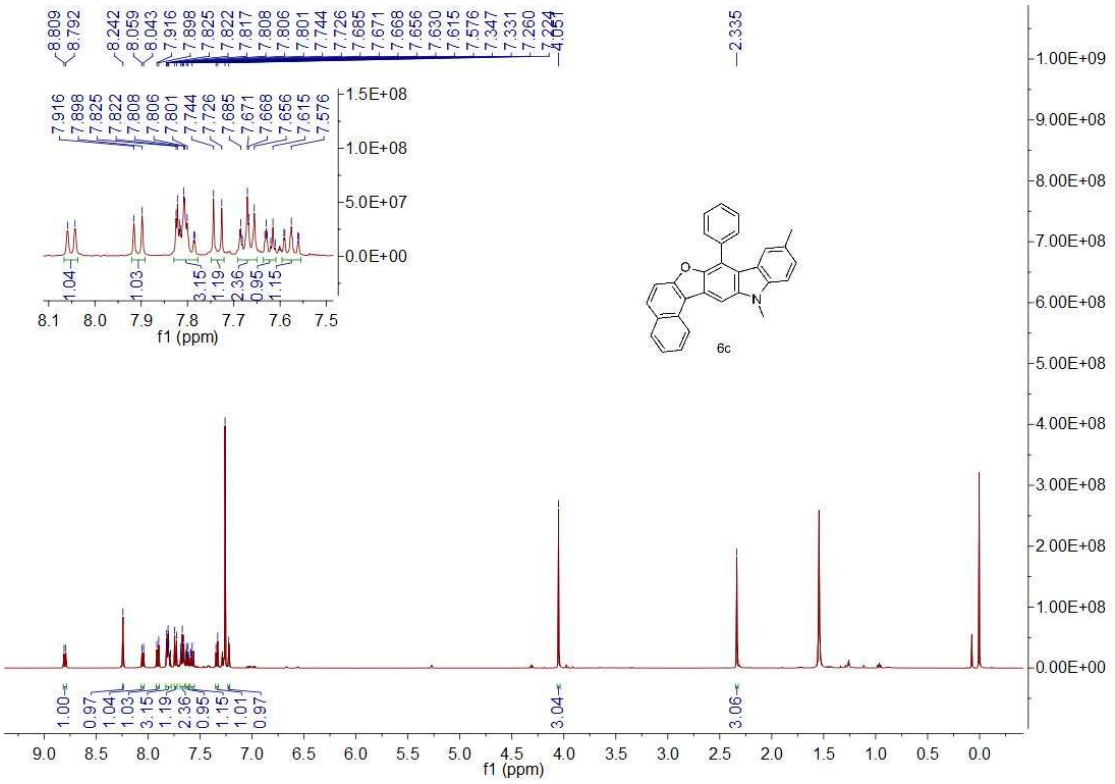
138.84
134.94
130.38
129.76
128.94
128.51
126.36
123.47
122.64
122.57
121.96
118.62
113.47
98.05
77.41
77.16
76.91
29.55
Br
O
N
5d
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

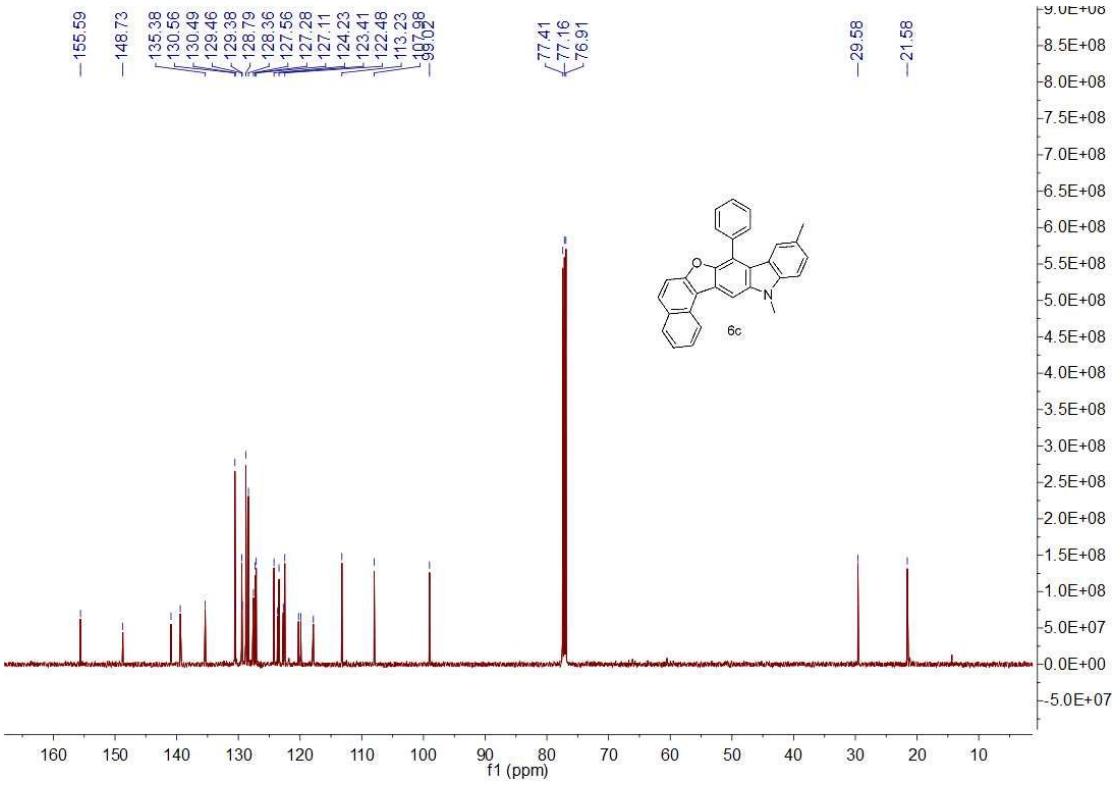

8.768
8.121
8.118
7.857
7.770
7.767
7.754
7.751
7.672
7.658
7.655
7.643
7.626
7.612
7.514
7.497
7.456
7.454
7.442
7.440
7.432
7.416
7.407
7.260
6.991
3.933
1.02
1.03
1.06
2.04
2.07
1.09
1.16
1.11
2.19
1.13
3.00
3.02
f1 (ppm)
5e

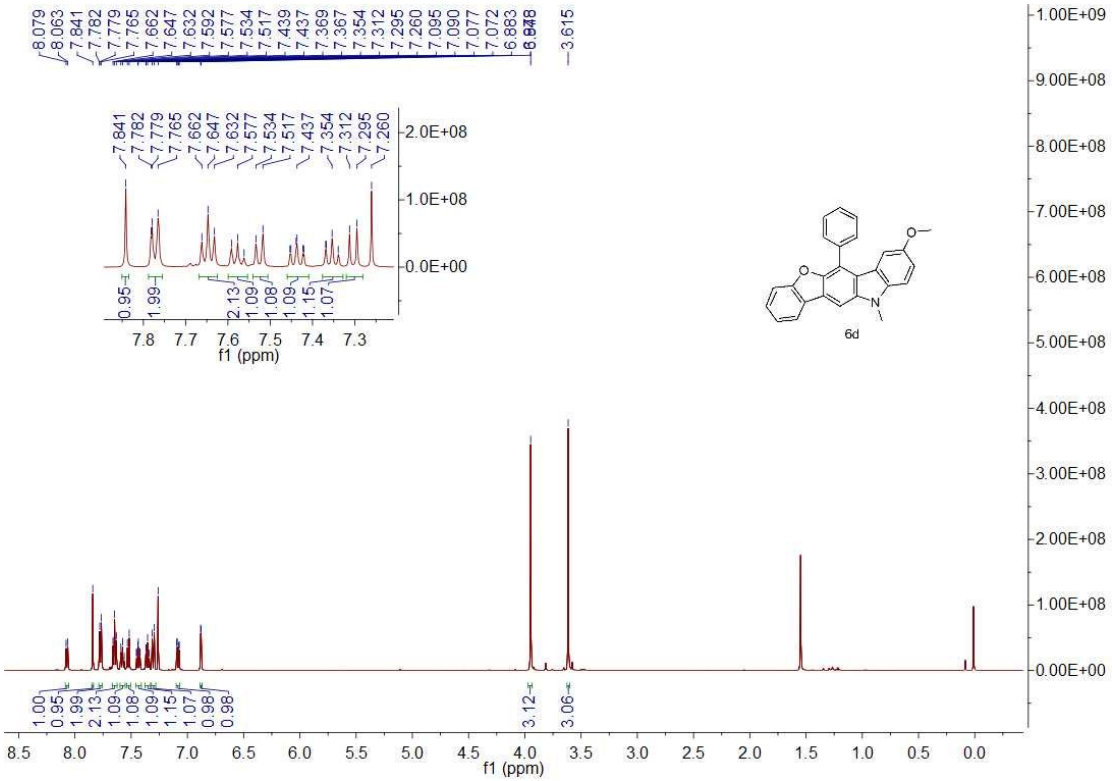

167.27
159.95
149.38
130.32
128.92
128.79
128.49
126.26
124.49
122.84
122.52
122.44
118.54
118.65
108.41
98.22
77.41
77.16
76.91
52.30
29.46
125.26
122.32
121.41
120.31
f1 (ppm)
5e

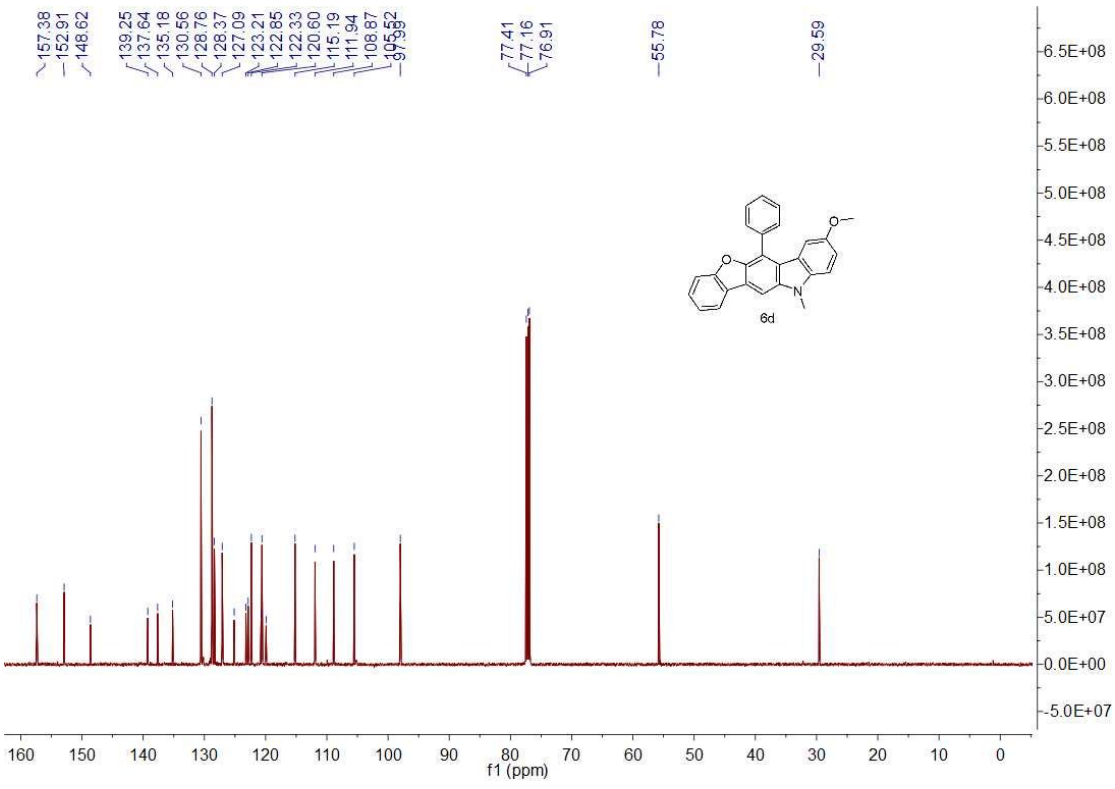

7.832
7.804
7.790
7.663
7.649
7.504
7.431
7.387
7.375
7.330
7.314
7.299
7.281
7.260
7.240
7.225
5.670
1.00
1.02
1.97
2.10
1.09
1.10
4.34
4.24
2.21
1.06
1.99
f1 (ppm)
6a Ph

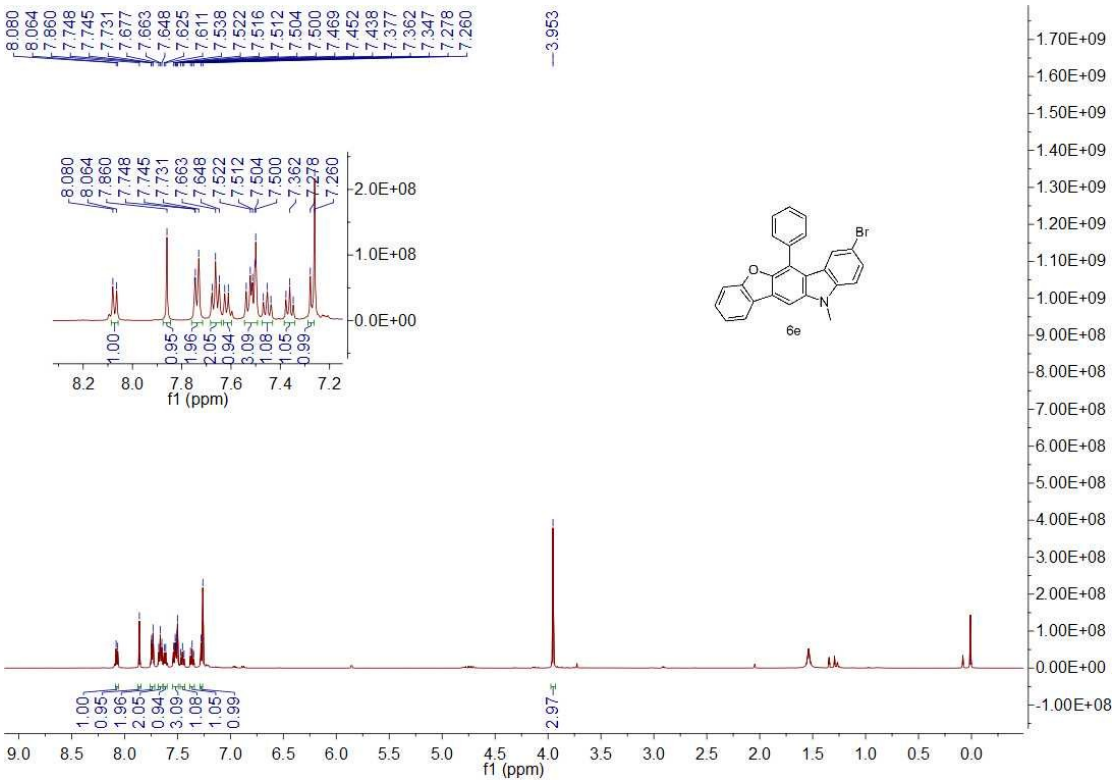

157.31
149.14
130.42
129.03
128.92
128.43
127.67
126.45
126.16
122.34
120.71
118.82
111.97
108.74
98.43
77.41
77.16
76.91
46.87
f1 (ppm)
6a Ph

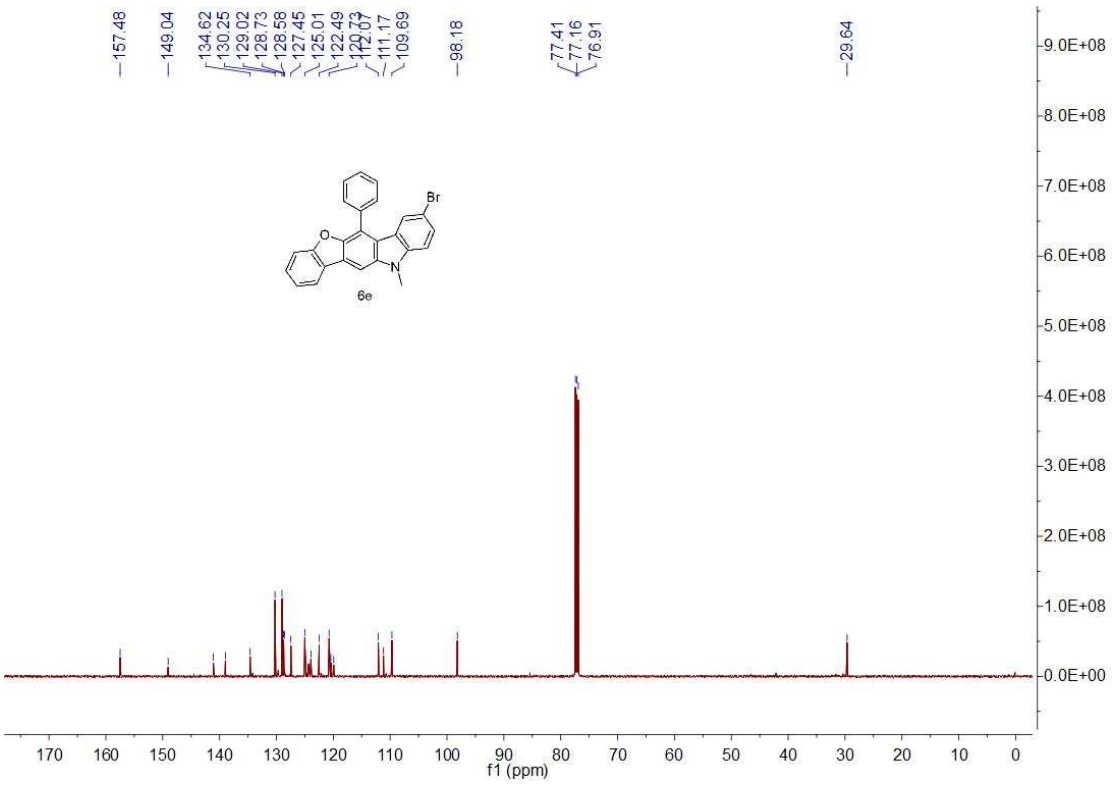

8.809
8.792
8.242
8.059
8.043
7.916
7.898
7.825
7.822
7.817
7.808
7.806
7.801
7.744
7.726
7.685
7.671
7.668
7.656
7.630
7.615
7.576
7.347
7.331
7.260
7.224
4.051
2.335
1.04
1.03
3.15
1.19
2.36
0.95
1.15
f1 (ppm)
6c
1.00
0.97
1.04
1.03
3.15
1.19
2.36
0.95
1.15
1.01
0.97
3.04
3.06
f1 (ppm)

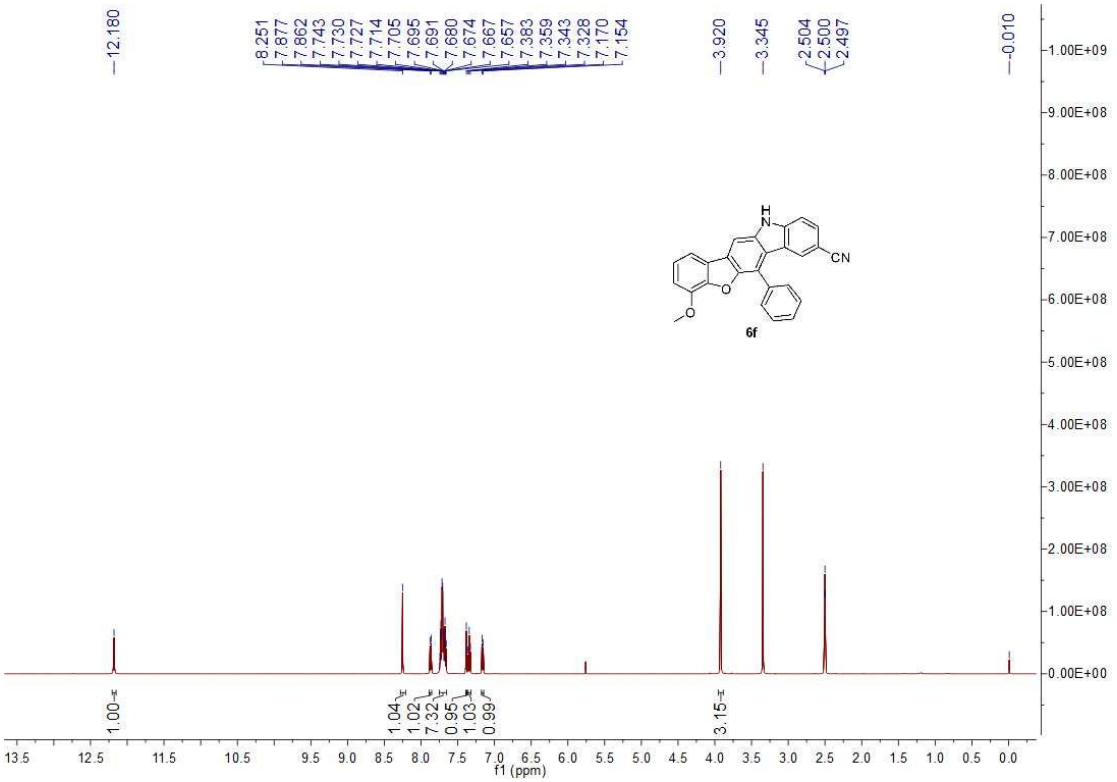

155.59
148.73
135.38
130.56
130.49
129.46
129.38
128.79
128.36
127.56
127.28
127.11
124.23
123.41
122.48
113.23
107.98
99.02
77.41
77.16
76.91
29.58
21.58
6c
f1 (ppm)

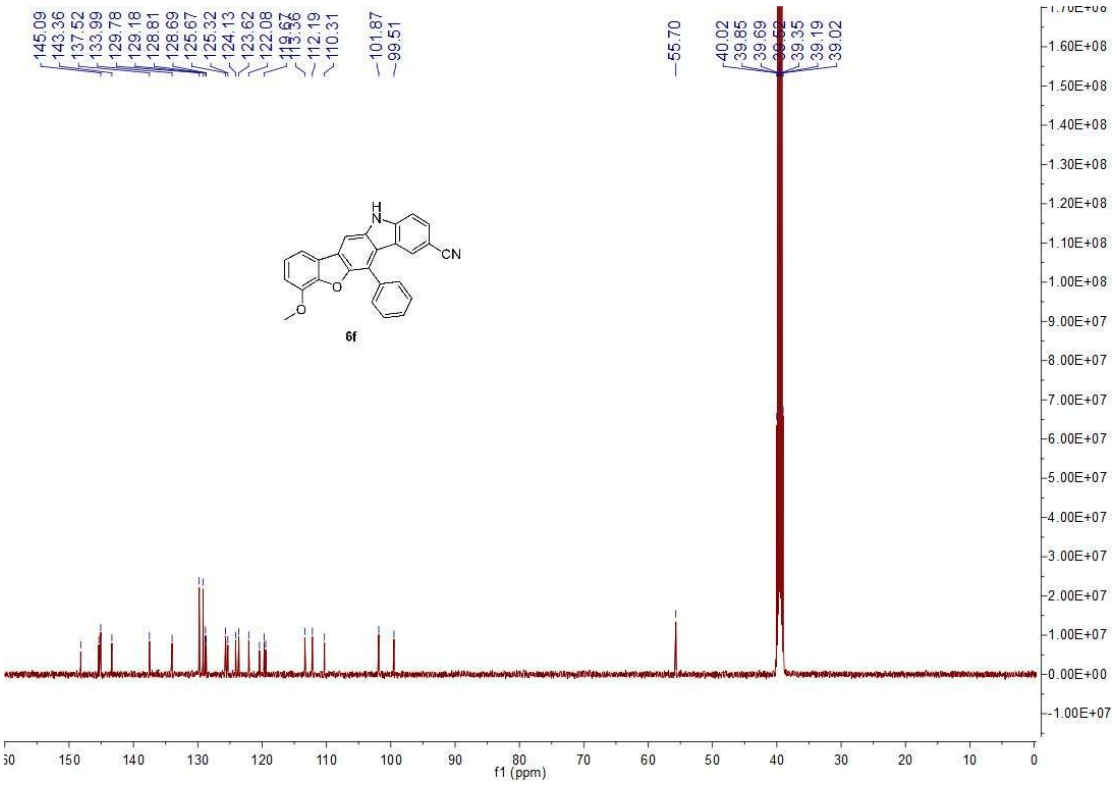

8.079
8.063
7.841
7.782
7.779
7.765
7.662
7.647
7.632
7.592
7.577
7.534
7.517
7.439
7.437
7.369
7.367
7.354
7.312
7.295
7.260
7.095
7.090
7.077
7.072
6.883
3.615
2.0E+08
1.0E+08
0.0E+00
0.95
1.99
2.13
1.09
1.08
1.09
1.15
1.07
7.8 7.7 7.6 7.5 7.4 7.3
f1 (ppm)
6d
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
1.00
0.95
1.99
2.13
1.09
1.08
1.09
1.15
1.07
0.98
0.98
3.12
3.06
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


157.38
152.91
148.62
139.25
137.64
135.18
130.56
128.76
128.37
127.09
123.21
122.85
122.33
120.60
115.19
111.94
108.87
105.52
97.99
77.41
77.16
76.91
55.78
29.59
6d
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.080
8.064
7.860
7.748
7.745
7.731
7.677
7.663
7.648
7.625
7.611
7.538
7.522
7.516
7.512
7.504
7.500
7.469
7.452
7.438
7.377
7.362
7.347
7.278
7.260
3.953
Br
O
N
6e
f1 (ppm)


157.48
149.04
134.62
130.25
129.02
128.73
128.58
127.45
125.01
122.49
120.07
111.17
109.69
98.18
77.41
77.16
76.91
29.64
Br
O
N
6e
f1 (ppm)


12.180
8.251
7.877
7.862
7.743
7.730
7.727
7.714
7.705
7.695
7.691
7.680
7.674
7.667
7.657
7.383
7.359
7.343
7.328
7.170
7.154
3.920
3.345
2.504
2.500
2.497
0.010
1.00
1.04
1.02
7.32
0.95
1.03
0.99
3.15
f1 (ppm)
6f


145.09
143.36
137.52
133.99
129.78
129.18
128.81
128.69
125.67
125.32
124.13
123.62
122.08
112.19
110.31
101.87
99.51
55.70
40.02
39.85
39.69
39.52
39.35
39.19
39.02
f1 (ppm)
6f